
signac Documentation

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Note: This is documentation for the **signac** *core package*, which is part of the **signac** framework. See [here](#) for a comprehensive introduction to the **signac** *framework*.

1.1 Installation

The recommended installation method for **signac** is via [conda](#) or [pip](#). The software is tested for Python versions 3.6+ and has minimal dependencies. Some features such as the HDF5 integration require additional packages. Supported Python and NumPy versions are determined according to the [NEP 29 deprecation policy](#).

1.1.1 Install with conda

You can install **signac** via conda (available on the [conda-forge](#) channel), with:

```
$ conda install -c conda-forge signac
```

All additional dependencies will be installed automatically. To upgrade the package, execute:

```
$ conda update signac
```

1.1.2 Install with pip

To install the package with the package manager [pip](#), execute

```
$ pip install signac --user
```

Note: It is highly recommended to install the package into the user space and not as superuser!

To upgrade the package, simply execute the same command with the `--upgrade` option.

```
$ pip install signac --user --upgrade
```

Consider installing optional dependencies:

```
$ pip install pymongo passlib bcrypt --user
```

1.1.3 Source Code Installation

Alternatively you can clone the [git repository](#) and execute the `setup.py` script to install the package.

```
git clone https://github.com/glotzerlab/signac.git
cd signac
python setup.py install --user
```

Consider installing *optional dependencies*.

1.1.4 Optional dependencies

Unless you install via [conda](#), optional dependencies are not installed automatically. In case you want to use extra features that require external packages, you need to install these manually.

Extra features with dependencies:

MongoDB database backend required: `pymongo`

recommended: `passlib`, `bcrypt`

HDF5 integration required: `h5py`

1.2 Command Line Interface

Overview

The following core **signac** functions are—in addition to the Python interface—accessible directly via the `$ signac` command.

1.2.1 init

```
usage: signac init [-h] [-w WORKSPACE] project_id

positional arguments:
  project_id            Initialize a project with the given project id.

optional arguments:
  -h, --help            show this help message and exit
  -w WORKSPACE, --workspace WORKSPACE
                        The path to the workspace directory.
```

1.2.2 project


```
usage: signac project [-h] [-w] [-i] [-a]
```

optional arguments:

```
-h, --help            show this help message and exit
-w, --workspace       Print the project's workspace path instead of the project
                        id.
-i, --index           Generate and print an index for the project.
-a, --access          Create access module for indexing.
```

1.2.3 job

```
usage: signac job [-h] [-w] [-c] [statepoint]
```

positional arguments:

```
statepoint            The job's statepoint in JSON format. Omit this argument to
                        read from STDIN.
```

optional arguments:

```
-h, --help            show this help message and exit
-w, --workspace       Print the job's workspace path instead of the job id.
-c, --create          Create the job's workspace directory if necessary.
```

1.2.4 statepoint

```
usage: signac statepoint [-h] [-p [PRETTY]] [-i [INDENT]] [-s]
                        [job_id [job_id ...]]
```

Print the statepoint(s) corresponding to one or more job ids.

positional arguments:

```
job_id                One or more job ids. The corresponding jobs must be
                        initialized.
```

optional arguments:

```
-h, --help            show this help message and exit
-p [PRETTY], --pretty [PRETTY]
                        Print state point in pretty format. An optional
                        argument to this flag specifies the maximal depth a
                        state point is printed.
-i [INDENT], --indent [INDENT]
                        Specify the indentation of the JSON formatted state
                        point.
-s, --sort            Sort the state point keys for output.
```

1.2.5 diff

```
usage: signac diff [-h] [-p [PRETTY]] [-i [INDENT]] [-f FILTER [FILTER ...]]
                  [-d DOC_FILTER [DOC_FILTER ...]]
                  [job_id [job_id ...]]
```

Find the difference among job state points.

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```
positional arguments:
  job_id                One or more job ids. The corresponding jobs must be
                        initialized.

optional arguments:
  -h, --help            show this help message and exit
  -p [PRETTY], --pretty [PRETTY]
                        Print state point in pretty format. An optional
                        argument to this flag specifies the maximal depth a
                        state point is printed.
  -i [INDENT], --indent [INDENT]
                        Specify the indentation of the JSON formatted state
                        point.
  -f FILTER [FILTER ...], --filter FILTER [FILTER ...]
                        Limit the diff to jobs matching this state point
                        filter.
  -d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
                        Show documents of jobs matching this document filter.
```

1.2.6 document

```
usage: signac document [-h] [-p [PRETTY]] [-i [INDENT]] [-s]
                        [-f FILTER [FILTER ...]]
                        [-d DOC_FILTER [DOC_FILTER ...]] [--index INDEX]
                        [job_id [job_id ...]]

Print the document(s) corresponding to one or more job ids.

positional arguments:
  job_id                One or more job ids. The job corresponding to a job id
                        must be initialized.

optional arguments:
  -h, --help            show this help message and exit
  -p [PRETTY], --pretty [PRETTY]
                        Print document in pretty format. An optional argument
                        to this flag specifies the maximal depth a document is
                        printed.
  -i [INDENT], --indent [INDENT]
                        Specify the indentation of the JSON formatted state
                        point.
  -s, --sort            Sort the document keys for output in JSON format.
  -f FILTER [FILTER ...], --filter FILTER [FILTER ...]
                        Show documents of jobs matching this state point
                        filter.
  -d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
                        Show documents of job matching this document filter.
  --index INDEX        The filename of an index file.
```

1.2.7 rm

```
usage: signac rm [-h] [-c] [-i] [-v] job_id [job_id ...]
```

positional arguments:

job_id One or more job ids of jobs to remove.

optional arguments:

-h, --help show this help message and exit
 -c, --clear Do not completely remove, but only clear the job.
 -i, --interactive Request confirmation before attempting to remove/clear
 each job.
 -v, --verbose Be verbose when removing/clearing files.

1.2.8 move

```
usage: signac move [-h] project job_id [job_id ...]
```

positional arguments:

project The root directory of the project to move one or more jobs to.
 job_id One or more job ids. The corresponding jobs must be initialized.

optional arguments:

-h, --help show this help message and exit

1.2.9 clone

```
usage: signac clone [-h] project job_id [job_id ...]
```

positional arguments:

project The root directory of the project to clone one or more jobs in.
 job_id One or more job ids. The corresponding jobs must be initialized.

optional arguments:

-h, --help show this help message and exit

1.2.10 index

```
usage: signac index [-h] [-t TAGS [TAGS ...]] [root]
```

positional arguments:

root Specify the root path from where the main index is to
 be compiled.

optional arguments:

-h, --help show this help message and exit
 -t TAGS [TAGS ...], --tags TAGS [TAGS ...]
 Specify tags for this main index compilation.

1.2.11 find

```
usage: signac find [-h] [-d DOC_FILTER [DOC_FILTER ...]] [-i INDEX]
                  [-s [SHOW]] [--sp [SP [SP ...]]] [--doc [DOC [DOC ...]]]
                  [-p [PRETTY]] [-1]
                  [filter [filter ...]]
```

All filter arguments may be provided either directly in JSON encoding or in a simplified form, e.g., `-- $ signac find a 42 --` is equivalent to `-- $ signac find '{"a": 42}'`.

positional arguments:

filter A JSON encoded state point filter (key-value pairs).

optional arguments:

-h, --help show this help message and exit

-d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
A document filter.

-i INDEX, --index INDEX
The filename of an index file.

-s [SHOW], --show [SHOW]
Show the state point and document of each job.
Equivalent to `--sp --doc --pretty 3`.

--sp [SP [SP ...]] Show the state point of each job. Can be passed the
list of state point keys to print (if they exist for a
given job).

--doc [DOC [DOC ...]] Show the document of each job. Can be passed the list
of document keys to print (if they exist for a given
job).

-p [PRETTY], --pretty [PRETTY]
Pretty print output when using `--sp`, `--doc`, or
`---show`. Argument is the depth to which keys are
printed.

-1, --one-line Print output in JSON and on one line.

1.2.12 view

```
usage: signac view [-h] [-f FILTER [FILTER ...]]
                  [-d DOC_FILTER [DOC_FILTER ...]] [-j JOB_ID [JOB_ID ...]]
                  [-i INDEX]
                  [prefix] [path]
```

Generate a human readable set of paths representing state points in the workspace, e.g.
`view/param_name_1/param_value_1/param_name_2/param_value_2/job`. The leaf nodes of this directory structure are symlinks (named "job") into the workspace directory for that parameter combination. Note that all positional arguments must be provided before any keyword arguments. In particular, the prefix and path must be specified before arguments such as the filters, e.g. `signac view $PREFIX $VIEW_PATH -f FILTERS -d DOC_FILTERS`.

positional arguments:

prefix The path where the view is to be created. Defaults to
view.

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```

path                The path used for the generation of the linked view
                    hierarchy, defaults to '{{auto}}' (see
                    Project.export_to for information on how this is
                    expanded).

optional arguments:
  -h, --help          show this help message and exit

select:
  -f FILTER [FILTER ...], --filter FILTER [FILTER ...]
                        Limit the view to jobs matching this state point
                        filter.
  -d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
                        Limit the view to jobs matching this document filter.
  -j JOB_ID [JOB_ID ...], --job-id JOB_ID [JOB_ID ...]
                        Limit the view to jobs with these job ids.
  -i INDEX, --index INDEX
                        The filename of an index file.

```

1.2.13 schema

```

usage: signac schema [-h] [-x] [-t DEPTH] [-p PRECISION] [-r MAX_NUM_RANGE]
                    [-f FILTER [FILTER ...]] [-d DOC_FILTER [DOC_FILTER ...]]
                    [-j JOB_ID [JOB_ID ...]]

optional arguments:
  -h, --help          show this help message and exit
  -x, --exclude-const  Exclude state point parameters, which are constant
                        over the complete project data space.
  -t DEPTH, --depth DEPTH
                        A non-zero value will format the schema in a nested
                        representation up to the specified depth. The default
                        is a flat view (depth=0).
  -p PRECISION, --precision PRECISION
                        Round all numerical values up to the given precision.
  -r MAX_NUM_RANGE, --max-num-range MAX_NUM_RANGE
                        The maximum number of entries shown for a value range,
                        defaults to 5.

select:
  -f FILTER [FILTER ...], --filter FILTER [FILTER ...]
                        Detect schema only for jobs that match the state point
                        filter.
  -d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
                        Detect schema only for jobs that match the document
                        filter.
  -j JOB_ID [JOB_ID ...], --job-id JOB_ID [JOB_ID ...]
                        Detect schema only for jobs with the given job ids.

```

1.2.14 shell

```

usage: signac shell [-h] [-c COMMAND] [-f FILTER [FILTER ...]]
                  [-d DOC_FILTER [DOC_FILTER ...]] [-j JOB_ID [JOB_ID ...]]

```

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```

                                [file]

positional arguments:
  file                Execute Python script in file.

optional arguments:
  -h, --help          show this help message and exit
  -c COMMAND, --command COMMAND
                      Execute Python program passed as string.

select:
  Specify one or more jobs to preset the `jobs` variable as a generator over
  all job handles associated with the given selection. If the selection
  contains only one job, an additional `job` variable is referencing that
  single job, otherwise it is `None`.

  -f FILTER [FILTER ...], --filter FILTER [FILTER ...]
                        Reduce selection to jobs that match the given filter.
  -d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
                        Reduce selection to jobs that match the given document
                        filter.
  -j JOB_ID [JOB_ID ...], --job-id JOB_ID [JOB_ID ...]
                        Reduce selection to jobs that match the given job ids.

```

1.2.15 sync

```

usage: signac sync [-h] [-v] [-a] [-r] [-l] [-p] [-o] [-g] [-t] [-x [EXCLUDE]]
                  [-I] [--size-only] [--round-times] [-n] [-u]
                  [-s {always,never,update,Ask}] [-k KEY] [--all-keys]
                  [--no-keys] [-w] [--force] [-m] [--parallel [PARALLEL]]
                  [--stats] [-H] [--json] [-f FILTER [FILTER ...]]
                  [-d DOC_FILTER [DOC_FILTER ...]] [-j JOB_ID [JOB_ID ...]]
                  source [destination]

```

Use this command to synchronize this project with another project; similar to the synchronization of two directories with `rsync`. Data is always copied from the source to the destination. For example: `signac sync /path/to/other/project -u --all-keys` means "Synchronize all jobs within this project with those in the other project; overwrite files if the source files is newer and overwrite all conflicting keys in the project and job documents."

```

positional arguments:
  source                The root directory of the project that this project
                        should be synchronized with.
  destination           Optional: The root directory of the project that
                        should be modified for synchronization, defaults to
                        the local project.

optional arguments:
  -h, --help          show this help message and exit
  -v, --verbosity     Set level of verbosity.
  -w, --allow-workspace
                      Allow the specification of a workspace (instead of a
                      project) directory as the destination path.
  --force             Ignore all warnings, just synchronize.

```

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```

-m, --merge          Clone all the jobs that are not present in destination
                     from source.
--parallel [PARALLEL] Use multiple threads for synchronization. You may
                     optionally specify how many threads to use, otherwise
                     all available processing units will be utilized.
--stats             Provide file transfer statistics.
-H, --human-readable Provide statistics with human readable formatting.
--json              Print statistics in JSON formatting.

copy options:
-a, --archive        archive mode; equivalent to: '-rltpog'
-r, --recursive      Do not skip sub-directories, but synchronize
                     recursively.
-l, --links          Copy symbolic links as symbolic links pointing to the
                     original source.
-p, --perms          Preserve permissions.
-o, --owner           Preserve owner.
-g, --group           Preserve group.
-t, --times           Preserve file modification times (requires -p).
-x [EXCLUDE], --exclude [EXCLUDE] Exclude all files matching the given pattern. Exclude
                     all files if this option is provided without any
                     argument.
-I, --ignore-times    Never rely on file meta data such as the size or the
                     modification time when determining file differences.
--size-only           Ignore modification times during file comparison.
                     Useful when synchronizing between file systems with
                     different timestamp resolution.
--round-times         Round modification times during file comparison.
                     Useful when synchronizing between file systems with
                     different timestamp resolution.
-n, --dry-run         Do not actually execute the synchronization. Increase
                     the output verbosity to see messages about what would
                     potentially happen.
-u, --update          Skip files with newer modification time stamp. This is
                     a short-cut for: --strategy=update.

sync strategy:
-s {always,never,update,Ask}, --strategy {always,never,update,Ask}
                     Specify a synchronization strategy, for differing
                     files.
-k KEY, --key KEY     Specify a regular expression for keys that should be
                     overwritten as part of the project and job document
                     synchronization.
--all-keys            Overwrite all conflicting keys. Equivalent to
                     '--key=.*'.
--no-keys             Never overwrite any conflicting keys.

select:
-f FILTER [FILTER ...], --filter FILTER [FILTER ...]
                     Only synchronize jobs that match the state point
                     filter.
-d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]
                     Only synchronize jobs that match the document filter.
-j JOB_ID [JOB_ID ...], --job-id JOB_ID [JOB_ID ...]
                     Only synchronize jobs with the given job ids.

```

1.2.16 import

```
usage: signac import [-h] [--move] [--sync] [--sync-interactive]
                    [origin] [schema_path]
```

Import an existing dataset into this project. Optionally provide a file path based schema to specify the state point metadata. Providing a path based schema is only necessary if the data set was not previously exported from a signac project.

positional arguments:

origin	The origin to import from. May be a path to a directory, a zipfile, or a tarball. Defaults to the current working directory.
schema_path	Specify an optional import path, such as 'foo/{foo:int}'. Possible type definitions include bool, int, float, and str. The type is assumed to be 'str' if no type is specified.

optional arguments:

-h, --help	show this help message and exit
--move	Move the data upon import instead of copying. Can only be used when importing from a directory.
--sync	Attempt recursive synchronization with default arguments.
--sync-interactive	Synchronize the project with the origin data space interactively.

1.2.17 export

```
usage: signac export [-h] [--move] [-f FILTER [FILTER ...]]
                    [-d DOC_FILTER [DOC_FILTER ...]] [-j JOB_ID [JOB_ID ...]]
                    target [schema_path]
```

Export the project data space (or a subset) to a directory, a zipfile, or a tarball.

positional arguments:

target	The target to export to. May be a path to a directory, a zipfile, or a tarball.
schema_path	Specify an optional export path, based on the job state point, e.g., 'foo/{job.sp.foo}'.

optional arguments:

-h, --help	show this help message and exit
--move	Move data to export target instead of copying. Can only be used when exporting to a directory target.

select:

-f FILTER [FILTER ...], --filter FILTER [FILTER ...]	Limit the jobs to export to those matching the state point filter.
-d DOC_FILTER [DOC_FILTER ...], --doc-filter DOC_FILTER [DOC_FILTER ...]	Limit the jobs to export to those matching this document filter.

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```
-j JOB_ID [JOB_ID ...], --job-id JOB_ID [JOB_ID ...]
    Limit the jobs to export to those matching the
    provided job ids.
```

1.2.18 config

```
usage: signac config [-h] [-g] [-l] [-f] {show,set,host,verify} ...

positional arguments:
  {show,set,host,verify}

optional arguments:
  -h, --help            show this help message and exit
  -g, --global          Modify the global configuration.
  -l, --local           Modify the local configuration.
  -f, --force           Skip sanity checks when modifying the configuration.
```

1.3 API Reference

This is the API for the **signac** (core) application.

1.3.1 The Project

Attributes

<code>Project.build_job_search_index(index[, _trust])</code>	Build a job search index.
<code>Project.build_job_statepoint_index([...])</code>	Build a state point index to identify jobs with specific parameters.
<code>Project.check()</code>	Check the project's workspace for corruption.
<code>Project.clone(job[, copytree])</code>	Clone job into this project.
<code>Project.config</code>	Get project's configuration.
<code>Project.create_access_module([filename, ...])</code>	Create the access module for indexing.
<code>Project.create_linked_view([prefix, ...])</code>	Create or update a persistent linked view of the selected data space.
<code>Project.detect_schema([exclude_const, ...])</code>	Detect the project's state point schema.
<code>Project.data</code>	Get data associated with this project.
<code>Project.doc</code>	Get document associated with this project.
<code>Project.document</code>	Get document associated with this project.
<code>Project.dump_statepoints(statepoints)</code>	Dump the state points and associated job ids.
<code>Project.export_to(target[, path, copytree])</code>	Export all jobs to a target location, such as a directory or a (compressed) archive file.
<code>Project.find_job_ids([filter, doc_filter, index])</code>	Find the <code>job_ids</code> of all jobs matching the filters.
<code>Project.find_jobs([filter, doc_filter])</code>	Find all jobs in the project's workspace.
<code>Project.fn(filename)</code>	Prepend a filename with the project's root directory path.

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<code>Project.get_id()</code>	Get the project identifier.
<code>Project.get_statepoint(jobid[, fn])</code>	Get the state point associated with a job id.
<code>Project.groupby([key, default])</code>	Group jobs according to one or more state point parameters.
<code>Project.groupbydoc([key, default])</code>	Group jobs according to one or more document values.
<code>Project.import_from([origin, schema, sync, ...])</code>	Import the data space located at origin into this project.
<code>Project.id</code>	Get the project identifier.
<code>Project.index([formats, depth, skip_errors, ...])</code>	Generate an index of the project's workspace.
<code>Project.isfile(filename)</code>	Check if a filename exists in the project's root directory.
<code>Project.min_len_unique_id()</code>	Determine the minimum length required for a job id to be unique.
<code>Project.num_jobs()</code>	Return the number of initialized jobs.
<code>Project.open_job([statepoint, id])</code>	Get a job handle associated with a state point.
<code>Project.read_statepoints([fn])</code>	Read all state points from a file.
<code>Project.repair([fn_statepoints, index, job_ids])</code>	Attempt to repair the workspace after it got corrupted.
<code>Project.reset_statepoint(job, new_statepoint)</code>	Overwrite the state point of this job while preserving job data.
<code>Project.root_directory()</code>	Return the project's root directory.
<code>Project.stores</code>	Get HDF5-stores associated with this project.
<code>Project.sync(other[, strategy, exclude, ...])</code>	Synchronize this project with the other project.
<code>Project.update_cache()</code>	Update the persistent state point cache.
<code>Project.update_statepoint(job, update[, ...])</code>	Change the state point of this job while preserving job data.
<code>Project.workspace()</code>	Return the project's workspace directory.
<code>Project.write_statepoints([statepoints, fn, ...])</code>	Dump state points to a file.

class `signac.Project` (*config=None, ignore_schema_version=False*)

Bases: `object`

The handle on a signac project.

Application developers should usually not need to directly instantiate this class, but use `get_project()` instead.

Parameters

- **config** – The project configuration to use. By default, it loads the first signac project configuration found while searching upward from the current working directory (Default value = None).
- **ignore_schema_version** (*bool*) – (Default value = False).

FN_CACHE = `'signac_sp_cache.json.gz'`

The default filename for the state point cache file.

FN_DOCUMENT = `'signac_project_document.json'`

The project's document filename.

FN_STATEPOINTS = `'signac_statepoints.json'`

The default filename to read from and write state points to.

KEY_DATA = `'signac_data'`

The project's datastore key.

build_job_search_index (*index*, *_trust=False*)

Build a job search index.

Parameters

- **index** (*list*) – A document index.
- **_trust** – (Default value = False).

Returns A job search index based on the provided index.

Return type JobSearchIndex

Deprecated since version 1.3: This will be removed in 2.0.

build_job_statepoint_index (*exclude_const=False*, *index=None*)

Build a state point index to identify jobs with specific parameters.

This method generates pairs of state point keys and mappings of values to a set of all corresponding job ids. The pairs are ordered by the number of different values. Since state point keys may be nested, they are represented as a tuple. For example:

```
>>> for i in range(4):
...     project.open_job({'a': i, 'b': {'c': i % 2}}).init()
...
>>> for key, value in project.build_job_statepoint_index():
...     print(key)
...     pprint.pprint(value)
...
('b', 'c')
defaultdict(<class 'set'>,
            {0: {'3a530c13bfaf57517b4e81ecab6aec7f',
                  '4e9a45a922eae6bb5d144b36d82526e4'},
             1: {'d49c6609da84251ab096654971115d0c',
                  '5c2658722218d48a5eb1e0ef7c26240b'}})
('a',)
defaultdict(<class 'set'>,
            {0: {'4e9a45a922eae6bb5d144b36d82526e4'},
             1: {'d49c6609da84251ab096654971115d0c'},
             2: {'3a530c13bfaf57517b4e81ecab6aec7f'},
             3: {'5c2658722218d48a5eb1e0ef7c26240b'}})
```

Values that are constant over the complete data space can be optionally ignored with the *exclude_const* argument set to True.

Parameters

- **exclude_const** (*bool*) – Exclude entries that are shared by all jobs that are part of the index (Default value = False).
- **index** – A document index.

Yields *tuple* – Pairs of state point keys and mappings of values to a set of all corresponding job ids (Default value = None).

Deprecated since version 1.3: This will be removed in 2.0. Use the `detect_schema()` function instead.

check ()

Check the project's workspace for corruption.

Raises `signac.errors.JobsCorruptedError` – When one or more jobs are identified as corrupted.

clone (*job*, *copytree*=<function copytree>)

Clone job into this project.

Create an identical copy of job within this project.

See [signac clone](#) for the command line equivalent.

Parameters

- **job** (*Job*) – The job to copy into this project.
- **copytree** – (Default value = `shutil.copytree()`)

Returns The job instance corresponding to the copied job.

Return type *Job*

Raises *DestinationExistsError* – In case that a job with the same id is already initialized within this project.

config

Get project's configuration.

Returns Dictionary containing project's configuration.

Return type `_ProjectConfig`

create_access_module (*filename*=None, *main*=True, *master*=None)

Create the access module for indexing.

This method generates the access module required to make this project's index part of a main index.

Parameters

- **filename** (*str*) – The name of the access module file. Defaults to the standard name and should usually not be changed.
- **main** (*bool*) – If True, add directives for the compilation of a master index when executing the module (Default value = True).
- **master** (*bool*) – Deprecated parameter. Replaced by main.

Returns Access module name.

Return type *str*

Deprecated since version 1.5: This will be removed in 2.0. Access modules are deprecated.

create_linked_view (*prefix*=None, *job_ids*=None, *index*=None, *path*=None)

Create or update a persistent linked view of the selected data space.

Similar to [export_to\(\)](#), this function expands the data space for the selected jobs, but instead of copying data will create symbolic links to the individual job workspace directories. This is primarily useful for browsing through the data space using a file-browser with human-interpretable directory paths.

By default, the paths of the view will be based on variable state point keys as part of the *implicit* schema of the selected jobs that we create the view for. For example, creating a linked view for a data space with schema

```
>>> print(project.detect_schema())
{
  'foo': 'int([0, 1, 2, ..., 8, 9], 10)',
}
```

by calling `project.create_linked_view('my_view')` will look similar to:

```
my_view/foo/0/job -> workspace/b8fcc6b8f99c56509eb65568922e88b8
my_view/foo/1/job -> workspace/b6cd26b873ae3624653c9268deff4485
...
```

It is possible to control the paths using the `path` argument, which behaves in the exact same manner as the equivalent argument for `export_to()`.

Note: The behavior of this function is almost equivalent to `project.export_to('my_view', copytree=os.symlink)` with the major difference that view hierarchies are actually *updated*, meaning that invalid links are automatically removed.

See [signac view](#) for the command line equivalent.

Parameters

- **prefix** (*str*) – The path where the linked view will be created or updated (Default value = None).
- **job_ids** (*iterable*) – If None (the default), create the view for the complete data space, otherwise only for this iterable of job ids.
- **index** – A document index (Default value = None).
- **path** – The path (function) used to structure the linked data space (Default value = None).

Returns A dictionary that maps the source directory paths to the linked directory paths.

Return type `dict`

data

Get data associated with this project.

This property should be used for large array-like data, which can't be stored efficiently in the project document. For examples and usage, see [Centralized Project Data](#).

Equivalent to:

```
return project.stores['signac_data']
```

See also:

[H5Store](#): Usage examples.

Returns An HDF5-backed datastore.

Return type [H5Store](#)

detect_schema (*exclude_const=False, subset=None, index=None*)

Detect the project's state point schema.

See [signac schema](#) for the command line equivalent.

Parameters

- **exclude_const** (*bool*) – Exclude all state point keys that are shared by all jobs within this project (Default value = False).
- **subset** – A sequence of jobs or job ids specifying a subset over which the state point schema should be detected (Default value = None).
- **index** – A document index (Default value = None).

Returns The detected project schema.

Return type `ProjectSchema`

doc

Get document associated with this project.

Alias for `document()`.

Returns The project document.

Return type `JSONDict`

document

Get document associated with this project.

Returns The project document.

Return type `JSONDict`

dump_statepoints (*statepoints*)

Dump the state points and associated job ids.

Equivalent to:

```
{project.open_job(sp).id: sp for sp in statepoints}
```

Parameters *statepoints* (*iterable*) – A list of state points.

Returns A mapping, where the key is the job id and the value is the state point.

Return type `dict`

export_to (*target*, *path=None*, *copytree=None*)

Export all jobs to a target location, such as a directory or a (compressed) archive file.

Use this function in combination with `find_jobs()` to export only a select number of jobs, for example:

```
project.find_jobs({'foo': 0}).export_to('foo_0.tar')
```

The `path` argument enables users to control how exactly the exported data space is to be expanded. By default, the path-function will be based on the *implicit* schema of the exported jobs. For example, exporting jobs that all differ by a state point key *foo* with `project.export_to('data/')`, the exported directory structure could look like this:

```
data/foo/0
data/foo/1
...
```

That would be equivalent to specifying `path=lambda job: os.path.join('foo', job.sp.foo)`.

Instead of a function, we can also provide a string, where fields for state point keys are automatically formatted. For example, the following two path arguments are equivalent: “foo/{foo}” and “foo/{job.sp.foo}”.

Any attribute of job can be used as a field here, so `job.doc.bar`, `job.id`, and `job.ws` can also be used as path fields.

A special `{{auto}}` field allows us to expand the path automatically with state point keys that have not been specified explicitly. So, for example, one can provide `path="foo/{foo}/{{{auto}}}"` to specify that the path shall begin with `foo/{foo}/`, but is then automatically expanded with all other state point

key-value pairs. How key-value pairs are concatenated can be controlled *via* the format-specifier, so for example, `path="{{auto: _ }}"` will generate a structure such as

```
data/foo_0
data/foo_1
...
```

Finally, providing `path=False` is equivalent to `path="{{job.id }}"`.

See also:

`import_from()` : Previously exported or non-signac data spaces can be imported.

`signac export` : See `signac export` for the command line equivalent.

Parameters

- **`target`** – A path to a directory to export to. The target can not already exist. Besides directories, possible targets are tar files (`.tar`), gzipped tar files (`.tar.gz`), zip files (`.zip`), bzip2-compressed files (`.bz2`), and xz-compressed files (`.xz`).
- **`path`** – The path (function) used to structure the exported data space. This argument must either be a callable which returns a path (str) as a function of `job`, a string where fields are replaced using the job-state point dictionary, or `False`, which means that we just use the job-id as path. Defaults to the equivalent of `{{auto}}`.
- **`copytree`** – The function used for the actual copying of directory tree structures. Defaults to `shutil.copytree()`. Can only be used when the target is a directory.

Returns A dict that maps the source directory paths, to the target directory paths.

Return type `dict`

`find_job_ids` (*filter=None, doc_filter=None, index=None*)

Find the `job_ids` of all jobs matching the filters.

The optional filter arguments must be a Mapping of key-value pairs and JSON serializable.

Note: Providing a pre-calculated index may vastly increase the performance of this function.

Parameters

- **`filter`** (*dict*) – A mapping of key-value pairs that all indexed job state points are compared against (Default value = None).
- **`doc_filter`** (*dict*) – A mapping of key-value pairs that all indexed job documents are compared against (Default value = None).
- **`index`** – A document index. If not provided, an index will be computed (Default value = None).

Returns

Return type The ids of all indexed jobs matching both filter(s)

Raises

- `TypeError` – If the filters are not JSON serializable.
- `ValueError` – If the filters are invalid.

- `RuntimeError` – If the filters are not supported by the index.

Deprecated since version 1.3: This will be removed in 2.0. Use `find_jobs()` instead, then access ids with `job.id`. Replicate the original behavior with `[job.id for job in project.find_jobs()]`

find_jobs (*filter=None, doc_filter=None*)

Find all jobs in the project’s workspace.

The optional filter arguments must be a Mapping of key-value pairs and JSON serializable. The *filter* argument is used to search against job state points, whereas the *doc_filter* argument compares against job document keys.

See [signac find](#) for the command line equivalent.

Parameters

- **filter** (*Mapping*) – A mapping of key-value pairs that all indexed job state points are compared against (Default value = None).
- **doc_filter** (*Mapping*) – A mapping of key-value pairs that all indexed job documents are compared against (Default value = None).

Returns JobsCursor of jobs matching the provided filter(s).

Return type *JobsCursor*

Raises

- `TypeError` – If the filters are not JSON serializable.
- `ValueError` – If the filters are invalid.
- `RuntimeError` – If the filters are not supported by the index.

fn (*filename*)

Prepend a filename with the project’s root directory path.

Parameters **filename** (*str*) – The name of the file.

Returns The joined path of project root directory and filename.

Return type *str*

get_id ()

Get the project identifier.

Returns The project id.

Return type *str*

Deprecated since version 1.3: This will be removed in 2.0. Use `project.id` instead.

classmethod get_job (*root=None*)

Find a Job in or above the current working directory (or provided path).

Parameters **root** (*str*) – The job root directory. If no root directory is given, the current working directory is assumed to be the job directory (Default value = None).

Returns The job instance.

Return type *Job*

Raises `LookupError` – When job cannot be found.

classmethod get_project (*root=None, search=True, **kwargs*)

Find a project configuration and return the associated project.

Parameters

- **root** (*str*) – The starting point to search for a project, defaults to the current working directory.
- **search** (*bool*) – If True, search for project configurations inside and above the specified root directory, otherwise only return projects with a root directory identical to the specified root argument (Default value = True).
- ****kwargs** – Optional keyword arguments that are forwarded to the *Project* class constructor.

Returns An instance of *Project*.

Return type *Project*

Raises *LookupError* – When project configuration cannot be found.

get_statepoint (*jobid*, *fn=None*)

Get the state point associated with a job id.

The state point is retrieved from the internal cache, from the workspace or from a state points file.

Parameters

- **jobid** (*str*) – A job id to get the state point for.
- **fn** (*str*) – The filename of the file containing the state points, defaults to *FN_STATEPOINTS*.

Returns The state point corresponding to jobid.

Return type *dict*

Raises

- *KeyError* – If the state point associated with jobid could not be found.
- *signac.errors.JobsCorruptedError* – If the state point manifest file corresponding to jobid is inaccessible or corrupted.

Deprecated since version 1.3: This will be removed in 2.0. Use `open_job(id=jobid).statepoint()` function instead.

groupby (*key=None*, *default=None*)

Group jobs according to one or more state point parameters.

This method can be called on any *JobsCursor* such as the one returned by `find_jobs()` or by iterating over a project.

Examples

```
# Group jobs by state point parameter 'a'.
for key, group in project.groupby('a'):
    print(key, list(group))

# Find jobs where job.sp['a'] is 1 and group them
# by job.sp['b'] and job.sp['c'].
for key, group in project.find_jobs({'a': 1}).groupby(('b', 'c')):
    print(key, list(group))

# Group by job.sp['d'] and job.document['count'] using a lambda.
```

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```

for key, group in project.groupby(
    lambda job: (job.sp['d'], job.document['count']))
):
    print(key, list(group))

```

If *key* is *None*, jobs are grouped by *id*, placing one job into each group.

Parameters

- **key** (*str*, *iterable*, or *callable*) – The state point grouping parameter(s) passed as a string, iterable of strings, or a callable that will be passed one argument, the job (Default value = *None*).
- **default** – A default value to be used when a given state point key is not present. The value must be sortable and is only used if not *None* (Default value = *None*).

Returns

- **key** (*str*) – Grouped key.
- **group** (*iterable of Jobs*) – Iterable of *Job* instances matching this group key.

groupbydoc (*key=None*, *default=None*)

Group jobs according to one or more document values.

This method can be called on any *JobsCursor* such as the one returned by *find_jobs()* or by iterating over a project.

Examples

```

# Group jobs by document value 'a'.
for key, group in project.groupbydoc('a'):
    print(key, list(group))

# Find jobs where job.sp['a'] is 1 and group them
# by job.document['b'] and job.document['c'].
for key, group in project.find_jobs({'a': 1}).groupbydoc(('b', 'c')):
    print(key, list(group))

# Group by whether 'd' is a field in the job.document using a lambda.
for key, group in project.groupbydoc(lambda doc: 'd' in doc):
    print(key, list(group))

```

If *key* is *None*, jobs are grouped by *id*, placing one job into each group.

Parameters

- **key** (*str*, *iterable*, or *callable*) – The document grouping parameter(s) passed as a string, iterable of strings, or a callable that will be passed one argument, *document* (Default value = *None*).
- **default** – A default value to be used when a given document key is not present. The value must be sortable and is only used if not *None* (Default value = *None*).

id

Get the project identifier.

Returns The project *id*.

Return type *str*

import_from (*origin=None, schema=None, sync=None, copytree=None*)

Import the data space located at *origin* into this project.

This function will walk through the data space located at *origin* and will try to identify data space paths that can be imported as a job workspace into this project.

The *schema* argument expects a function that takes a path argument and returns a state point dictionary. A default function is used when no argument is provided. The default schema function will simply look for state point manifest files—usually named `signac_statepoint.json`—and then import all data located within that path into the job workspace corresponding to the state point specified in the manifest file.

Alternatively the *schema* argument may be a string, that is converted into a schema function, for example: Providing `foo/{foo:int}` as *schema* argument means that all directories under `foo/` will be imported and their names will be interpreted as the value for `foo` within the state point.

Tip: Use `copytree=os.replace` or `copytree=shutil.move` to move dataspaces on import instead of copying them.

Warning: Imports can fail due to conflicts. Moving data instead of copying may therefore lead to inconsistent states and users are advised to apply caution.

See also:

`export_to()` : Export the project data space.

signac import : See `signac import` for the command line equivalent.

Parameters

- **origin** – The path to the data space origin, which is to be imported. This may be a path to a directory, a zip file, or a tarball archive (Default value = `None`).
- **schema** – An optional schema function, which is either a string or a function that accepts a path as its first and only argument and returns the corresponding state point as dict. (Default value = `None`).
- **sync** – If `True`, the project will be synchronized with the imported data space. If a dict of keyword arguments is provided, the arguments will be used for `sync()` (Default value = `None`).
- **copytree** – Specify which exact function to use for the actual copytree operation. Defaults to `shutil.copytree()`.

Returns A dict that maps the source directory paths to the target directory paths.

Return type `dict`

index (*formats=None, depth=0, skip_errors=False, include_job_document=True*)

Generate an index of the project's workspace.

This generator function indexes every file in the project's workspace until the specified *depth*. The job document if it exists, is always indexed, other files need to be specified with the *formats* argument.

See `signac project -i` for the command line equivalent.

```
for doc in project.index({r'*.txt', 'TextFile'}):
    print(doc)
```

Parameters

- **formats** (*str*, *dict*) – The format definitions as a pattern string (e.g. `r'*.*\.\txt'`) or a mapping from pattern strings to formats (e.g. `'TextFile'`). If `None`, only the job document is indexed (Default value = `None`).
- **depth** (*int*) – Specifies the crawling depth. A value of 0 means no limit (Default value = 0).
- **skip_errors** (*bool*) – Skip all errors which occur during indexing. This is useful when trying to repair a broken workspace (Default value = `False`).
- **include_job_document** (*bool*) – Include the contents of job documents (Default value = `True`).

Yields *dict* – Index document.

classmethod **init_project** (*name*, *root=None*, *workspace=None*, *make_dir=True*)

Initialize a project with the given name.

It is safe to call this function multiple times with the same arguments. However, a *RuntimeError* is raised if an existing project configuration would conflict with the provided initialization parameters.

See *signac init* for the command line equivalent.

Parameters

- **name** (*str*) – The name of the project to initialize.
- **root** (*str*) – The root directory for the project. Defaults to the current working directory.
- **workspace** (*str*) – The workspace directory for the project. Defaults to a subdirectory *workspace* in the project root.
- **make_dir** (*bool*) – Create the project root directory if it does not exist yet (Default value = `True`).

Returns Initialized project, an instance of *Project*.

Return type *Project*

Raises *RuntimeError* – If the project root path already contains a conflicting project configuration.

isfile (*filename*)

Check if a filename exists in the project's root directory.

Parameters **filename** (*str*) – The name of the file.

Returns `True` if filename exists in the project's root directory.

Return type *bool*

min_len_unique_id ()

Determine the minimum length required for a job id to be unique.

This method's runtime scales with the number of jobs in the workspace.

Returns Minimum string length of a unique job identifier.

Return type *int*

num_jobs ()

Return the number of initialized jobs.

Returns Count of initialized jobs.

Return type *int*

open_job (*statepoint=None, id=None*)

Get a job handle associated with a state point.

This method returns the job instance associated with the given state point or job id. Opening a job by a valid state point never fails. Opening a job by id requires a lookup of the state point from the job id, which may fail if the job was not previously initialized.

Parameters

- **statepoint** (*dict*) – The job’s unique set of state point parameters (Default value = None).
- **id** (*str*) – The job id (Default value = None).

Returns The job instance.

Return type *Job*

Raises

- *KeyError* – If the attempt to open the job by id fails.
- *LookupError* – If the attempt to open the job by an abbreviated id returns more than one match.

read_statepoints (*fn=None*)

Read all state points from a file.

See also:

dump_statepoints() Dump the state points and associated job ids.

write_statepoints() Dump state points to a file.

Parameters **fn** (*str*) – The filename of the file containing the state points, defaults to *FN_STATEPOINTS*.

Returns State points.

Return type *dict*

repair (*fn_statepoints=None, index=None, job_ids=None*)

Attempt to repair the workspace after it got corrupted.

This method will attempt to repair lost or corrupted job state point manifest files using a state points file or a document index or both.

Parameters

- **fn_statepoints** (*str*) – The filename of the file containing the state points, defaults to *FN_STATEPOINTS*.
- **index** – A document index (Default value = None).
- **job_ids** – An iterable of job ids that should get repaired. Defaults to all jobs.

Raises *signac.errors.JobsCorruptedError* – When one or more corrupted job could not be repaired.

reset_statepoint (*job, new_statepoint*)

Overwrite the state point of this job while preserving job data.

This method will change the job id if the state point has been altered.

Danger: Use this function with caution! Resetting a job's state point, may sometimes be necessary, but can possibly lead to incoherent data spaces.

Parameters

- **job** (*Job*) – The job that should be reset to a new state point.
- **new_statepoint** (*mapping*) – The job's new state point.

Raises

- *DestinationExistsError* – If a job associated with the new state point is already initialized.
- *OSError* – If the move failed due to an unknown system related error.

Deprecated since version 1.3: This will be removed in 2.0. Use `job.reset_statepoint()` instead.

root_directory ()

Return the project's root directory.

Returns Path of project directory.

Return type *str*

stores

Get HDF5-stores associated with this project.

Use this property to access an HDF5 file within the project's root directory using the *H5Store* dict-like interface.

This is an example for accessing an HDF5 file called `'my_data.h5'` within the project's root directory:

```
project.stores['my_data']['array'] = np.random((32, 4))
```

This is equivalent to:

```
H5Store(project.fn('my_data.h5'))['array'] = np.random((32, 4))
```

Both the *project.stores* and the *H5Store* itself support attribute access. The above example could therefore also be expressed as:

```
project.stores.my_data.array = np.random((32, 4))
```

Returns The HDF5-Store manager for this project.

Return type *H5StoreManager*

sync (*other*, *strategy=None*, *exclude=None*, *doc_sync=None*, *selection=None*, ***kwargs*)

Synchronize this project with the other project.

Try to clone all jobs from the other project to this project. If a job is already part of this project, try to synchronize the job using the optionally specified strategies.

See *signac sync* for the command line equivalent.

Parameters

- **other** (*Project*) – The other project to synchronize this project with.
- **strategy** – A file synchronization strategy (Default value = None).

- **exclude** – Files with names matching the given pattern will be excluded from the synchronization (Default value = None).
- **doc_sync** – The function applied for synchronizing documents (Default value = None).
- **selection** – Only sync the given jobs (Default value = None).
- ****kwargs** – This method also accepts the same keyword arguments as the `sync_projects()` function.

Raises

- `DocumentSyncConflict` – If there are conflicting keys within the project or job documents that cannot be resolved with the given strategy or if there is no strategy provided.
- `FileSyncConflict` – If there are differing files that cannot be resolved with the given strategy or if no strategy is provided.
- `SchemaSyncConflict` – In case that the `check_schema` argument is `True` and the detected state point schema of this and the other project differ.

temporary_project (*name=None, dir=None*)

Context manager for the initialization of a temporary project.

The temporary project is by default created within the root project’s workspace to ensure that they share the same file system. This is an example for how this method can be used for the import and synchronization of external data spaces.

```
with project.temporary_project() as tmp_project:
    tmp_project.import_from('/data')
    project.sync(tmp_project)
```

Parameters

- **name** (*str*) – An optional name for the temporary project. Defaults to a unique random string.
- **dir** (*str*) – Optionally specify where the temporary project root directory is to be created. Defaults to the project’s workspace directory.

Returns An instance of `Project`.

Return type `Project`

to_dataframe (**args, **kwargs*)

Export the project metadata to a pandas `DataFrame`.

The arguments to this function are forwarded to `to_dataframe()`.

Parameters

- ***args** – Forwarded to `to_dataframe()`.
- ****kwargs** – Forwarded to `to_dataframe()`.

Returns

Return type `DataFrame`

update_cache ()

Update the persistent state point cache.

This function updates a persistent state point cache, which is stored in the project root directory. Most data space operations, including iteration and filtering or selection are expected to be significantly faster after calling this function, especially for large data spaces.

update_statepoint (*job*, *update*, *overwrite=False*)

Change the state point of this job while preserving job data.

By default, this method will not change existing parameters of the state point of the job.

This method will change the job id if the state point has been altered.

Warning: While appending to a job's state point is generally safe, modifying existing parameters may lead to data inconsistency. Use the `overwrite` argument with caution!

Parameters

- **job** (*Job*) – The job whose state point shall be updated.
- **update** (*mapping*) – A mapping used for the state point update.
- **overwrite** (*bool*, *optional*) – If True, this method will set all existing and new parameters to a job's statepoint, making it equivalent to `reset_statepoint()`. Use with caution! (Default value = False).

Raises

- `KeyError` – If the update contains keys, which are already part of the job's state point and `overwrite` is False.
- `DestinationExistsError` – If a job associated with the new state point is already initialized.
- `OSError` – If the move failed due to an unknown system related error.

Deprecated since version 1.3: This will be removed in 2.0. Use `job.update_statepoint()` instead.

workspace ()

Return the project's workspace directory.

The workspace defaults to `project_root/workspace`. Configure this directory with the 'workspace_dir' attribute. If the specified directory is a relative path, the absolute path is relative from the project's root directory.

Note: The configuration will respect environment variables, such as `$HOME`.

See `signac project -w` for the command line equivalent.

Returns Path of workspace directory.

Return type `str`

write_statepoints (*statepoints=None*, *fn=None*, *indent=2*)

Dump state points to a file.

If the file already contains state points, all new state points will be appended, while the old ones are preserved.

See also:

`dump_statepoints()` Dump the state points and associated job ids.

Parameters

- **statepoints** (*iterable*) – A list of state points, defaults to all state points which are defined in the workspace.
- **fn** (*str*) – The filename of the file containing the state points, defaults to `FN_STATEPOINTS`.
- **indent** (*int*) – Specify the indentation of the JSON file (Default value = 2).

1.3.2 The JobsCursor class

Attributes

<code>JobsCursor.export_to(target[, path, copytree])</code>	Export all jobs to a target location, such as a directory or a (zipped) archive file.
<code>JobsCursor.groupby([key, default])</code>	Group jobs according to one or more state point parameters.
<code>JobsCursor.groupbydoc([key, default])</code>	Group jobs according to one or more document values.
<code>JobsCursor.to_dataframe([sp_prefix, ...])</code>	Convert the selection of jobs to a pandas <code>DataFrame</code> .

class `signac.contrib.project.JobsCursor` (*project, filter, doc_filter*)

Bases: `object`

An iterator over a search query result.

Application developers should not directly instantiate this class, but use `find_jobs()` instead.

Enables simple iteration and grouping operations.

Parameters

- **project** (*Project*) – Project handle.
- **filter** (*dict*) – A mapping of key-value pairs that all indexed job state points are compared against (Default value = None).
- **doc_filter** (*dict*) – A mapping of key-value pairs that all indexed job documents are compared against (Default value = None).

export_to (*target, path=None, copytree=None*)

Export all jobs to a target location, such as a directory or a (zipped) archive file.

See also:

`export_to()` : For full details on how to use this function.

Parameters

- **target** (*str*) – A path to a directory or archive file to export to.
- **path** (*str or callable*) – The path (function) used to structure the exported data space (Default value = None).
- **copytree** (*callable*) – The function used for copying of directory tree structures. Defaults to `shutil.copytree()`. Can only be used when the target is a directory (Default value = None).

Returns A dictionary that maps the source directory paths to the target directory paths.

Return type `dict`

groupby (*key=None, default=None*)

Group jobs according to one or more state point parameters.

This method can be called on any *JobsCursor* such as the one returned by *find_jobs()* or by iterating over a project.

Examples

```
# Group jobs by state point parameter 'a'.
for key, group in project.groupby('a'):
    print(key, list(group))

# Find jobs where job.sp['a'] is 1 and group them
# by job.sp['b'] and job.sp['c'].
for key, group in project.find_jobs({'a': 1}).groupby(('b', 'c')):
    print(key, list(group))

# Group by job.sp['d'] and job.document['count'] using a lambda.
for key, group in project.groupby(
    lambda job: (job.sp['d'], job.document['count'])
):
    print(key, list(group))
```

If *key* is *None*, jobs are grouped by id, placing one job into each group.

Parameters

- **key** (*str, iterable, or callable*) – The state point grouping parameter(s) passed as a string, iterable of strings, or a callable that will be passed one argument, the job (Default value = *None*).
- **default** – A default value to be used when a given state point key is not present. The value must be sortable and is only used if not *None* (Default value = *None*).

groupbydoc (*key=None, default=None*)

Group jobs according to one or more document values.

This method can be called on any *JobsCursor* such as the one returned by *find_jobs()* or by iterating over a project.

Examples

```
# Group jobs by document value 'a'.
for key, group in project.groupbydoc('a'):
    print(key, list(group))

# Find jobs where job.sp['a'] is 1 and group them
# by job.document['b'] and job.document['c'].
for key, group in project.find_jobs({'a': 1}).groupbydoc(('b', 'c')):
    print(key, list(group))

# Group by whether 'd' is a field in the job.document using a lambda.
for key, group in project.groupbydoc(lambda doc: 'd' in doc):
    print(key, list(group))
```

If *key* is *None*, jobs are grouped by id, placing one job into each group.

Parameters

- **key** (*str, iterable, or callable*) – The document grouping parameter(s) passed as a string, iterable of strings, or a callable that will be passed one argument, *document* (Default value = None).
- **default** – A default value to be used when a given document key is not present. The value must be sortable and is only used if not None (Default value = None).

next()

Return the next element.

This function is deprecated. Users should use `next(iter(...))` instead. .. deprecated:: 0.9.6

to_dataframe (*sp_prefix='sp.', doc_prefix='doc.', usecols=None, flatten=False*)

Convert the selection of jobs to a pandas `DataFrame`.

This function exports the job metadata to a `pandas.DataFrame`. All state point and document keys are prefixed by default to be able to distinguish them.

Parameters

- **sp_prefix** (*str, optional*) – Prefix state point keys with the given string. Defaults to “sp.”.
- **doc_prefix** (*str, optional*) – Prefix document keys with the given string. Defaults to “doc.”.
- **usecols** (*list-like or callable, optional*) – Used to select a subset of columns. If list-like, must contain strings corresponding to the column names that should be included. For example, `['sp.a', 'doc.notes']`. If callable, the column will be included if the function called on the column name returns True. For example, `lambda x: 'sp.' in x`. Defaults to None, which uses all columns from the state point and document. Note that this filter is applied *after* the doc and sp prefixes are added to the column names.
- **flatten** (*bool, optional*) – Whether nested state points or document keys should be flattened. If True, `{'a': {'b': 'c'}}` becomes a column named `a.b` with value `c`. If False, it becomes a column named `a` with value `{'b': 'c'}`. Defaults to False.

Returns A pandas `DataFrame` with all job metadata.

Return type `DataFrame`

1.3.3 The Job class

Attributes

<code>Job.clear()</code>	Remove all job data, but not the job itself.
<code>Job.close()</code>	Close the job and switch to the previous working directory.
<code>Job.data</code>	Get data associated with this job.
<code>Job.doc</code>	Alias for <code>document</code> .
<code>Job.document</code>	Get document associated with this job.
<code>Job.fn(filename)</code>	Prepend a filename with the job’s workspace directory path.
<code>Job.get_id()</code>	Job’s state point unique identifier.
<code>Job.id</code>	Get the unique identifier for the job’s state point.
<code>Job.init([force])</code>	Initialize the job’s workspace directory.

Continued on next page

Table 3 – continued from previous page

<code>Job.isfile(filename)</code>	Return True if file exists in the job's workspace.
<code>Job.move(project)</code>	Move this job to project.
<code>Job.open()</code>	Enter the job's workspace directory.
<code>Job.remove()</code>	Remove the job's workspace including the job document.
<code>Job.reset()</code>	Remove all job data, but not the job itself.
<code>Job.reset_statepoint(new_statepoint)</code>	Overwrite the state point of this job while preserving job data.
<code>Job.sp</code>	Alias for <code>statepoint</code> .
<code>Job.statepoint</code>	Get the job's state point.
<code>Job.stores</code>	Get HDF5 stores associated with this job.
<code>Job.sync(other[, strategy, exclude, doc_sync])</code>	Perform a one-way synchronization of this job with the other job.
<code>Job.update_statepoint(update[, overwrite])</code>	Change the state point of this job while preserving job data.
<code>Job.workspace()</code>	Return the job's unique workspace directory.
<code>Job.ws</code>	Alias for <code>workspace()</code> .

class `signac.contrib.job.Job` (*project*, *statepoint=None*, *_id=None*)

Bases: `object`

The job instance is a handle to the data of a unique state point.

Application developers should not directly instantiate this class, but use `open_job()` instead.

Jobs can be opened by `statepoint` or `_id`. If both values are provided, it is the user's responsibility to ensure that the values correspond.

Parameters

- **project** (*Project*) – Project handle.
- **statepoint** (*dict*) – State point for the job. (Default value = None)
- **_id** (*str*) – The job identifier. (Default value = None)

FN_DOCUMENT = `'signac_job_document.json'`

The job's document filename.

FN_MANIFEST = `'signac_statepoint.json'`

The job's manifest filename.

The job manifest is a human-readable file containing the job's state point that is stored in each job's workspace directory.

KEY_DATA = `'signac_data'`

The job's datastore key.

clear()

Remove all job data, but not the job itself.

This function will do nothing if the job was not previously initialized.

See `signac rm -c` for the command line equivalent.

close()

Close the job and switch to the previous working directory.

data

Get data associated with this job.

This property should be used for large array-like data, which can't be stored efficiently in the job document. For examples and usage, see [Job Data Storage](#).

Equivalent to:

```
return job.stores['signac_data']
```

Returns An HDF5-backed datastore.

Return type *H5Store*

doc

Alias for *document*.

Warning: If you need a deep copy that will not modify the underlying persistent JSON file, use *document* instead of *doc*. For more information, see *statepoint* or *JSONDict*.

document

Get document associated with this job.

Warning: If you need a deep copy that will not modify the underlying persistent JSON file, use *document* instead of *doc*. For more information, see *statepoint* or *JSONDict*.

See *signac document* for the command line equivalent.

Returns The job document handle.

Return type *JSONDict*

fn (filename)

Prepend a filename with the job's workspace directory path.

Parameters **filename** (*str*) – The name of the file.

Returns The full workspace path of the file.

Return type *str*

get_id()

Job's state point unique identifier.

Returns The job id.

Return type *str*

Deprecated since version 1.3: This will be removed in 2.0. Use *job.id* instead.

id

Get the unique identifier for the job's state point.

Returns The job id.

Return type *str*

init (force=False)

Initialize the job's workspace directory.

This function will do nothing if the directory and the job manifest already exist.

Returns the calling job.

See *signac job -c* for the command line equivalent.

Parameters **force** (*bool*) – Overwrite any existing state point’s manifest files, e.g., to repair them if they got corrupted (Default value = False).

Returns The job handle.

Return type *Job*

isfile (*filename*)

Return True if file exists in the job’s workspace.

Parameters **filename** (*str*) – The name of the file.

Returns True if file with filename exists in workspace.

Return type *bool*

move (*project*)

Move this job to project.

This function will attempt to move this instance of job from its original project to a different project.

See *signac move* for the command line equivalent.

Parameters **project** (*Project*) – The project to move this job to.

open ()

Enter the job’s workspace directory.

You can use the *Job* class as context manager:

```
with project.open_job(my_statepoint) as job:
    # manipulate your job data
```

Opening the context will switch into the job’s workspace, leaving it will switch back to the previous working directory.

remove ()

Remove the job’s workspace including the job document.

This function will do nothing if the workspace directory does not exist.

See *signac rm* for the command line equivalent.

reset ()

Remove all job data, but not the job itself.

This function will initialize the job if it was not previously initialized.

reset_statepoint (*new_statepoint*)

Overwrite the state point of this job while preserving job data.

This method will change the job id if the state point has been altered.

For more information, see [Modifying the State Point](#).

Danger: Use this function with caution! Resetting a job’s state point may sometimes be necessary, but can possibly lead to incoherent data spaces.

Parameters **new_statepoint** (*dict*) – The job’s new state point.

spAlias for `statepoint`.**statepoint**

Get the job's state point.

Warning: The state point object behaves like a dictionary in most cases, but because it persists changes to the filesystem, making a copy requires explicitly converting it to a dict. If you need a modifiable copy that will not modify the underlying JSON file, you can access a dict copy of the state point by calling it, e.g. `sp_dict = job.statepoint()` instead of `sp = job.statepoint`. For more information, see : `JSONDict`.

See `signac statepoint` for the command line equivalent.**Returns** Returns the job's state point.**Return type** `dict`**stores**

Get HDF5 stores associated with this job.

Use this property to access an HDF5 file within the job's workspace directory using the `H5Store` dict-like interface.

This is an example for accessing an HDF5 file called 'my_data.h5' within the job's workspace:

```
job.stores['my_data']['array'] = np.random((32, 4))
```

This is equivalent to:

```
H5Store(job.fn('my_data.h5'))['array'] = np.random((32, 4))
```

Both the `stores` and the `H5Store` itself support attribute access. The above example could therefore also be expressed as:

```
job.stores.my_data.array = np.random((32, 4))
```

Returns The HDF5-Store manager for this job.**Return type** `H5StoreManager`**sync** (*other*, *strategy=None*, *exclude=None*, *doc_sync=None*, ***kwargs*)

Perform a one-way synchronization of this job with the other job.

By default, this method will synchronize all files and document data with the other job to this job until a synchronization conflict occurs. There are two different kinds of synchronization conflicts:

1. The two jobs have files with the same, but different content.
2. The two jobs have documents that share keys, but those keys are associated with different values.

A file conflict can be resolved by providing a 'FileSync' *strategy* or by *excluding* files from the synchronization. An unresolvable conflict is indicated with the raise of a `FileSyncConflict` exception.A document synchronization conflict can be resolved by providing a `doc_sync` function that takes the source and the destination document as first and second argument.**Parameters**

- **other** (`Job`) – The other job to synchronize from.

- **strategy** – A synchronization strategy for file conflicts. If no strategy is provided, a `SyncConflict` exception will be raised upon conflict (Default value = None).
- **exclude** (*str*) – An filename exclude pattern. All files matching this pattern will be excluded from synchronization (Default value = None).
- **doc_sync** – A synchronization strategy for document keys. If this argument is None, by default no keys will be synchronized upon conflict.
- **dry_run** – If True, do not actually perform the synchronization.
- ****kwargs** – Extra keyword arguments will be forward to the `sync_jobs()` function which actually excutes the synchronization operation.

Raises `FileSyncConflict` – In case that a file synchronization results in a conflict.

update_statepoint (*update*, *overwrite=False*)

Change the state point of this job while preserving job data.

By default, this method will not change existing parameters of the state point of the job.

This method will change the job id if the state point has been altered.

For more information, see [Modifying the State Point](#).

Warning: While appending to a job’s state point is generally safe, modifying existing parameters may lead to data inconsistency. Use the `overwrite` argument with caution!

Parameters

- **update** (*dict*) – A mapping used for the state point update.
- **overwrite** (*bool*, *optional*) – If True, this method will set all existing and new parameters to a job’s statepoint, making it equivalent to `reset_statepoint()`. Use with caution! (Default value = False).

Raises

- `KeyError` – If the update contains keys, which are already part of the job’s state point and `overwrite` is False.
- `DestinationExistsError` – If a job associated with the new state point is already initialized.
- `OSError` – If the move failed due to an unknown system related error.

workspace ()

Return the job’s unique workspace directory.

See `signac job -w` for the command line equivalent.

Returns The path to the job’s workspace directory.

Return type `str`

WS

Alias for `workspace()`.

1.3.4 The Collection

class `signac.Collection` (*docs=None*, *primary_key='_id'*, *compresslevel=0*, *_trust=False*)

A collection of documents.

The Collection class manages a collection of documents in memory or in a file on disk. A document is defined as a dictionary mapping of key-value pairs.

An instance of collection may be used to manage and search documents. For example, given a collection with member data, where each document contains a *name* entry and an *age* entry, we can find the name of all members that are at age 32 like this:

```
members = [
    {'name': 'John', 'age': 32},
    {'name': 'Alice', 'age': 28},
    {'name': 'Kevin', 'age': 32},
    # ...
]

member_collection = Collection(members)
for doc in member_collection.find({'age': 32}):
    print(doc['name'])
```

To iterate over all documents in the collection, use:

```
for doc in collection:
    print(doc)
```

By default a collection object will reside in memory. However, it is possible to manage a collection associated to a file on disk. To open a collection which is associated with a file on disk, use the `Collection.open()` class method:

```
with Collection.open('collection.txt') as collection:
    for doc in collection.find({'age': 32}):
        print(doc)
```

The collection file is by default opened in *a+* mode, which means it can be read from and written to and will be created if it does not exist yet.

Parameters

- **docs** (*iterable*) – Initialize the collection with these documents.
- **primary_key** (*str*) – The name of the key which serves as the primary index of the collection. Selecting documents by primary key has time complexity of $O(N)$ in the worst case and $O(1)$ on average. All documents must have a primary key value. The default primary key is *_id*.
- **compresslevel** (*int*) – The level of compression to use. Any positive value implies compression and is used by the underlying gzip implementation. Default value is 0 (no compression).

Raises `ValueError` – When first argument is a string.

clear()

Remove all documents from the collection.

close()

Close this collection instance.

In case that the collection is associated with a file-object, all changes are flushed to the file and the file is closed.

It is not possible to re-open the same collection instance after closing it.

delete_many (*filter*)

Delete all documents that match the filter.

Parameters **filter** (*dict*) – A document that should be deleted must match this filter.

delete_one (*filter*)

Delete one document that matches the filter.

Parameters **filter** (*dict*) – The document that should be deleted must match this filter.

dump (*file=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='UTF-8'>*)

Dump the collection in JSON-encoding to file.

The file argument defaults to `sys.stdout`, which means the encoded blob will be printed to screen in case that no file argument is provided.

For example, to dump to a file on disk, one could write:

```
with open('my_collection.txt', 'w') as file:
    collection.dump(file)
```

Parameters **file** – The file to write the encoded blob to (Default value = `sys.stdout`).

find (*filter=None, limit=0*)

Find all documents matching filter, but not more than limit.

This function searches the collection for all documents that match the given filter and returns a result vector. For example:

```
for doc in collection.find(my_filter):
    print(doc)
```

Nested values should be searched using the `.` operator, for example:

```
docs = collection.find({'nested.value': 42})
```

will return documents with a nested structure: `{'nested': {'value': 42}}`.

The result of `find()` can be stored and iterated over multiple times. In addition, the result vector can be queried for its size:

```
docs = collection.find(my_filter)

print(len(docs))    # the number of documents matching

for doc in docs:    # iterate over the result vector
    pass
```

Arithmetic Operators

- *\$eq*: equal
- *\$ne*: not equal
- *\$gt*: greater than
- *\$gte*: greater or equal than

- *\$lt*: less than
- *\$lte*: less or equal than

```
project.find({"a": {"$lt": 5})
```

Matches all docs with *a* less than 5.

Logical Operators

That includes *\$and* and *\$or*; both expect a list of expressions.

```
project.find({"$or": [{"a": 4}, {"b": {"$gt": 3}}]})
```

Matches all docs, where *a* is 4 or *b* is greater than 3.

Exists operator

Determines whether a specific key exists, or not, e.g.:

```
project.find({"a": {"$exists": True}})
```

Array operator

To determine whether specific elements are in (*\$in*), or not in (*\$nin*) an array, e.g.:

```
project.find({"a": {"$in": [0, 1, 2]}})
```

Matches all docs, where *a* is either 0, 1, or 2. Usage of *\$nin* is equivalent.

Regular expression operator

Allows the “on-the-fly” evaluation of regular expressions, e.g.:

```
project.find({"protocol": {"$regex": "foo"}})
```

Will match all docs with a protocol that contains the term ‘foo’.

\$type operator

Matches when a value is of specific type, e.g.:

```
project.find({"protocol": {"$type": str}})
```

Finds all docs, where the value of protocol is of type str. Other types that can be checked are: *int*, *float*, *bool*, *list*, and *null*.

\$where operator

Matches an arbitrary python expression, e.g.:

```
project.find({"foo": {"$where": "lambda x: x.startswith('bar')"}}
↪)
```

Matches all docs, where the value for foo starts with the word ‘bar’.

Parameters

- **filter** (*dict*) – All documents must match the given filter (Default value = None).
- **limit** (*int*) – Do not return more than limit number of documents. A limit value of 0 (the default) means no limit.

Returns A result object that iterates over all matching documents.

Return type `_CollectionSearchResults`

Raises `ValueError` – In case that the filter argument is invalid.

find_one (*filter=None*)

Return one document that matches the filter or None.

```
doc = collection.find_one(my_filter)
if doc is None:
    print("No result found for filter", my_filter)
else:
    print("Doc matching filter:", my_filter, doc)
```

Parameters **filter** (*dict*) – The returned document must match the given filter (Default value = None).

Returns A matching document or None.

Return type `dict`

Raises `ValueError` – In case that the filter argument is invalid.

flush ()

Write all changes to the associated file.

If the collection instance is associated with a file-object, calling the `flush()` method will write all changes to this file.

This method is also called when the collection is explicitly or implicitly closed.

ids

Get an iterator over the primary key in the collection.

Returns iterator over the primary key in the collection.

Return type `iterable`

index (*key, build=False*)

Get (and optionally build) the index for a given key.

An index allows to access documents by a specific key with minimal time complexity, e.g.:

```
age_index = member_collection.index('age')
for _id in age_index[32]:
    print(member_collection[_id]['name'])
```

This means we can access documents by the ‘age’ key in $O(1)$ time on average in addition to the primary key. Using the `find()` method will automatically build all required indexes for the particular search.

Once an index has been built, it will be internally managed by the class and updated with subsequent changes. An index returned by this method is always current with the latest state of the collection.

Parameters

- **key** (*str*) – The primary key of the requested index.
- **build** (*bool*) – If True, build a non-existing index if necessary, otherwise raise `KeyError` (Default value = False).

Returns Index for the given key.

Return type `dict`

Raises `KeyError` – In case the build is `False` and the index has not been built yet or no index is present for the key.

insert_one (*doc*)

Insert one document into the collection.

If the document does not have a value for the collection's primary key yet, it will be assigned one.

```
_id = collection.insert_one(doc)
assert _id in collection
```

Note: The document will be directly updated in case that it has no primary key and must therefore be mutable!

Parameters `doc` (*dict*) – The document to be inserted.

Returns The `_id` of the inserted documented.

Return type `str`

main ()

Start a command line interface for this Collection.

Use this function to interact with this instance of Collection on the command line. For example, executing the following script:

```
# find.py
with Collection.open('my_collection.txt') as c:
    c.main()
```

will enable us to search for documents on the command line like this:

```
$ python find.py '{"age": 32}'
{"name": "John", "age": 32}
{"name": "Kevin", "age": 32}
```

Raises `ValueError` – When both `-id` or `-indent` are selected.

classmethod `open` (*filename*, *mode=None*, *compresslevel=None*)

Open a collection associated with a file on disk.

Using this factory method will return a collection that is associated with a collection file on disk. For example:

```
with Collection.open('collection.txt') as collection:
    for doc in collection:
        print(doc)
```

will read all documents from the `collection.txt` file or create the file if it does not exist yet.

Modifications to the file will be written to the file when the `flush()` method is called or the collection is explicitly closed by calling the `Collection.close()` method or implicitly by leaving the `with`-clause:

```
with Collection.open('collection.txt') as collection:
    collection.update(my_docs)
# All changes to the collection have been written to collection.txt.
```

The open-modes work as expected, so for example to open a collection file in *read-only* mode, use `Collection.open('collection.txt', 'r')`.

Opening a gzip (*.gz) file also works as expected. Because gzip does not support a combined read and write mode, *mode=** is not available. Be sure to open the file in read, write, or append mode as required. Due to the manner in which gzip works, opening a file in *mode=wt* will effectively erase the current file, so take care using *mode=wt*.

Parameters

- **filename** (*str*) – Name of file to read the documents from or create the file if it does not exist.
- **mode** (*str*) – Open the file with mode (Default value = None).
- **compresslevel** (*int*) – The level of compression to use. Any positive value implies compression and is used by the underlying gzip implementation. (Default value = None)

Returns An instance of *Collection*.

Return type *Collection*

Raises *RuntimeError* – File open-mode is not None for in-memory collection or compressed collections are not opened in binary mode.

primary_key

Get the name of the collection's primary key (default='_id').

classmethod read_json (*file=None*)

Construct an instance of *Collection* from a JSON file.

Parameters **file** – The json file to read, provided as either a filename or a file-like object (Default value = None).

Returns A *Collection* containing the JSON file

Return type *Collection*

replace_one (*filter, replacement, upsert=False*)

Replace one document that matches the given filter.

The first document matching the filter will be replaced by the given replacement document. If the *upsert* argument is True, the replacement will be inserted in case that no document matches the filter.

Parameters

- **filter** (*dict*) – A document that should be replaced must match this filter.
- **replacement** (*dict*) – The replacement document.
- **upsert** (*bool*) – If True, insert the replacement document in the case that no document matches the filter (Default value = False).

Returns The id of the replaced (or upserted) document.

Return type *str*

Raises *ValueError* – In case that the filter argument is invalid.

to_json (*file=None*)

Dump the collection as a JSON file.

This function returns the JSON-string directly if the file argument is None.

Parameters **file** – The filename or a file-like object to write the JSON string to (Default value = None).

Returns JSON-string when file argument is not provided.

Return type JSON

update (*docs*)

Update the collection with these documents.

Any existing documents with the same primary key will be replaced.

Parameters **docs** (*iterable*) – A sequence of documents to be upserted into the collection.

1.3.5 The JSONDict

This class implements the interface for the job's *statepoint* and *document* attributes, but can also be used stand-alone:

class signac.JSONDict (*filename=None, write_concern=False, parent=None*)

A dict-like mapping interface to a persistent JSON file.

The JSONDict is a *MutableMapping* and therefore behaves similarly to a *dict*, but all data is stored persistently in the associated JSON file on disk.

```
doc = JSONDict('data.json', write_concern=True)
doc['foo'] = "bar"
assert doc.foo == doc['foo'] == "bar"
assert 'foo' in doc
del doc['foo']
```

This class allows access to values through key indexing or attributes named by keys, including nested keys:

```
>>> doc['foo'] = dict(bar=True)
>>> doc
{'foo': {'bar': True}}
>>> doc.foo.bar = False
{'foo': {'bar': False}}
```

Warning: While the JSONDict object behaves like a dictionary, there are important distinctions to remember. In particular, because operations are reflected as changes to an underlying file, copying (even deep copying) a JSONDict instance may exhibit unexpected behavior. If a true copy is required, you should use the `_as_dict()` method to get a dictionary representation, and if necessary construct a new JSONDict instance: `new_dict = JSONDict(old_dict._as_dict())`.

Parameters

- **filename** – The filename of the associated JSON file on disk.
- **write_concern** – Ensure file consistency by writing changes back to a temporary file first, before replacing the original file. Default is False.
- **parent** – A parent instance of JSONDict or None.

buffered()

Context manager for buffering read and write operations.

This context manager activates the “buffered” mode, which means that all read operations are cached, and all write operations are deferred until the buffered mode is deactivated.

clear() → None. Remove all items from D.

get(k[, d]) → D[k] if k in D, else d. d defaults to None.

items() → a set-like object providing a view on D’s items

keys() → a set-like object providing a view on D’s keys

pop(k[, d]) → v, remove specified key and return the corresponding value.
If key is not found, d is returned if given, otherwise `KeyError` is raised.

popitem() → (k, v), remove and return some (key, value) pair
as a 2-tuple; but raise `KeyError` if D is empty.

reset(data)

Replace the document contents with data.

setdefault(k[, d]) → D.get(k,d), also set D[k]=d if k not in D

update([E], **F) → None. Update D from mapping/iterable E and F.

If E present and has a `.keys()` method, does: for k in E: D[k] = E[k] If E present and lacks `.keys()` method, does: for (k, v) in E: D[k] = v In either case, this is followed by: for k, v in F.items(): D[k] = v

values() → an object providing a view on D’s values

1.3.6 The H5Store

This class implements the interface to the job’s `data` attribute, but can also be used stand-alone:

class `signac.H5Store(filename, **kwargs)`

An HDF5-backed container for storing array-like and dictionary-like data.

The `H5Store` is a `MutableMapping` and therefore behaves similar to a `dict`, but all data is stored persistently in the associated HDF5 file on disk.

Supported types include:

- built-in types (int, float, str, bool, `NoneType`, array)
- numpy arrays
- pandas data frames (requires pandas and pytables)
- mappings with values that are supported types

Values can be accessed as attributes (`h5s.foo`) or via key index (`h5s['foo']`).

Examples

```
>>> from signac import H5Store
>>> with H5Store('file.h5') as h5s:
...     h5s['foo'] = 'bar'
...     assert 'foo' in h5s
...     assert h5s.foo == 'bar'
...     assert h5s['foo'] == 'bar'
>>>
```


The H5Store can be used as a context manager to ensure that the underlying file is opened, however most built-in types (excluding arrays) can be read and stored without the need to `_explicitly_` open the file. **To access arrays (reading or writing), the file must always be opened!**

To open a file in read-only mode, use the `open()` method with `mode='r'`:

```
>>> with H5Store('file.h5').open(mode='r') as h5s:
...     pass
>>>
```

Parameters

- **filename** (*str*) – The filename of the underlying HDF5 file.
- ****kwargs** – Additional keyword arguments to be forwarded to the `h5py.File` constructor. See the documentation for the [h5py.File constructor](#) for more information.

`clear()`

Remove all data from this store.

Danger: All data will be removed, this action cannot be reversed!

`close()`

Close the underlying HDF5 file.

file

Access the underlying instance of `h5py.File`.

This property exposes the underlying `h5py.File` object enabling use of functions such as `create_dataset()` or `requires_dataset()`.

Note: The store must be open to access this property!

Returns The `h5py` file-object that this store is operating on.

Return type `h5py.File`

Raises **H5StoreClosedError** – When the store is closed at the time of accessing this property.

filename

Return the H5Store filename.

`flush()`

Flush the underlying HDF5 file.

get (*k*, *d*) → *D*[*k*] if *k* in *D*, else *d*. *d* defaults to `None`.

items () → a set-like object providing a view on *D*'s items

keys () → a set-like object providing a view on *D*'s keys

mode

Return the default opening mode of this H5Store.

open (*mode=None*)

Open the underlying HDF5 file.

Parameters *mode* – The file open mode to use. Defaults to ‘a’ (append).

Returns This H5Store instance.

pop (*k*, *d*) → *v*, remove specified key and return the corresponding value.

If key is not found, *d* is returned if given, otherwise `KeyError` is raised.

popitem () → (*k*, *v*), remove and return some (key, value) pair as a 2-tuple; but raise `KeyError` if *D* is empty.

setdefault (*key*, *value*)

Set a value for a key if that key is not already set.

update ([*E*], ***F*) → `None`. Update *D* from mapping/iterable *E* and *F*.

If *E* present and has a `.keys()` method, does: for *k* in *E*: *D*[*k*] = *E*[*k*] If *E* present and lacks `.keys()` method, does: for (*k*, *v*) in *E*: *D*[*k*] = *v* In either case, this is followed by: for *k*, *v* in *F*.items(): *D*[*k*] = *v*

values () → an object providing a view on *D*’s values

1.3.7 The H5StoreManager

This class implements the interface to the job’s `stores` attribute, but can also be used stand-alone:

class `signac.H5StoreManager` (*prefix*)

Bases: `signac.core.dict_manager.DictManager`

Helper class to manage multiple instances of `H5Store` within a directory.

Example (assuming that the ‘stores/’ directory exists):

```
>>> stores = H5StoreManager('stores/')
>>> stores.data
<H5Store(filename=stores/data.h5)>
>>> stores.data.foo = True
>>> dict(stores.data)
{'foo': True}
```

Parameters *prefix* – The directory prefix shared by all stores managed by this class.

cls

alias of `H5Store`

keys ()

Return an iterable of keys.

prefix

Return the prefix.

1.3.8 Top-level functions

The signac framework aids in the management of large and heterogeneous data spaces.

It provides a simple and robust data model to create a well-defined, indexable storage layout for data and metadata. This makes it easier to operate on large data spaces, streamlines post-processing and analysis, and makes data collectively accessible.

`signac.TemporaryProject` (*name=None*, *cls=None*, ***kwargs*)

Context manager for the generation of a temporary project.

This is a factory function that creates a Project within a temporary directory and must be used as context manager, for example like this:

```
with TemporaryProject() as tmp_project:
    tmp_project.import_from('/data')
```

Parameters

- **name** (*str*) – An optional name for the temporary project. Defaults to a unique random string.
- **cls** – The class of the temporary project. Defaults to *Project*.
- ****kwargs** – Optional keyword arguments that are forwarded to the TemporaryDirectory class constructor, which is used to create a temporary root directory.

Yields *Project* – An instance of *Project*.

`signac.get_project` (*root=None, search=True, **kwargs*)

Find a project configuration and return the associated project.

Parameters

- **root** (*str*) – The starting point to search for a project, defaults to the current working directory.
- **search** (*bool*) – If True, search for project configurations inside and above the specified root directory, otherwise only return projects with a root directory identical to the specified root argument (Default value = True).
- ****kwargs** – Optional keyword arguments that are forwarded to `get_project()`.

Returns An instance of *Project*.

Return type *Project*

Raises *LookupError* – If no project configuration can be found.

`signac.init_project` (*name, root=None, workspace=None, make_dir=True*)

Initialize a project with the given name.

It is safe to call this function multiple times with the same arguments. However, a *RuntimeError* is raised if an existing project configuration would conflict with the provided initialization parameters.

Parameters

- **name** (*str*) – The name of the project to initialize.
- **root** (*str*) – The root directory for the project. Defaults to the current working directory.
- **workspace** (*str*) – The workspace directory for the project. Defaults to a subdirectory *workspace* in the project root.
- **make_dir** (*bool*) – Create the project root directory, if it does not exist yet (Default value = True).

Returns The initialized project instance.

Return type *Project*

Raises *RuntimeError* – If the project root path already contains a conflicting project configuration.

`signac.get_job` (*root=None*)

Find a Job in or above the current working directory (or provided path).

Parameters `root` (*str*) – The job root directory. If no root directory is given, the current working directory is assumed to be within the current job workspace directory (Default value = None).

Returns Job handle.

Return type *Job*

Raises `LookupError` – If this job cannot be found.

Examples

When the current directory is a job workspace directory:

```
>>> signac.get_job()
signac.contrib.job.Job(project=..., statepoint={...})
```

`signac.diff_jobs(*jobs)`

Find differences among a list of jobs' state points.

The resulting diff is a dictionary where the keys are job ids and the values are each job's state point minus the intersection of all provided jobs' state points. The comparison is performed over the combined set of keys and values.

See *signac diff* for the command line equivalent.

Parameters `*jobs` (sequence[*Job*]) – Sequence of jobs to diff.

Returns A dictionary where the keys are job ids and values are the unique parts of that job's state point.

Return type *dict*

Examples

```
>>> import signac
>>> project = signac.init_project('project_name')
>>> job1 = project.open_job({'constant': 42, 'diff1': 0, 'diff2': 1}).init()
>>> job2 = project.open_job({'constant': 42, 'diff1': 1, 'diff2': 1}).init()
>>> job3 = project.open_job({'constant': 42, 'diff1': 2, 'diff2': 2}).init()
>>> print(job1)
c4af2b26f1fd256d70799ad3ce3bdad0
>>> print(job2)
b96b21fada698f8934d58359c72755c0
>>> print(job3)
e4289419d2b0e57e4852d44a09f167c0
>>> signac.diff_jobs(job1, job2, job3)
{'c4af2b26f1fd256d70799ad3ce3bdad0': {'diff2': 1, 'diff1': 0},
 'b96b21fada698f8934d58359c72755c0': {'diff2': 1, 'diff1': 1},
 'e4289419d2b0e57e4852d44a09f167c0': {'diff2': 2, 'diff1': 2}}
>>> signac.diff_jobs(*project)
{'c4af2b26f1fd256d70799ad3ce3bdad0': {'diff2': 1, 'diff1': 0},
 'b96b21fada698f8934d58359c72755c0': {'diff2': 1, 'diff1': 1},
 'e4289419d2b0e57e4852d44a09f167c0': {'diff2': 2, 'diff1': 2}}
```

`signac.get_database(name, hostname=None, config=None)`

Get a database handle.

The database handle is an instance of *Database*, which provides access to the document collections within one database.

```
db = signac.db.get_database('MyDatabase')
docs = db.my_collection.find()
```

Please note, that a collection which did not exist at the point of access, will automatically be created.

Parameters

- **name** (*str*) – The name of the database to get.
- **hostname** (*str*) – The name of the configured host. Defaults to the first configured host, or the host specified by *default_host*.
- **config** (`common.config.Config`) – The config object to retrieve the host configuration from. Defaults to the global configuration.

Returns The database handle.

Return type `pymongo.database.Database`

See also:

<https://api.mongodb.org/python/current/api/pymongo/database.html>

Deprecated since version 1.3: This will be removed in 2.0. The database package is deprecated.

`signac.fetch(doc_or_id, mode='r', mirrors=None, num_tries=3, timeout=60, ignore_local=False)`

Fetch the file associated with this document or file id.

This function retrieves a file associated with the provided index document or file id and behaves like the built-in `open()` function, e.g.:

```
for doc in index:
    with signac.fetch(doc) as file:
        do_something_with(file)
```

Parameters

- **doc_or_id** – A file_id or a document with a file_id value.
- **mode** – Mode to use for opening files.
- **mirrors** – An optional set of mirrors to fetch the file from.
- **num_tries** (*int*) – The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) – The time in seconds to wait before an automatic retry attempt.

Returns The file associated with the document or file id.

Return type A file-like object

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.export_one(doc, index, mirrors=None, num_tries=3, timeout=60)`

Export one document to index and an optionally associated file to mirrors.

Parameters

- **doc** – A document with a file_id entry.
- **docs** – The index collection to export to.
- **mirrors** – An optional set of mirrors to export files to.

- **num_tries** (*int*) – The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) – The time in seconds to wait before an automatic retry attempt.

Returns The id and file id after successful export.

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.export(docs, index, mirrors=None, update=False, num_tries=3, timeout=60, **kwargs)`

Export docs to index and optionally associated files to mirrors.

The behavior of this function is equivalent to:

```
for doc in docs:
    export_one(doc, index, mirrors, num_tries)
```

If the *update* argument is set to True, the export algorithm will automatically identify stale index documents, that means documents that refer to files or state points that have been removed and are no longer part of the data space. Any document which shares the *root*, but not the *_id* field with any of the updated documents is considered stale and removed. Using *update* in combination with an empty docs sequence will raise *ExportError*, since it is not possible to identify stale documents in that case.

Note: This function will automatically delegate to specialized implementations for special index types. For example, if the index argument is a MongoDB document collection, the index documents will be exported via `export_pymongo()`.

Parameters

- **docs** – The index documents to export.
- **index** – The collection to export the index to.
- **mirrors** – An optional set of mirrors to export files to.
- **update** (*bool*) – If True, remove stale index documents, that means documents that refer to files or state points that no longer exist.
- **num_tries** (*int*) – The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) – The time in seconds to wait before an automatic retry attempt.
- **kwargs** – Optional keyword arguments to pass to delegate implementations.

Raises *ExportError* – When using the update argument in combination with an empty docs sequence.

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.export_to_mirror(doc, mirror, num_tries=3, timeout=60)`

Export a file associated with doc to mirror.

Parameters

- **doc** – A document with a file_id entry.
- **mirror** – A file-system object to export the file to.
- **num_tries** (*int*) – The number of automatic retry attempts in case of mirror connection errors.

- **timeout** (*int*) – The time in seconds to wait before an automatic retry attempt.

Returns The file id after successful export.

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.export_pymongo(docs, index, mirrors=None, update=False, num_tries=3, timeout=60, chunk-size=100)`

Optimized `export()` function for pymongo index collections.

The behavior of this function is roughly equivalent to:

```
for doc in docs:
    export_one(doc, index, mirrors, num_tries)
```

Note: All index documents must be JSON-serializable to be able to be exported to a MongoDB collection.

Parameters

- **docs** – The index documents to export.
- **index** (`pymongo.collection.Collection`) – The database collection to export the index to.
- **num_tries** (*int*) – The number of automatic retry attempts in case of mirror connection errors.
- **timeout** (*int*) – The time in seconds to wait before an automatic retry attempt.
- **chunksize** (*int*) – The buffer size for export operations.

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.index_files(root='.', formats=None, depth=0)`

Generate a file index.

This generator function yields file index documents, where each index document corresponds to one file.

To index all files in the current working directory, simply execute:

```
for doc in signac.index_files():
    print(doc)
```

A file associated with a file index document can be fetched via the `fetch()` function:

```
for doc in signac.index_files():
    with signac.fetch(doc) as file:
        print(file.read())
```

This is especially useful if the file index is part of a collection (`Collection`) which can be searched for specific entries.

To limit the file index to files with a specific filename formats, provide a regular expression as the `formats` argument. To index all files that have file ending `.txt`, execute:

```
for doc in signac.index_files(formats='.*\\.txt'):
    print(doc)
```

We can specify specific formats by providing a dictionary as `formats` argument, where the key is the filename pattern and the value is an arbitrary formats string, e.g.:

```
for doc in signac.index_files(formats=
    {r'.*\.txt': 'TextFile', r'.*\.zip': 'ZipFile'}):
    print(doc)
```

Parameters

- **root** (*str*) – The directory to index, defaults to the current working directory.
- **formats** – Limit the index to files that match the given regular expression and optionally associate formats with given patterns.
- **depth** (*int*) – Limit the search to the specified directory depth.

Yields The file index documents as dicts.

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.index` (*root='.', tags=None, depth=0, **kwargs*)
Generate a main index.

A main index is compiled from other indexes by searching for modules named `signac_access.py` and compiling all indexes which are yielded from a function `get_indexes(root)` defined within that module as well as the indexes generated by crawlers yielded from a function `get_crawlers(root)` defined within that module.

This is a minimal example for a `signac_access.py` file:

```
import signac

def get_indexes(root):
    yield signac.index_files(root, r'.*\.txt')
```

Internally, this function constructs an instance of `MainCrawler` and all extra key-word arguments will be forwarded to the constructor of said main crawler.

Parameters

- **root** (*str*) – Look for access modules under this directory path.
- **tags** – If tags are provided, do not execute subcrawlers that don't match the same tags.
- **depth** (*int*) – Limit the search to the specified directory depth.
- **kwargs** – These keyword-arguments are forwarded to the internal `MainCrawler` instance.

Yields The main index documents as instances of dict.

Deprecated since version 1.3: This will be removed in 2.0. The indexing module is deprecated.

`signac.buffered` (*buffer_size=33554432, force_write=False*)
Enter a global buffer mode for all `JSONDict` instances.

All future write operations are written to the buffer, read operations are performed from the buffer whenever possible.

All write operations are deferred until the `flush_all()` function is called, the buffer overflows, or upon exiting the buffer mode.

This context may be entered multiple times, however the buffer size can only be set *once*. Any subsequent specifications of the buffer size are ignored.

Parameters **buffer_size** (*int*) – Specify the maximum size of the read/write buffer. Defaults to `DEFAULT_BUFFER_SIZE`. A negative number indicates to not restrict the buffer size.

`signac.is_buffered()`
Return true if in buffered read/write mode.

`signac.flush()`
Execute all deferred JSONDict write operations.

`signac.get_buffer_size()`
Return the current maximum size of the read/write buffer.

`signac.get_buffer_load()`
Return the current actual size of the read/write buffer.

1.3.9 Submodules

signac.cite module

Functions to support citing this software.

`signac.cite.bibtex` (*file=None*)
Generate bibtex entries for signac.

The bibtex entries will be printed to screen unless a filename or a file-like object are provided, in which case they will be written to the corresponding file.

Note: A full reference should also include the version of this software. Please refer to the documentation on how to cite a specific version.

Parameters `file` – A str or file-like object. Defaults to `sys.stdout`.

`signac.cite.reference` (*file=None*)
Generate formatted reference entries for signac.

The references will be printed to screen unless a filename or a file-like object are provided, in which case they will be written to the corresponding file.

Note: A full reference should also include the version of this software. Please refer to the documentation on how to cite a specific version.

Parameters `file` – A str or file-like object. Defaults to `sys.stdout`.

signac.sync module

Synchronization of jobs and projects.

Jobs may be synchronized by copying all data from the source job to the destination job. This means all files are copied and the documents are synchronized. Conflicts, that means both jobs contain conflicting data, may be resolved with a user defined strategy.

The synchronization of projects is in essence the synchronization of all jobs which are in the destination project with the ones in the source project and the sync synchronization of the project document. If a specific job does not exist yet at the destination it is simply cloned, otherwise it is synchronized.

A sync strategy is a function (or functor) that takes the source job, the destination job, and the name of the file generating the conflict as arguments and returns the decision whether to overwrite the file as Boolean. There are some default strategies defined within this module as part of the `FileSync` class. These are the default strategies:

1. `always` – Always overwrite on conflict.
2. `never` – Never overwrite on conflict.
3. `update` – Overwrite when the modification time of the source file is newer.
4. `Ask` – Ask the user interactively about each conflicting filename.

For example, to synchronize two projects resolving conflicts by modification time, use:

```
dest_project.sync(source_project, strategy=sync.FileSync.update)
```

Unlike files, which are always either overwritten as a whole or not, documents can be synchronized more fine-grained with a *sync function*. Such a function (or functor) takes the source and the destination document as arguments and performs the synchronization. The user is encouraged to implement their own sync functions, but there are a few default functions implemented as part of the `DocSync` class:

1. `NO_SYNC` – Do not perform any synchronization.
2. `COPY` – Apply the same strategy used to resolve file conflicts.
3. `update` – Equivalent to `dst.update(src)`.
4. `ByKey` – Synchronize the source document key by key, more information below.

This is how we could synchronize two jobs, where the documents are synchronized with a simple update function:

```
dst_job.sync(src_job, doc_sync=sync.DocSync.update)
```

The `DocSync.ByKey` functor attempts to synchronize the destination document with the source document without overwriting any data. That means this function behaves similar to `update()` for a non-intersecting set of keys, but in addition will preserve nested mappings without overwriting values. In addition, any key conflict, that means keys that are present in both documents, but have differing data, will lead to the raise of a `DocumentSyncConflict` exception. The user may explicitly decide to overwrite certain keys by providing a “key-strategy”, which is a function that takes the conflicting key as argument, and returns the decision whether to overwrite that specific key as Boolean. For example, to sync two jobs, where conflicting keys should only be overwritten if they contain the term ‘foo’, we could execute:

```
dst_job.sync(src_job, doc_sync=sync.DocSync.ByKey(lambda key: 'foo' in key))
```

This means that all documents are synchronized ‘key-by-key’ and only conflicting keys that contain the word “foo” will be overwritten, any other conflicts would lead to the raise of a `DocumentSyncConflict` exception. A key-strategy may also be a regular expression, so the synchronization above could also be achieved with:

```
dst_job.sync(src_job, doc_sync=sync.DocSync.ByKey('foo'))
```

class `signac.sync.FileSync`

Bases: `object`

Collection of file synchronization strategies.

class `Ask`

Bases: `object`

Resolve sync conflicts by asking whether a file should be overwritten interactively.

static `always(src, dst, fn)`

Resolve sync conflicts by always overwriting.

classmethod keys()

Return keys.

static never(*src*, *dst*, *fn*)

Resolve sync conflicts by never overwriting.

static update(*src*, *dst*, *fn*)

Resolve sync conflicts based on newest modified timestamp.

class `signac.sync.DocSync`

Bases: `object`

Collection of document synchronization functions.

class `ByKey`(*key_strategy*=None)

Bases: `object`

Synchronize documents key by key.

COPY = 'copy'

Copy (and potentially overwrite) documents like any other file.

NO_SYNC = False

Do not synchronize documents.

static update(*src*, *dst*)

Perform a simple update.

`signac.sync.sync_jobs`(*src*, *dst*, *strategy*=None, *exclude*=None, *doc_sync*=None, *recursive*=False, *follow_symlinks*=True, *preserve_permissions*=False, *preserve_times*=False, *preserve_owner*=False, *preserve_group*=False, *deep*=False, *dry_run*=False)

Synchronize the dst job with the src job.

By default, this method will synchronize all files and document data of dst job with the src job until a synchronization conflict occurs. There are two different kinds of synchronization conflicts:

1. The two jobs have files with the same name, but different content.
2. The two jobs have documents that share keys, but those keys are mapped to different values.

A file conflict can be resolved by providing a 'FileSync' *strategy* or by *excluding* files from the synchronization. An unresolvable conflict is indicated with the raise of a `FileSyncConflict` exception.

A document synchronization conflict can be resolved by providing a *doc_sync* function that takes the source and the destination document as first and second argument.

Parameters

- **src** (*Job*) – The src job, data will be copied from this job's workspace.
- **dst** (*Job*) – The dst job, data will be copied to this job's workspace.
- **strategy** (*callable*) – A synchronization strategy for file conflicts. The strategy should be a callable with signature `strategy(src, dst, filepath)` where *src* and *dst* are the source and destination instances of `Project` and *filepath* is the filepath relative to the project root. If no strategy is provided, a `errors.SyncConflict` exception will be raised upon conflict. (Default value = None)
- **exclude** (*str*) – A filename exclusion pattern. All files matching this pattern will be excluded from the synchronization process. (Default value = None)
- **doc_sync** (attribute or callable from `DocSync`) – A synchronization strategy for document keys. The default is to use a safe key-by-key strategy that will not overwrite any values on conflict, but instead raises a `DocumentSyncConflict` exception.

- **recursive** (*bool*) – Recursively synchronize sub-directories encountered within the job workspace directories. (Default value = False)
- **follow_symlinks** (*bool*) – Follow and copy the target of symbolic links. (Default value = True)
- **preserve_permissions** (*bool*) – Preserve file permissions (Default value = False)
- **preserve_times** (*bool*) – Preserve file modification times (Default value = False)
- **preserve_owner** (*bool*) – Preserve file owner (Default value = False)
- **preserve_group** (*bool*) – Preserve file group ownership (Default value = False)
- **dry_run** (*bool*) – If True, do not actually perform any synchronization operations. (Default value = False)
- **deep** (*bool*) – (Default value = False)

```
signac.sync.sync_projects(source, destination, strategy=None, exclude=None, doc_sync=None,
                          selection=None, check_schema=True, recursive=False, follow_symlinks=True,
                          preserve_permissions=False, preserve_times=False, preserve_owner=False,
                          preserve_group=False, deep=False, dry_run=False, parallel=False, collect_stats=False)
```

Synchronize the destination project with the source project.

Try to clone all jobs from the source to the destination. If the destination job already exist, try to synchronize the job using the optionally specified strategy.

Parameters

- **source** (class:~.Project) – The project presenting the source for synchronization.
- **destination** (class:~.Project) – The project that is modified for synchronization.
- **strategy** (*callable*) – A synchronization strategy for file conflicts. The strategy should be a callable with signature `strategy(src, dst, filepath)` where `src` and `dst` are the source and destination instances of *Project* and `filepath` is the filepath relative to the project root. If no strategy is provided, a *errors.SyncConflict* exception will be raised upon conflict. (Default value = None)
- **exclude** (*str*) – A filename exclusion pattern. All files matching this pattern will be excluded from the synchronization process. (Default value = None)
- **doc_sync** (attribute or callable from *DocSync*) – A synchronization strategy for document keys. The default is to use a safe key-by-key strategy that will not overwrite any values on conflict, but instead raises a *DocumentSyncConflict* exception.
- **selection** (sequence of *Job* or job ids (*str*)) – Only synchronize the given selection of jobs. (Default value = None)
- **check_schema** (*bool*) – If True, only synchronize if this and the other project have a matching state point schema. See also: `detect_schema()`. (Default value = True)
- **recursive** (*bool*) – Recursively synchronize sub-directories encountered within the job workspace directories. (Default value = False)
- **follow_symlinks** (*bool*) – Follow and copy the target of symbolic links. (Default value = True)
- **preserve_permissions** (*bool*) – Preserve file permissions (Default value = False)
- **preserve_times** (*bool*) – Preserve file modification times (Default value = False)
- **preserve_owner** (*bool*) – Preserve file owner (Default value = False)

- **preserve_group** (*bool*) – Preserve file group ownership (Default value = False)
- **dry_run** (*bool*) – If True, do not actually perform the synchronization operation, just log what would happen theoretically. Useful to test synchronization strategies without the risk of data loss. (Default value = False)
- **deep** (*bool*) – (Default value = False)
- **parallel** (*bool*) – (Default value = False)
- **collect_stats** (*bool*) – (Default value = False)

Returns Returns stats if `collect_stats` is True, else None.

Return type `NoneType` or `FileTransferStats`

Raises

- *DocumentSyncConflict* – If there are conflicting keys within the project or job documents that cannot be resolved with the given strategy or if there is no strategy provided.
- *FileSyncConflict* – If there are differing files that cannot be resolved with the given strategy or if no strategy is provided.
- *SchemaSyncConflict* – In case that the `check_schema` argument is True and the detected state point schema of this and the other project differ.

signac.warnings module

Module for signac deprecation warnings.

exception `signac.warnings.SignacDeprecationWarning`

Bases: `UserWarning`

Indicates the deprecation of a signac feature, API or behavior.

This class indicates a user-relevant deprecation and is therefore a `UserWarning`, not a `DeprecationWarning` which is hidden by default.

signac.errors module

Errors raised by signac.

exception `signac.errors.AuthenticationError`

Bases: `signac.core.errors.Error`, `RuntimeError`

Authentication error.

exception `signac.errors.BufferException`

Bases: `signac.core.errors.Error`

An exception occurred in buffered mode.

exception `signac.errors.BufferedFileError` (*files*)

Bases: `signac.core.jsondict.BufferException`

Raised when an error occurred while flushing one or more buffered files.

files

A dictionary of files that caused issues during the flush operation, mapped to a possible reason for the issue or None in case that it cannot be determined.

exception `signac.errors.ConfigError`

Bases: `signac.core.errors.Error`, `RuntimeError`

Error with parsing or reading a configuration file.

exception `signac.errors.DestinationExistsError` (*destination*)

Bases: `signac.core.errors.Error`, `RuntimeError`

The destination for a move or copy operation already exists.

Parameters *destination* – The destination object causing the error.

exception `signac.errors.DocumentSyncConflict` (*keys*)

Bases: `signac.errors.SyncConflict`

Raised when a synchronization operation fails due to a document conflict.

keys = None

The keys that caused the conflict.

exception `signac.errors.Error`

Bases: `Exception`

Base class used for signac Errors.

exception `signac.errors.ExportError`

Bases: `signac.core.errors.Error`, `RuntimeError`

Error exporting documents to a mirror.

exception `signac.errors.FetchError`

Bases: `FileNotFoundError`

Error in fetching data.

exception `signac.errors.FileSyncConflict` (*filename*)

Bases: `signac.errors.SyncConflict`

Raised when a synchronization operation fails due to a file conflict.

filename = None

The filename of the file that caused the conflict.

exception `signac.errors.IncompatibleSchemaVersion`

Bases: `signac.core.errors.Error`

The project's schema version is incompatible with this version of signac.

exception `signac.errors.InvalidKeyError`

Bases: `ValueError`

Raised when a user uses a non-conforming key.

exception `signac.errors.JobsCorruptedError` (*job_ids*)

Bases: `signac.core.errors.Error`, `RuntimeError`

The state point manifest file of one or more jobs cannot be opened or is corrupted.

Parameters *job_ids* – The job id(s) of the corrupted job(s).

exception `signac.errors.SchemaSyncConflict` (*schema_src*, *schema_dst*)

Bases: `signac.errors.SyncConflict`

Raised when a synchronization operation fails due to schema differences.

exception `signac.errors.StatepointParsingError`

Bases: `signac.core.errors.Error`, `RuntimeError`

Indicates an error that occurred while trying to identify a state point.

exception `signac.errors.SyncConflict`

Bases: `signac.core.errors.Error`, `RuntimeError`

Raised when a synchronization operation fails.

exception `signac.errors.WorkspaceError` (*error*)

Bases: `signac.core.errors.Error`, `OSError`

Raised when there is an issue creating or accessing the workspace.

Parameters *error* – The underlying error causing this issue.

1.4 Changelog

The **signac** package follows [semantic versioning](#).

1.4.1 Version 1

[1.6.0] – 2020-01-24

Added

- Implemented `JobsCursor.__contains__` check (#449).
- Added documentation for `JobsCursor` class (#475).

Changed

- Optimized job hash and equality checks (#442, #455).
- Optimized `H5Store` initialization (#443).
- State points are loaded lazily when `Job` is opened by id (#238, #239).
- Optimized `Job` and `Project` classes to cache internal properties and initialize on access (#451).
- Python 3.6 is only tested with oldest dependencies (#474).
- Improved documentation for updating and resetting state points (#444).

Deprecated

- Deprecate `syncutil.copytree` method (#439).

Fixed

- Zero-dimensional NumPy arrays can be used in state points and documents (#449).

[1.5.1] – 2020-12-19

Added

- Support for h5py version 3 (#411).
- Added pyupgrade to pre-commit hooks (#413).
- Code is formatted with `black` and `isort` pre-commit hooks (#415).
- Added macOS to CircleCI testing pipeline (#281, #414).
- Official support for Python 3.9 (#417).

Changed

- Optimized internal function `_mkdir_p` (#421).
- Optimized performance of job initialization (#422).
- Optimized performance of buffer storage (#428).
- Optimized performance of creating/loading synced data structures (#429).

[1.5.0] – 2020-09-20

Added

- Type annotations are validated during continuous integration (#313).
- Added `_repr_html_` method in `ProjectSchema` class (#314, #324).
- Allow grouping by variables that are not present in all jobs in the project in `JobsCursor.groupby` (#321, #323).
- Added parameters `usecols` and `flatten` to allow selection of columns and flattening of nested data when converting signac data into a pandas `DataFrame` (#327, #330).
- Added support for `pre-commit` hooks (#355, #358).
- Expanded CLI documentation (#187, #359, #377).

Changed

- Docstrings are now written in `numpydoc` style.

Fixed

- Fix the `signac config verify` command (previously broken) (#301, #302).
- Warnings now appear when raised by the `signac` CLI (#317, #308).
- Fix dots in synchronization error messages (#375, #376).

Deprecated

- Deprecate the `create_access_modules` method in `Project`, to be removed in 2.0 (#303, #308).
- The `MainCrawler` class has replaced the `MasterCrawler` class. Both classes are deprecated (#342).

Removed

- Dropped support for Python 3.5 (#340). The signac project will follow the [NEP 29 deprecation policy](#) going forward.
- Removed dependency on `pytest-subtests` (#379).

[1.4.0] – 2020-02-28

Added

- Added Windows to platforms tested with continuous integration (#264, #266).
- Add command line option `-m/--merge` for `signac sync` (#280, #230).

Changed

- Workspace directory is created when `Project` is initialized (#267, #271).
- Changed testing framework from `unittest` to `pytest` (#212, #275).
- Refactored internal use of deprecated `get_statepoint` function (#227, #282).

Fixed

- Fixed issues on Windows with `H5Store`, project import/export, and operations that move files (#264, #266).
- Calling `items` or `values` on `_SyncedDict` objects does not mutate nested dictionaries (#234, #269).
- Fixed issue with `project.data` access from separate instances of `H5StoreManager` (#274, #278).
- Fixed error when launching `signac shell` if permissions are denied for `.signac_shell_history` (#279).

Removed

- Removed vendored `tqdm` module and replaced it with a requirement (#289).
- Removed support for `rapidjson` as an alternative JSON library (#285, #287).
- Removed tuple of keys implementation of nested dictionaries (#272, #296).

[1.3.0] – 2019-12-20

Added

- Official support for Python 3.8 (#258).
- Add properties `Project.id` and `Job.id` (#250).
- Add `signac.diff_jobs` function to compare two or more state points (#248, #247).
- Add function to initialize a sample data space for testing purposes (#215).
- Add schema version to ensure compatibility and enable migrations in future package versions (#165, #253).

Changed

- Implemented `Project.__contains__` check in constant time (#231).

Fixed

- Attempting to create a linked view for a `Project` on Windows now raises an informative error message (#214, #236).
- `Project` configuration is initialized using `ConfigObj`, allowing the configuration to include commas and special characters (#251, #252).

Deprecated

- Deprecate the `get_id` method in `Project` and `Job` classes in favor of the `id` property, to be removed in 2.0 (#250).
- In-memory modification of the project configuration, to be removed in 2.0 (#246).

Removed

- Dropped support for Python 2.7 (#232).

[1.2.0] – 2019-07-22

Added

- Keep `signac` shell command history on a per-project basis (#134, #194).
- Add `read_json()` and `to_json()` methods to `Collection` class (#104, #200).

Fixed

- Fix issue where shallow copies of instances of `Job` would behave incorrectly (#153, #207).
- Fix issue causing a failure of the automatic conversion of valid key types (#168, #205).
- Improve the ‘dots in keys’ error message to make it easier to fix related issues (#170, #205).

- Update the `__repr__` and `__repr_html__` implementations of the `Project`, `Job`, and `JobsCursor` classes (#193).
- Reduce the logging verbosity about a missing default host key in the configuration (#201).
- Fix issue with incorrect detection of dict-like files managed with the `DictManager` class (e.g. `job.stores`) (#203).
- Fix issue with generating views from the command line for projects with only one job (#208, #211).
- Fix issue with heterogeneous types in state point values that are lists (#209, #210).

Deprecated

- Support for Python 2.7 is deprecated with this version and will be removed in the next minor release. See the [Python 3 Statement](#).

[1.1.0] – 2019-05-19

Added

- Add command line options `--sp` and `--doc` for `signac find` that allow users to display key-value pairs of the state point and document in combination with the job id (#97, #146).
- Improve the representation (return value of `repr()`) of instances of `H5Group` and `SyncedAttrDict`.

Fixed

- Fix: Searches for whole numbers will match all numerically matching integers regardless of whether they are stored as decimals or whole numbers (#169).
- Fix: Passing an instance of dict to `H5Store.setdefault()` will return an instance of `H5Group` instead of a dict (#180).
- Fix error with storing numpy arrays and scalars in a synced dictionary (e.g. `job.statepoint`, `job.document`) (#184).
- Fix issue with `ResourceWarning` originating from unclosed instance of `Collection` (#186).
- Fix issue with using the `get_project()` function with a relative path and `search=False` (#191).

Removed

- Support for Python version 3.4 (no longer tested).

[1.0.0] – 2019-02-28

Added

- Official support for Python 3.7.
- The `H5Store` and `H5StoreManager` classes, which are useful for storing (numerical) array-like data with an HDF5-backend. These classes are exposed within the root namespace.

- The `job.data` and `project.data` properties which present an instance of `H5Store` to access numerical data within the job workspace and project root directory.
- The `job.stores` and `project.stores` properties, which present an instance of `H5StoreManager` to manage multiple instances of `H5Store` to store numerical array-like data within the project workspace and project root directory.
- The `signac.get_job()` and the `signac.Project.get_job()` functions that allow users to get a job handle by switching into or providing the job's workspace directory.
- The `job` variable is automatically set when opening a `signac shell` from within a job's workspace directory.
- Add the `signac shell -c` option which allows the direct specification of Python commands to be executed within the shell.
- Automatic cast of `numpy` arrays to lists when storing them within a `JSONDict`, e.g., a `job.statepoint` or `job.document`.
- Enable `Collection` class to manage collections stored in compressed files (gzip, zip, etc.).
- Enable deleting of `JSONDict` keys through the attribute interface, e.g., `del job.doc.foo`.
- Pretty HTML representation of instances of `Project` and `JobsCursor` targeted at Jupyter Notebooks (requires `pandas`, automatically enabled when installed).
- The `to_dataframe()` function to export the job state point and document data of a `Project` or a `JobsCursor`, e.g., the result of `Project.find_jobs()`, as a `pandas.DataFrame` (requires `pandas`).

Changed

- Dots (`.`) in keys are no longer allowed for `JSONDict` and `Collection` keys (previously deprecated).
- The `JSONDict` module is exposed in the root namespace, which is useful for storing text-serializable data with a JSON-backend similar to the `job.statepoint` or `job.document`, etc.
- The `Job.init()` method returns the job to allow one-line job creation and initialization.
- The `search` argument was added to the `signac.get_project()` function, which when `True` (the default), will cause `signac` to search for a project within *and above* a specified root directory, not only within the root directory. The behavior without any arguments remains unchanged.

Fixed

- Fix `Collection.update()` behavior such that existing documents with identical primary key are updated. Previously, a `KeyError` would be raised.
- Fix issue where the `Job.move()` would trigger a confusing `DestinationExists` exception when trying to move jobs across devices / file systems.
- Fix issue that caused failures when the `python-rapidjson` package is installed. The `python-rapidjson` package is used as the primary JSON-backend when installed.
- Fix issue where schema with multiple keys would subset incorrectly if the list of jobs or statepoints was provided as an iterator rather than a sequence.

Removed

- Removes the obsolete and deprecated `core.search_engine` module.
- The previously deprecated `Project.find_statepoints()` and `Project.find_job_documents()` functions have been removed.
- The `Project.find_jobs()` no longer accepts the obsolete `index` argument.

1.4.2 Version 0.9

[0.9.5] – 2019-01-31

Fixed

- Ensure that the `next()` function can be called for a `JobsIterator`, e.g., `project.find()`.
- Pickling issue that occurs when a `_SyncedDict` (`job.statepoint`, `job.document`, etc.) contains a list.
- Issue with the `readline` module that would cause `signac shell` to fail on Windows operating systems.

[0.9.4] – 2018-10-24

Added

- Adds the `$ signac import` command and the `Project.import_from()` method for the import of data spaces into a project workspace, such as a directory, a tarball, or a zip file.
- Adds the `$ signac export` command and the `Project.export_to()` method for the export of project workspaces to an external location, such as a directory, a tarball, or a zip file.
- Adds functionality for the rapid initialization of temporary projects with the `signac.TemporaryProject` context manager.
- Adds the `signac.Project.temporary_project()` context manager which creates a temporary project within the root project workspace.
- Add `signac` to the default namespace when invoking `signac shell`.
- Add option to specify a custom view path for the `signac view/Project.create_linked_view()` function.
- Iterables of documents used to construct a `Collection` no longer require an `_id` field.

Changed

- The default path for linked views has been adjusted to match the one used for data exports.

Fixed

- Fix issue where differently typed integer values stored within a `Collection` under the same key would not be indexed correctly. This issue affected the correct function of the `$type` operator for aforementioned cases and would lead to incorrect types in the Project schema detection algorithm for integer values.
- Fix issue where jobs that are migrated (state point change), but are not initialized, were not properly updated.

- Fix issue where changes to lists as part of synchronized dictionary, for example a state point or document would not be saved.
- Fix non-deterministic issue occurring on network file systems when trying to open jobs where the user has no write access to the job workspace directory.

[0.9.3] – 2018-06-14

Added

- Add *\$near* operator to express queries for numerical values that match up to a certain precision.
- Add the *\$signac shell* sub command to directly launch a Python interpreter within a project directory.

Fixed

- Fix issue where a job instance would not be properly updated after more than one state point reset.

[0.9.2] – 2017-12-18

Added

- Add provisional feature (persistent state point caching); calling the `Project.update_cache()` method will generate and store a persistent state point cache in the project root directory, which will increase the speed of many project iteration, search, and selection operations.
- Add `Project.check()` method which checks for workspace corruption, but does not make any attempt to repair it.
- The `Project.repair()` method will attempt to repair jobs, that have been corrupted by manually renaming the job's workspace directory.

Changed

- Enable the *write_concern* flag for the `job.document`.
- Allow to omit the specification of an authentication mechanism in the MongoDB host configuration.

Fixed

- Fix critical issue in the `JSONDict` implementation that would previously overwrite the underlying file when attempting to store values that are not JSON serializable.
- Fix issue where the `Project.export()` function would ignore the update argument when the index to export to would be a MongoDB collection.

[0.9.1] – 2017-11-07

Fixed

- Fix critical issue in the `SyncedAttrDict` implementation that would previously overwrite the underlying file if the first operation was a `__setitem__()` operation.

[0.9.0] – 2017-10-28

Added

- Introduction of `$ signac sync`, `Project.sync()`, and `Job.sync()` for the simplified and fine-grained synchronization of multiple project data spaces.
- Introduction of `$ signac schema` and `Project.detect_schema()` for the automatic detection of the implicit and semi-structured state point schema of a project data space.
- Simplified aggregation of jobs over projects and `Project.find_jobs()` results with the `Project.groupby()` function.
- Support for project-centralized data with the `Project.document` attribute and the `Project.fn()` method for the wrapping of filenames within the project root directory.
- Added the `Job.clear()` and the `Job.reset()` methods to clear or reset a job's workspace data.

Changed

- Both `Job.statepoint` and `Job.document` now use the same underlying data structure and provide the exact same API (copy with `()` and access of keys as attributes).
- The `Collection` class uses an internal counter instead of UUIDs for the generation of primary keys (resulting in improved performance).
- Major performance improvements (faster `Collection`, improved caching)
- Overhaul of the reference documentation.

1.4.3 Version 0.8

[0.8.7] – 2017-10-05

Fixed

- Fix an issue where the creation of linked views was non-deterministic in some cases.
- Fix an issue where the creation of linked views would fail when the project contains job with state points that have lists as values.

[0.8.6] – 2017-08-25

Fixed

- Fix `Collection` append truncation issue (see issue #66).

[0.8.5] – 2017-06-07

Changed

- The signac ids in the *signac find –show* view are no longer enclosed by quotation marks.

Fixed

- Fix compatibility issue that broke the *signac find –view* and all *–pretty* commands on Python 2.7.
- Fix issue where view directories would be incomplete in combination with heterogeneous state point schemas.

[0.8.4] – 2017-05-19

Added

- All search queries on project and collection objects support various operators including: *\$and*, *\$or*, *\$gt*, *\$gte*, *\$lt*, *\$lte*, *\$eq*, *\$ne*, *\$exists*, *\$regex*, *\$where*, *\$in*, *\$nin*, and *\$type*.
- The `$ signac find` command supports a simple filter syntax, where key value pairs can be provided as individual arguments.
- The `$ signac find` command is extended by a *–show* option, to display the state point and the document contents directly. The contents are truncated to an adjustable depth to reduce output noise.
- The `$ signac view` command has an additional filter option to select a sub data space directly without needing to pipe job ids.
- The new `$ signac document` command can be used to display a job's document directly.

Changed

- Minor performance improvements.

[0.8.3] – 2017-05-10

Changed

- Raise `ExportError` when updating with an empty index.

Fixed

- Fix command line logic issue with `$signac config host`.
- Fix bug, where `Collection.replace_one()` would ignore the upsert argument under specific conditions.

[0.8.2] – 2017-04-19

Fixed

- Fixes a `TypeError` which occurred under specific conditions when calling `Collection.find()` with nested filter arguments.

[0.8.1] – 2017-04-17

Fixed

- Fixes wide-spread typo (*indeces* -> *indexes*).

[0.8.0] – 2017-04-16

Overall major simplification of the generation of indexes and the management and searching of index collections without external database.

Added

- Introduction of the `Collection` class for the management of document collections, such as indexes in memory and on disk.
- Generation of file indexes directly via the `signac.index_files()` function.
- Generation of main indexes directly via the `signac.index()` function and the `$ signac index` command.
- The API of `signac_access.py` files has been simplified, including the possibility to use a blank file for a minimal configuration.
- Use the `$ signac project --access` command to create a minimal access module in addition to `Project.create_access_module()`.
- The update of existing index collections has been simplified by using the `export()` function with the `update=True` argument, which means that stale documents (the associated file or state point no longer exists) are automatically identified and removed.
- Added the `Job.ws` attribute, as short-cut for `Job.workspace()`.
- The `Job.sp` interface has a `get()` function which can be used to specify a default value in case that the requested key is not part of the state point.

Changed (breaking API)

- The `$ signac index` command generates a main index instead of a project index. To generate a project index from the command line use `$ signac project --index` instead.
- The `SignacProjectCrawler` class expects the project's root directory as first argument, not the workspace directory.
- The `get_crawlers()` function defined within a `signac_access.py` access module is expected to yield crawler instances directly, not a mapping of crawler ids and instances.

- The simplification of the `signac_access.py` module API is reflected in a reduction of arguments to the `Project.create_access_module()` method.

Changed (non-breaking)

- The `RegexFileCrawler`, `SignacProjectCrawler` and `MainCrawler` classes were moved into the root namespace.
- If a `MainCrawler` object is instantiated with the `raise_on_error` argument set to `True`, any errors encountered during crawling are raised instead of ignored and skipped; this simplifies the debugging of erroneous access modules.
- Improved error message for invalid configuration files.
- Better error messages for invalid `$ signac find` queries.
- Check a host configuration on the command line via `$ signac host --test`.
- A MongoDB database host configuration defaults to *none* when no authentication method is explicitly specified.
- Using the `--debug` option in combination with `$ signac index` will show the traceback of errors encountered during indexing instead of ignoring them.
- Instances of `Job` are hashable, making it possible to use them as dict keys for instance.
- The representation of `Job` instances via `repr()` can actually serves as copy constructor command.
- The project interface implementation performs all non-trivial search operations on an internally management index collection, which improves performance and simplifies the code base.

Deprecated

- The `DocumentSearchEngine` class has been deprecated, its functionality is now provided by the `Collection` class.

Fixed

- An issue related to exporting documents to MongoDB collections via `pymongo` in combination with Python 2.7 has been fixed.

1.4.4 Version 0.7

[0.7.1] – 2017-01-09

Added

- When the `python-rapidjson` package is installed, it will be used for JSON encoding/decoding (experimental).

Changed

- All job move-related methods raise `DestinationExistsError` in case of destination conflicts.
- Optimized `$ signac find` command.

Fixed

- Fixed bug in `$ signac statepoint`.
- Suppress ‘broken pipe error’ message when using `$ signac find` for example in combination with `$ head`.

[0.7.0] – 2017-01-04

Added

- Add support for Python version 3.6.
- Add support for PyPy and PyPy3.
- Simplified iteration over project data spaces.
- An existing linked view can be updated by executing the view command again.
- Add attribute interface for the access and modification of job state points: `Job.sp`.
- Add function for moving and copying of jobs between projects.
- All project related iterators support the `len`-operator.
- Enable iteration over all jobs with: `for job in project:`
- Make `len(project)` an alias for `project.num_jobs()`.
- Add `in`-operator to determine whether a job is initialized within a project.
- Add `Job.sp` attribute to access and modify a job’s state point.
- The `Project.open_job()` method accepts abbreviated job ids.
- Add `Project.min_len_unique_id()` method to determine the minimum length of job ids to be unique within the project’s data space.
- Add `Job.move()` method to move jobs between projects.
- Add `Project.clone()` method to copy jobs between projects.
- Add `$ signac move` and `$ signac clone` command line functions.
- Add `Job.reset_statepoint()` method to reset a job’s state point.
- Add `Job.update_statepoint()` method to update a job’s state point.
- Add a `Job.FN_DOCUMENT` constant which defines the default filename of the job document file
- The `$ signac find` command accepts a `-d/--doc-filter` option to filter by job document contents.
- Add the `Project.create_linked_view()` method as replacement for the previously deprecated `Project.create_view()` method.

Changed

- Linked views use relative paths.
- The *Guide* documentation chapter has been renamed to *Reference* and generally overhauled.
- The *Quick Reference* documentation chapter has been extended.

Fixed

- Fix error when using an instance of `Job` after calling `Job.remove()`.
- A project created in one the standard config directories (such as the home directory) does not take prevalence over project configurations in or above the current working directory.

Removed

- The *signac-gui* component has been removed.
- The `Project.create_linked_view()` *force* argument is removed.
- The `Project.find_variable_parameters()` method has been removed

1.4.5 Version 0.6

[0.6.2] – 2017-12-15

Added

- Add instructions on how to acknowledge **signac** in publications to documentation.
- Add cite module for the auto-generation of formatted references and BibTeX entries.

Removed

- Remove SSL authentication support.

[0.6.1] – 2017-11-26

Changed

- The `Project.create_view()` method triggers a `DeprecationWarning` instead of a `PendingDeprecationWarning`.
- The `Project.find_variable_parameters()` method triggers a `DeprecationWarning` instead of a `PendingDeprecationWarning`.

Fixed

- Make package more robust against PySide import errors.
- Fix `Project.__repr__` method.
- Fix critical bug in `fs.GridFS` class, which rendered it unusable.
- Fix issue in `indexing.fetch()` previously resulting in local paths being ignored.
- Fix error `signac.__all__` namespace directive.

[0.6.0] – 2016-11-18

Added

- Add the `export_to_mirror()` function for mirroring files.
- Introduction of the `signac.fs` namespace to simplify the configuration of mirror filesystems.
- Add `errors` module to root namespace. Many exceptions raised inherit from the base exception types defined within that module, making it easier to catch signac related errors.
- Add the `export_one()` function for the export of a single index document; simplifies the implementation of custom export functions.
- Opening an instance of `Job` with the `open_job()` method multiple times and entering a job context recursively is now well-defined behavior: Opening a job now adds the current working directory onto a stack, closing it switches into the directory on top of the stack.
- The return type of `Project.open_job()` can be configured to make it easier to specialize projects with custom job types.

Changed

- The `MainCrawler` logic has been simplified; their primary function is the compilation of index documents from subcrawlers, all export logic, including data mirroring is now provided by the `signac.export()` function.
- Each index document is now uniquely coupled with only one file or data object, which is why `signac.fetch()` replaces `signac.fetch_one()` and the latter one has been deprecated and is currently an alias of the former one.
- The `signac.fetch()` function always returns a file-like object, regardless of format definition.
- The format argument in the `crawler.define()` function is now optional and has now very well defined behavior for str types. It is encouraged to define a format with a str constant rather than a file-like object type.
- The `TextFile` file-like object class definition in the `formats` module has been replaced with a constant of type `str`.
- The `signac.export()` function automatically delegates to specialized implementations such as `export_pymongo()` and is more robust against errors, such as broken connections.
- The `export_pymongo()` function makes multiple automatic restart attempts when encountering errors.
- Documentation: The tutorial is now based on signac-examples jupyter notebooks.
- The `contrib.crawler` module has been renamed to `contrib.indexing` to better reflect the semantic context.
- The `signac.export()` function now implements the logic for data linking and mirroring.
- Provide default argument for ‘-indent’ option for `$ signac statepoint` command.
- Log, but do not reraise exceptions during `MainCrawler` execution, making the compilation of main indexes more robust against errors.
- The object representation of `Job` and `Project` instances is simplified.
- The warning verbosity has been reduced when importing modules with optional dependencies.

Removed

- All modules related to the stale *conversion framework* feature have been removed resulting in a removal of the optional `networkx` dependency.
- Multiple modules related to the *conversion framework* feature have been removed, including: `contrib.formats_network`, `contrib.conversion`, and `contrib.adapters`.

Fixed

- Opening instances of `Job` with the `Job.open()` method multiple times, equivalently entering the job context recursively, does not cause an error anymore, but instead the behavior is well-defined.

1.4.6 Version 0.5

[0.5.0] – 2016-08-31

Added

- New function: `signac.init_project()` simplifies project initialization within Python
- Added optional `root` argument to `signac.get_project()` to simplify getting a project handle outside of the current working directory
- Added optional argument to `signac.get_project()`, to allow fetching of projects outside of the current working directory.
- Added two class factory methods to *Project*: `get_project()` and `init_project()`.

Changed

- The performance of project indexing and crawling has been improved.

1.4.7 Version 0.4

[0.4.0] – 2016-08-05

Added

- The performance of find operations can be greatly improved by using pre-generated job indexes.
- New top-level commands: `$ signac find`, `$ signac index`, `$ signac statepoint`, and `$ signac view`.
- New method: `Project.create_linked_view()`
- New method: `Project.build_job_statepoint_index()`
- New method: `Project.build_job_search_index()`
- The `Project.find_jobs()` method allows to filter by job document.

Changed

- The `SignacProjectCrawler` indexes all jobs, not only those with non-empty job documents.
- The `signac.fetch_one()` function returns `None` if no associated object can be fetched.
- The tutorial is restructured into multiple parts.
- Instructions for installation are separated from the guide.

Removed

- Remove previously deprecated `crawl` keyword argument in index export functions.
- Remove previously deprecated function `common.config.write_config()`.

1.4.8 Version 0.3

[0.3.0] – 2016-06-23

Added

- Add contributing agreement and guidelines.

Changed

- Change license from MIT to BSD 3-clause license.

1.4.9 Version 0.2

[0.2.9] – 2016-06-06

Added

- Addition of the `signac config` command line API.
- Password updates are encrypted with `bcrypt` when `passlib` is installed.
- The user is prompted to enter missing credentials (username/password) in case that they are not stored in the configuration.
- The `$ signac config` tool provides the `--update-pw` argument, which allows users to update their own password.
- Added MIT license, in addition, all source code files contain a short licensing header.

Changed

- Improved documentation on how to configure `signac`.
- The OSI classifiers are updated, including an upgrade of the development status to ‘4 - beta’.

Fixed

- Nested job state points can no longer get corrupted. This bug occurred when trying to operate on nested state point mappings.

Deprecated

- Deprecated pymongo versions 2.x are no longer supported.

[0.2.8] – 2016-04-18

Added

- `Project` is now in the root namespace.
- Add `index()` method to *Project*.
- Add `create_access_module()` method to *Project*.
- Add `find_variable_parameters()` method to *Project*.
- Add `fn()` method to *Job*, which prepends the job's workspace path to a filename.
- The documentation contains a comprehensive tutorial

Changed

- The `crawl()` function yields only the index documents and not a tuple of `(_id, doc)`.
- `export()` and `export_pymongo()` expect the index documents as first argument, not a crawler instance. The old API is still supported, but will trigger a `DeprecationWarning`.

[0.2.7] – 2016-02-29

Added

- Add `job.isfile()` method

Changed

- Optimize `project.find_statepoints()` and `project.repair()` functions.

[0.2.6] – 2016-02-20

Added

- Add `job.reset_statepoint()` and `job.update_statepoint()`
- Add `job.remove()` function

Changed

- Sanitize filter argument in all `project.find_*` methods.
- The `job.statepoint()` function accurately represents saved statepoints, e.g. tuples are represented as lists, as there is no difference between tuples and lists in JSON.
- `signac-gui` does not block on database operations.
- `signac-gui` allows reload of databases and collections of connected hosts.

Fixed

- `RegexFileCrawler.define()` class function only acts upon the actual specialization and not globally on all `RegexFileCrawler` classes.
- `signac-gui` does not crash when replica sets are configured.

[0.2.5] – 2016-02-10

Added

- Added `signac.get_project()`, `signac.get_database()`, `signac.fetch()` and `signac.fetch_one()` to top-level namespace.
- Added basic shell commands, see `$ signac --help`.
- Allow opening of jobs by id: `project.open_job(id='abc123...')`.
- Mirror data while crawling.
- Use extra sources for `fetch()` and `fetch_one()`.
- Add file system handler: `LocalFS`, handler for local file system.
- Add file system handler: `GridFS`, handler for MongoDB GridFS file system.
- Crawler tags, to control which crawlers are used for a specific index.
- Allow explicit job workspace creation with `job.init()`.
- Forwarding of pymongo host configuration via **signac** configuration.

Changed

- Major reorganization of the documentation, split into: Overview, Guide, Quick Reference and API.
- Documentation: Add notes for system administrators about advanced indexing.
- Warn about outdated pymongo versions.
- Set `zip_safe` flag to true in `setup.py`.
- Remove dependency on `six` module, by adding it to the common subpackage.

Deprecated

Fixed

- Fixed hard import of pymongo bug (issue #24).
- Crawler issues with malformed documents.

[0.2.4] – 2016-01-11

Added

- Implement `Project.repair()` function for projects with corrupted workspaces.
- Allow environment variables in workspace path definition.
- Check and fix config permission errors.

Changed

- Increase robustness of job manifest file creation.

Fixed

- Fix project crawler deep directory issue (hotfix).

[0.2.3] – 2015-12-09

Fixed

- Fix a few bugs related to project views.

[0.2.2] – 2015-11-30

Fixed

- Fix `SignacProjectCrawler.super()` bug.

[0.2.1] – 2015-11-29

Added

- Add support for Python 2.7
- Add signac-gui (early alpha)
- Allow specification of relative and default workspace paths
- Add the ability to create project views
- Add `Project.find_*` functions to search the workspace

- Add function to write and read state point hash tables

[0.2.0] – 2015-11-05

- Major consolidation of the package.
- Remove all hard dependencies, but six.

1.5 Support and Development

To get help using the **signac** package, either send an email to signac-support@umich.edu or join the [signac gitter chatroom](#).

The **signac** package is hosted on [GitHub](#) and licensed under the open-source BSD 3-Clause license. Please use the [repository's issue tracker](#) to report bugs or request new features.

1.5.1 Code contributions

This project is open-source. Users are highly encouraged to contribute directly by implementing new features and fixing issues. Development for packages as part of the **signac** framework should follow the general development guidelines outlined [here](#).

A brief summary of contributing guidelines are outlined in the [CONTRIBUTING.md](#) file as part of the repository. All contributors must agree to the [Contributor Agreement](#) before their pull request can be merged.

Set up a development environment

Start by [forking](#) the project.

We highly recommend to setup a dedicated development environment, for example with [venv](#):

```
~ $ python -m venv ~/envs/signac-dev
~ $ source ~/envs/signac-dev/bin/activate
(signac-dev) ~ $ pip install pre-commit
```

or alternatively with [conda](#):

```
~ $ conda create -n signac-dev -c conda-forge python=3 pre-commit
~ $ conda activate signac-dev
```

Then clone your fork and install the package from source with:

```
(signac-dev) ~ $ cd path/to/my/fork/of/signac
(signac-dev) signac $ pip install -e .
```

The `-e` option stands for *editable*, which means that the package is directly loaded from the source code repository. That means any changes made to the source code are immediately reflected upon reloading the Python interpreter.

The [pre-commit](#) tool is used to enforce code style guidelines. To install the tool and configure pre-commit hooks, execute:

```
(signac-dev) signac $ pip install pre-commit
(signac-dev) signac $ pre-commit install
```

With the pre-commit hook, your code will be checked for syntax and style before you make a commit. The continuous integration pipeline for the package will perform these checks as well, so running these tests before committing / pushing will prevent the pipeline from failing due to style-related issues.

The development workflow

Prior to working on a patch, it is advisable to create an [issue](#) that describes the problem or proposed feature. This means that the code maintainers and other users get a chance to provide some input on the scope and possible limitations of the proposed changes, as well as advise on the actual implementation.

All code changes should be developed within a dedicated git branch and must all be related to each other. Unrelated changes, such as minor fixes to unrelated bugs encountered during implementation, spelling errors, and similar typographical mistakes must be developed within a separate branch.

Branches should be named after the following pattern: `<prefix>/issue-<#>-optional-short-description`. Choose from one of the following prefixes depending on the type of change:

- `fix/`: Any changes that fix the code and documentation.
- `feature/`: Any changes that introduce a new feature.
- `release/`: Reserved for release branches.

If your change does not seem to fall into any of the above mentioned categories, use `misc/`.

Once you are content with your changes, push the new branch to your forked repository and create a pull request into the main repository. Feel free to push a branch before completion to get input from the maintainers and other users, but make sure to add a comment that clarifies that the branch is not ready for merge yet.

Testing

Prior to fixing an issue, implement unit tests that *fail* for the described problem. New features must be tested with unit and integration tests. To run tests, execute:

```
(signac-dev) signac $ python -m pytest tests/
```

Building documentation

Building documentation requires the [sphinx](#) package which you will need to install into your development environment.

```
(signac-dev) signac $ pip install Sphinx sphinx_rtd_theme
```

Then you can build the documentation from within the `doc/` directory as part of the source code repository:

```
(signac-dev) signac $ cd doc/
(signac-dev) doc $ make html
```

Note: Documentation as part of the package should be largely limited to the API. More elaborate documentation on how to integrate **signac** into a computational workflow should be documented as part of the [framework documentation](#), which is maintained [here](#).

Updating the changelog

To update the changelog, add a one-line description to the `changelog.txt` file within the `next` section. For example:

```
next
----

- Fix issue with launching rockets to the moon.

[0.6.3] -- 2018-08-22
-----

- Fix issue related to dynamic data spaces, ...
```

Just add the `next` section in case it doesn't exist yet.

CHAPTER 2

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