PyPads

Release 0.1.20

Install PyPads:

1		All PyPads How To Install	3			
2	Getting started					
	2.1	Getting started with PyPads	8			
3	PyPa	ads	17			
	3.1	PyPads application class	17			
	3.2	Logging functions	21			
	3.3	Utilities	22			
	3.4	Mapping Files	22			
4	Exte	nsions	27			
	4.1	Extensions and plugins	27			
5	Rela	ted Projects	29			
	5.1	Related Projects	29			
6	Cha	ngelog	31			
	6.1	0.2.0 (2020-06-22)	31			
	6.2	0.1.20 (2020-05-19)	31			
	6.3	0.1.19 (2020-05-19)	31			
	6.4	0.1.18 (2020-05-19)	31			
	6.5	About Us	31			
Рy	thon]	Module Index	33			
In	dex		35			

Building on the MLFlow toolset, PyPaDS aims to extend the existing tracking functionality, make logging as easy as possible for the user. The production of structured results is an additional goal of the extension.

Install PyPads:

2 Install PyPads:

CHAPTER 1

Install PyPads

Logging your experiments manually can be overwhelming and exhaustive? PyPads is a tool to help automate logging as much information as possible by tracking the libraries of your choice.

• Installing PyPads: With pip | From source

1.1 How To Install

There are different ways to install pypads:

- *Install the latest official release*. This is the best approach for most users. It will provide a stable version and pre-built packages are available for most platforms.
- Building the package from source. This is best for users who want the latest features and aren't afraid of running brand-new code. This is also needed for users who wish to contribute to the project.

1.1.1 Installing the latest release with pip

The lastest stable version of pypads can be downloaded and installed from PyPi:

pip install pypads

Note that in order to avoid potential conflicts with other packages it is strongly recommended to use a virtual environment, e.g. python3 virtualenv (see python3 virtualenv documentation) or conda environments.

Using an isolated environment makes possible to install a specific version of pypads and its dependencies independently of any previously installed Python packages. In particular under Linux is it discouraged to install pip packages alongside the packages managed by the package manager of the distribution (apt, dnf, pacman...).

Note that you should always remember to activate the environment of your choice prior to running any Python command whenever you start a new terminal session.

Warning: Pypads requires Python 3.6 or newer.

1.1.2 Installing pypads from source

This section introduces how to install the **master branch** of pypads. This can be done by building from source.

Building from source

Building from source is required to work on a contribution (bug fix, new feature, code or documentation improvement).

1. Use Git to check out the latest source from the pypads repository on Github.:

```
git clone git@github.com:padre-lab-eu/pypads.git # add --depth 1 if your_ 

--connection is slow
cd pypads
```

If you plan on submitting a pull-request, you should clone from your fork instead.

2. Install poetry tool for dependency management for your platform. See instructions in the Official documentation.:

```
pip install poetry
```

- 3. Optional (but recommended): create and activate a dedicated virtualenv or conda environment.
- 4. Build the project with poetry, this will generate a whl and a tar file under dist/:

```
poetry build
```

5. Install pypads using one of the two generated files:

```
pip install dist/pypads-X.X.X.tar.gz
OR
pip install dist/pypads-X.X.X-py3-none-any.whl
```

If the package is available on pypi but can't be found with poetry you might want to delete your local poetry cache: poetry cache clear –all pypi

Dependencies

Runtime dependencies

Pypads requires the following dependencies both at build time and at runtime:

- Python (>= 3.6),
- cloudpickle (>= 1.3.3),
- mlflow (>= 1.6.0),
- boltons (>= 19.3.0),
- loguru (>=0.4.1)

Those dependencies are automatically installed by poetry if they were missing when building pypads from source.

Build dependencies

Building PyPads also requires:

• Poetry >= 0.12.

Test dependencies

Running tests requires:

- pytest >= 5.2.5,
- scikit-learn >= 0.21.3,
- tensorflow \Rightarrow = 2.0.0b1,
- psutil >= 5.7.0,
- networkx >= 2.4,
- keras >= 2.3.1.

Some tests also require numpy.

1.1. How To Install 5

CHAPTER 2

Getting started

Learn more about how to use pypads, configuring your tracking events and hooks, mapping your custom logging function and some of the core features of PyPads.

- Usage example Decision Tree Iris classification
- **Mapping file example for Scikit-learn** A *mapping file* is where we define the classes and functions to be tracked from the library of our choice. It includes the defined hooks.
- · Hooks and events
 - Events are defined primarily by listeners which are, in our case, hooks. When triggered, the corresponding loggers are called. Logging functions are linked to these events via a mapping dictionary passed to the base class.
 - Hooks help the user to define what triggers those events (e.g. what functions or classes should trigger a specific event).
- **Loggers** Logging functions are functions called around when any tracked method or class triggers their corresponding event. Mapping events to logging functions is done by passing a dictionary **mapping** as a parameter to the *PyPads class*.

The following tables show the default loggers of pypads.

• Event Based loggers

Logger	Event	Hook	Description
LogInit	init	'pypads_init'	Debugging purposes
Log	log	'pypads_log'	Debugging purposes
Parameters	parameters	'pypads_fit'	tracks parameters of the tracked
			function call
Cpu,Ram,Dis	k hardware	'pypads_fit'	track usage information, properties
			and other info on CPU, Memory
			and Disk.
Input	input	'pypads_fit'	tracks the input parameters of the
			current tracked function call.
Output	output	'pypads_predict', 'pypads_fit'	Logs the output of the current
			tracked function call.
Metric	metric	'pypads_metric'	tracks the output of the tracked
			metric function.
PipelineTrackepipeline		'pypads_fit','pypads_predict',	tracks the workflow of execution
		'pypads_transform', 'py-	of the different pipeline elements
		pads_metrics'	of the experiment.

• Pre/Post run loggers

Logger	Pre/Post	Description
IGit	Pre	Source code management and tracking
ISystem	Pre	System information (os,version,machine)
ICpu	Pre	Cpu information (Nbr of cores, max/min frequency)
IRam	Pre	Memory information (Total RAM, SWAP)
IDisk	Pre	Disk information (disk total space)
IPid	Pre	Process information (ID, command, cpu usage, memory
		usage)
ISocketInfo	Pre	Network information (hostname, ip address)
IMacAddress	Pre	Mac address

2.1 Getting started with PyPads

PyPads is a tracking framework for your python programs. It implements an infrastructure featuring the possibilities for:

- Community driven mapping files
- · Logging injection by importlib extension
- · Timekeeping
- Full access to the current state in logging functions
- Prefabricated tracking functions and formats
- · Data and control flow manipulation with actuators
- · Run based data caching for loggers

The framework was developed for machine learning experiments and is based on mlflow. The main focus for PyPads is based in its ulterior, but pythonic manner of use. PyPads aims to deliver a way to harmonize results of a multitude of libraries in a structured way, while stepping out of the way if needed. Most dependencies of PyPads are to be considered as optional and are only used to extend on more sophisticated logging functions.

In its core app, PyPads allows for registering plugin extensions. These can be used to define packages introducing new loggers, validators, actuators, decorators etc.

2.1.1 Quick start

Install PyPads assuming Python 3 is already installed:

```
$ pip install pypads
```

Usage

Activating PyPads for tracking in its default setting is as easy as adding two lines to your experiment.

A simple example looks like the following.

```
from pypads.app.base import PyPads
PyPads (autostart=True)

# An example
from sklearn import datasets, metrics
from sklearn.tree import DecisionTreeClassifier

# load the iris datasets
dataset = datasets.load_iris()

# fit a model to the data
model = DecisionTreeClassifier()
model.fit(dataset.data, dataset.target) # pypads will track the parameters, output,
and input of the model fit function.
# get the predictions
predicted = model.predict(dataset.data) # pypads will track only the output of the
amodel predict function.
```

Results

By default results can be found in the .mlruns folder in the home directory of the executing user. While this can be changed when initializing the app, you can also specify the environment variable MLFLOW_PATH to define a custom location.

2.1.2 Concepts

PyPads includes a set of concepts, of which some are to be followed because of technical reasons, while others only impose semantical meaning.

Actuators

Actuators are features of PyPads manipulating experiments. When using an actuator the result of the experiment may be or is impacted. Actuators can include changes to the underlying machine learning code, setup and more. An exemplary actuator is an actuator enforcing a random seed setup. Custom, new or other actuators can be added to an IActuators plugin exposing them to PyPads.

```
@actuator
def set_random_seed(self, seed=None):
    # Set seed if needed
    if seed is None:
        import random
        # Numpy only allows for a max value of 2**32 - 1
        seed = random.randrange(2 ** 32 - 1)
        self.pypads.cache.run_add('seed', seed)

from pypads.injections.analysis.randomness import set_random_seed
    set_random_seed(seed)
```

To call an actuator you can use the app.

```
from pypads.app.base import PyPads
tracker = PyPads (autostart=True)
tracker.actuators.set_random_see (seed=1)
```

API

The PyPads API delivers standard functionality of PyPads. This also pipes some of mlflow features. You can start, stop runs, log artifacts, metrics or parameters, set tags and write meta information about them. Additionally the PyPads API inroduces setup and teardown (also called pre and post run) functions to be called and also to manually mark functions for tracking. A full documentation can be found here. To call the api you can use the app.

```
from pypads.app.base import PyPads
tracker = PyPads(autostart=True)
tracker.api.set_tag("foo", "bar")
```

Validators

Validators are to be used if the experimental status or code has to be checked on some properties. These should normally not log anything, but a validation report. A validation report should be an optional tag or at max a text file. In general validators should inform the user on runtime about errors and problems. It is planned to add the possibility to interrupt an execution if validators fail in the future. Some validators will be logging functions bound to library functions. An examplary validator which will want to be bound to the usage of pytorch is the determinism check for pytorch.

```
@validator
def determinism(self):
    check_determinism()
```

To call the api you can use the app.

```
from pypads.app.base import PyPads
tracker = PyPads (autostart=True)
tracker.validators.set_tag("foo", "bar")
```

Setup / Teardown functions

Setup or teardown functions are to be called when a run starts or ends. These mostly are used to log meta information about the experiment including data about git, hardware and the environment. A list of currently defined decorators can be found here.

Configuring setup or teardown functions can be done via the app constructor or api.

```
from pypads.app.base import PyPads
tracker = PyPads(setup_fns=[ICpu()], autostart=True)
# tracker.api.register_setup("custom_cpu", ICpu())
```

MappingFiles

Mapping files deliver hooks into libraries to trigger tracking functionality. They are written in yml and defining a syntax to markup functions, classes and modules.

Decorators

Decorators can be used instead of a mapping file to denote hooks in code. Because most libraries are not to be changed directly they are currently used sparingly. In PyPads defined decorators can be found here.

Logging functions

Logging functions are the generic functions performing tracking tasks bound to hooked functions of libraries. Everything not fitting into other concepts is just called logging function. Following function would track the input to the hooked function.

```
class Input(LoggingFunction):
    """
Function logging the input parameters of the current pipeline object function call.
    """

def __pre__(self, ctx, *args, _pypads_write_format=WriteFormats.pickle, _pypads_env:_
    LoggingEnv, **kwargs):
    """
    :param ctx:
    :param args:
    :param _pypads_write_format:
    :param kwargs:
    :return:
    """
    for i in range(len(args)):
        arg = args[i]
```

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Configuring logging functions can be achieved by providing mappings to the constructor of the app. Mapping files provide hooks (generally prepended by "pypads" in their naming) and logging functions are mapped to events. A hook can subsequently trigger multiple events and thus logging functions. To pass an event to function mapping a simple dict can be used.

```
from pypads.app.base import PyPads
event_function_mapping = {
    "parameters": Parameters(),
    "output": Output(_pypads_write_format=WriteFormats.text.name),
    "input": Input(_pypads_write_format=WriteFormats.text.name)
}
tracker = PyPads(events=event_function_mapping, autostart=True)
```

Additionally a hook to event mapping can be defined.

Defining hooks can be done via api, mappings, mapping files or decorators. Decorators are a sensible approach for local custom code.

```
from pypads.app.base import PyPads
tracker = PyPads(autostart=True)

@tracker.decorator.track(event="pypads_fit")
def fit_function_to_track(foo: str):
    return foo + "bar"
```

The same holds true for api based tracking.

```
from pypads.app.base import PyPads
tracker = PyPads(autostart=True)

def fit_function_to_track(foo: str):
    return foo + "bar"

tracker.api.track(ctx=get_class_that_defined_method(fit_function_to_track), fn=fit_
    function_to_track, hooks=["pypads_fit"])
```

Mapping files or mappings are a more permanent, shareable and modular approach.

Check points

Check points are currently not implemented. They will introduce a structured way to denote cache able states. By defining check points we hope to be able to define marks from which an experiment can be rerun in the future.

2.1.3 Examples

Sklearn DecisionTree example

Following shows how PyPads can be used to track the parameters, input and output of a sklearn experiment.

```
# define the configuration, in this case we want to track the parameters,
# outputs and the inputs of each called function included in the hooks (pypads_fit,_
→pypads_predict)
events = {
    "parameters": {"on": ["pypads_fit"]},
    "output": {"on": ["pypads_fit", "pypads_predict"]},
    "input": {"on": ["pypads_fit"]}
# A simple initialization of the class will activate the tracking
PyPads (events=events)
# An example
from sklearn import datasets, metrics
from sklearn.tree import DecisionTreeClassifier
# load the iris datasets
dataset = datasets.load_iris()
# fit a model to the data
model = DecisionTreeClassifier()
model.fit(dataset.data, dataset.target) # pypads will track the parameters, output,
→and input of the model fit function.
# get the predictions
```

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```
predicted = model.predict(dataset.data) # pypads will track only the output of the → model predict function.
```

The used hooks for each event are defined in the mapping yml file where each event includes the functions to listen to.

Mapping file example

For the previous example, the sklearn mapping yml file would look like the following.

```
metadata:
  author: "Thomas Weißgerber"
  version: "0.1.0"
  library:
    name: "sklearn"
    version: "0.19.1"
mappings:
  !!python/pPath sklearn:
    !!python/pPath base.BaseEstimator:
        concepts: ["algorithm"]
    !!python/pPath __init__:
      hooks: "pypads_init"
    !!python/rSeg (fit|.fit_predict|fit_transform)$:
      hooks: "pypads_fit"
    !!python/rSeg (fit_predict|predict|score)$:
      hooks: "pypads_predict"
    !!python/rSeg (fit_transform|transform)$:
      hooks: "pypads_transform"
```

For example, "pypads_fit" is an event listener on any **fit, fit_predict and fit_transform** function call made by any tracked class with those methods.

Defining a hook for an event

A hook can be defined in the mapping file via the "hooks" attribute. It is composed of the given name and path defined by the keys in the yml file. Muliple hooks can use the same name and therefore trigger the same functions.

Define an event

Once the hooks are defined, they are then linked to the events we want them to trigger. Following the example below, the hook **pypads_metric** will be linked to an event we call **Metrics** for example. This is done via passing a dictionary as the parameter **config** to the *PyPads class*

```
events = {
         "Metrics" : {"on": ["pypads_metrics"]}
}
```

PyPads loggers

PyPads has a set of built-in logging functions that are mapped by default to some pre-defined events. Check the default setting of PyPads *here*. The user can also define custom logging functions for custom events. Details on how to do

that can be found *here*.

2.1.4 External resources

Currently there are unfortunately not too many external resources available fo PyPads. Additional examples are to be added in the next steps of the road map. You can find an IPython Notebook and an Code example on these repositories.

TODO Please add links to two repositories with example code (We can use the stuff for the data science lab)

CHAPTER 3

PyPads

3.1 PyPads application class

This class represents the app. To start and activate the tracking of your modules, classes and functions, the app class has to be instantiated.

Warning: It is recommended to initialize the tracking **before** importing the modules to be tracked. While extending the importlib and reloading the modules may work sometimes doing so may result in unforeseen issues.

```
class pypads.app.base.PyPads (uri=None, folder=None, mappings:

List[pypads.importext.mappings.MappingCollection] = None,
hooks=None, events=None, setup_fns=None, config=None,
pre_initialized_cache: pypads.app.misc.caches.PypadsCache =
None, disable plugins=None, autostart=None)
```

PyPads app. Serves as the main entrypoint to PyPads. After constructing this app tracking is activated.

 $\begin{tabular}{ll} \textbf{activate_tracking} (reload_modules=False, & reload_warnings=True, & clear_imports=False, & affected_modules=None) \\ \end{tabular}$

Function to duck punch all objects defined in the mapping files. This should at best be called before importing any libraries. :param affected_modules: Affected modules of the mapping files. :param clear_imports: Clear imports after punching. CAREFUL THIS IS EXPERIMENTAL! :param reload_warnings: Show warnings of affected modules which were already imported before the importlib was extended. :param reload_modules: Force a reload of affected modules. CAREFUL THIS IS EXPERIMENTAL! :return:

actuators

Access the actuators of pypads. :return: PyPadsActuators

add atexit fn(fn)

Add function to be executed before stopping your process. This function is also added to pypads and errors are caught to not impact the experiment itself. Deactivating pypads should be able to run some of the atExit fns declared for pypads.

api

Access the api of pypads. :return: PyPadsAPI

static available_actuators()

Return a list of available actuators in the current installation of PyPads. :return: Actuator classes

static available anchors()

Return a list of available anchors in the current installation of PyPads. Anchors are names for hooks. :return: Anchors

static available cmds()

Return a list of available api commands in the current installation of PyPads. :return: API commands classes

static available_decorators()

Return a list of available decorators in the current installation of PyPads. :return: Decorator classes

static available_events()

Return a list of available events (event types) in the current installation of PyPads. Events are triggered by hooks and map to functions. :return: Event types

static available_loggers()

Return a list of available LoggingFunctions for mappings in the current installation of PyPads. :return: Logging function classes

static available_setup_functions()

Return a list of available setup function in the current installation of PyPads. :return: Setup function classes

static available_teardown_functions()

Return a list of available setup function in the current installation of PyPads. :return: Teardown function classes

static available_validators()

Return a list of available validators in the current installation of PyPads. :return: Validator classes

backend

Return the backend of PyPads. This is currently hardcoded to mlflow. :return: Backend

cache

Return the cache of pypads. This holds generic cache data and run cache data. :return:

call_tracker

Return the call tracker of PyPads. This is used to keep track of the calls of hooked functions. :return: CallTracker

config

Return the configuration of pypads. :return: Configuration dict

deactivate_tracking(run_atexits=False, reload_modules=True)

Deacticate the current tracking and cleanup. :param run_atexits: Run the registered atexit functions of pypads :param reload_modules: Force a reload of affected modules :return:

decorators

Access the decorators of pypads. :return: PyPadsDecorators

events

Get the to the constructor passed event / logging function mappings. :return: Hook configuration.

folder

Return the local folder pypads uses for its temporary storage, configuration etc. :return:

function_registry

Access the function registry holding all mappings of events to logging functions :return: Function registry

hook registry

Access the hook registry holding all mappings of anchors/hooks to events :return: Hook registry

hooks

Get the to the constructor passed hook / event mappings. :return: Hook configuration.

is_affected_module (name, affected_modules=None)

Check if a given module name is in the list of affected modules. You can pass a list of affected modules or take the one of the wrap_manager. :param name: Name of the module to check :param affected_modules: The list of affected modules (can be None and will be extracted automatically) :return:

managed_git_factory

Return Git manager of PyPads. This used to create and manages git repositories. :return: ManagedGitFactory

mapping_registry

Access the mapping registry holding all references to mapping files etc. :return: Mapping registry

mappings

Get the to the constructor passed mappings. :return: Additional mapping files.

mlf

Return a mlflow client to interact with stored data. :return: MlflowClient

```
start_track (experiment_name=None, disable_run_init=False)
```

Start a new run to track. :param experiment_name: The name of the mlflow experiment :param disable_run_init: Flag to indicate if the run_init functions are to be run on an already existing run. :return:

uri

Return the tracking uri pypads uses for mlflow. :return:

validators

Access the validators of pypads. :return: PyPadsValidators

wrap_manager

Return the wrap manager of PyPads. This is used to wrap modules, functions and classes. :return: Wrap-Manager

3.1.1 Default settings

The app includes default values for configuration, hook/event mappings, event/function mappings etc.

Default Anchors

Anchors are names for repeating types of hooks. Fit functions for example are existing on multiple libraries.

Default Event Types

Event types represent strategies to react to an anchor / hook.

```
DEFAULT_EVENT_TYPES = [EventType("parameters", "Track the parameters for given model.

→"),

EventType("output", "Track the output of the function."),

EventType("input", "Track the input of the function."),

EventType("hardware", "Track current hardware load on function.

→execution."),

EventType("metric", "Track a metric."),

EventType("autolog", "Activate mlflow autologging."),

EventType("pipeline", "Track a pipeline step."),

EventType("log", "Log the call to console.")]
```

Default Config

The configuration for PyPads

```
DEFAULT_CONFIG = {
    "track_sub_processes": False, # Activate to track spawned subprocesses by_
    extending the joblib
    "recursion_identity": False, # Activate to ignore tracking on recursive calls of_
    the same function with the same mapping
    "recursion_depth": -1, # Limit the tracking of recursive calls
    "log_on_failure": True, # Log the stdout / stderr output when the execution of_
    the experiment failed
    "include_default_mappings": True # Include the default mappings additionally to_
    the passed mapping if a mapping is passed
}
```

Default Hook Mapping

The hook mapping, maps hooks (anchors) to the events (event types).

```
DEFAULT_HOOK_MAPPING = {
    "init": {"on": ["pypads_init"]},
    "parameters": {"on": ["pypads_fit"]},
    "hardware": {"on": ["pypads_fit"]},
    "output": {"on": ["pypads_fit", "pypads_predict"]},
    "input": {"on": ["pypads_fit"], "with": {"_pypads_write_format": WriteFormats.
    \text.name}},
    "metric": {"on": ["pypads_metric"]},
    "pipeline": {"on": ["pypads_fit", "pypads_predict", "pypads_transform", "pypads_\text.orm"]},
    "log": {"on": ["pypads_log"]}
}
```

Default Event Mapping

Defines which logging functions should be run for events.

```
DEFAULT_LOGGING_FNS = {
    "parameters": Parameters(),
    "output": Output(_pypads_write_format=WriteFormats.text.name),
    "input": Input(_pypads_write_format=WriteFormats.text.name),
```

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3.2 Logging functions

3.2.1 LoggingFunction base class

To develop custom loggers, we need to write a class that inherits from the base class **LoggingFunction**. Then, those custom loggers can be mapped to events of the user choice in the parameter **mapping** of the *PyPads class*.

3.2.2 Pre and Post run loggers

Another type of logging functions supported by Pypads is the pre/post run loggers which are executed before and after the run execution respectively.

· Pre Run loggers

```
class pypads.app.injections.run_loggers.PreRunFunction(*args, **kwargs)
     This class should be used to define new pre run functions
     _call (pads, *args, **kwargs)
          Function where to add you custom code to execute before starting or ending the run.
              Parameters pads – the current instance of PyPads.
     _check_dependencies()
          Raise error if dependencies are missing.
     static needed packages()
          Overwrite this to provide your package names. :return: List of needed packages by the logger.

    Post Run loggers

class pypads.app.injections.run_loggers.PostRunFunction(*args, **kwargs)
     This class should be used to define new post run functions
     _call (pads, *args, **kwargs)
          Function where to add you custom code to execute before starting or ending the run.
              Parameters pads – the current instance of PyPads.
     _check_dependencies()
```

Overwrite this to provide your package names. :return: List of needed packages by the logger.

Raise error if dependencies are missing.

static needed packages()

3.2.3 Mlflow autolog (experimental)

Pypads also support mlflow autologging functionalities. More on that can be found at MLflow.

```
 \textbf{class} \text{ pypads.injections.loggers.mlflow.mlflow\_autolog.} \textbf{MlflowAutologger} (*args, order = -1, **kwargs)
```

MlflowAutologger is the intergration of the mlflow autologging functionalities into PyPads tracking system.

```
__call_wrapped__(ctx, *args, _args, _kwargs, _pypads_autologgers=None, _pypads_env=<class 'pypads.injections.analysis.call_tracker.LoggingEnv'>, **kwargs)
```

Note: Experimental: This method may change or be removed in a future release without warning.

Function used to enable autologgers of mlflow.

identity

Return the identity of the logger. This should be unique for the same functionality across multiple versions.

3.3 Utilities

```
pypads.utils.util.dict_merge(*dicts)
     Simple merge of dicts :param dicts: :return:
pypads.utils.util.dict_merge_caches(*dicts)
     Merge two dicts. Entries are overwritten if not mergeable. Cache is supported. :param dicts: dicts to merge
     :return:
pypads.utils.util.get_class_that_defined_method(meth)
     Try to find the class / module which defined given method. :param meth: Method for which we search an origin.
     :return:
pypads.utils.util.inheritors(clazz)
     Function getting all subclasses of given class. :param clazz: Clazz to search for :return:
pypads.utils.util.is_package_available (name)
     Check if given package is available. :param name: Name of the package :return:
pypads.utils.util.local_uri_to_path(uri)
     Convert URI to local filesystem path.
pypads.utils.util.sizeof_fmt (num, suffix='B')
     Get the mem / disk size in a human readable way. :param num: :param suffix: :return:
pypads.utils.util.string_to_int(s)
     Build a int from a given string. :param s: :return:
```

3.4 Mapping Files

22

PyPads using the concept of mapping files to track which functions should be logged. These files are written in YAML. YAML (YAML Ain't A Markup Language) is a human readable data serialization language. YAML has features such as comments and anchors these features make it desirable.

The mapping file can be divided broadly into different parts like metadata, fragments and mappings. Each section is explained in detail below. Following excerpts show possible mapping files. While the keras file uses implicit syntax for the path matchers marked by a prepending:, the sklearn version depicts how to use YAML typing with <code>!!python/pPath</code>, <code>!!python/rSeg</code> or <code>!!python/pSeg</code>.

```
metadata:
  author: "Thomas Weißgerber"
  version: "0.1.0"
  library:
    name: "keras"
    version: "2.3.1"
mappings:
  :keras.metrics.Metric:
   hooks: ["pypads_metric"]
   data:
      concepts: ["keras classification metrics"]
  :keras.engine.training.Model:
    :___init___:
     hooks: ["pypads_init"]
    :{re:(fit|fit_generator)$}:
      hooks: ["pypads_fit"]
    :predict_classes:
      hooks: ["pypads_predict"]
```

```
metadata:
  author: "Thomas Weißgerber"
  version: "0.1.0"
  library:
   name: "sklearn"
    version: ">= 0.19.1"
fragments:
  default_model:
    !!python/pPath __init__:
      hooks: "pypads_init"
    !!python/rSeg (fit|.fit_predict|fit_transform)$:
      hooks: "pypads_fit"
    !!python/rSeg (fit_predict|predict|score)$:
      hooks: "pypads_predict"
    !!python/rSeg (fit_transform|transform)$:
      hooks: "pypads_transform"
mappings:
  !!python/pPath sklearn:
    !!python/pPath base.BaseEstimator:
      ;default_model: ~
      data:
        concepts: ["algorithm"]
    !!python/pPath metrics.classification:
      !!python/rSeg .*:
        hooks: "pypads_metric"
          concepts: ["Sklearn provided metric"]
    !!python/pPath tree.tree.DecisionTreeClassifier:
      ;default_model: ~
```

(continues on next page)

3.4. Mapping Files 23

(continued from previous page)

```
data:
       name: decision tree classifier
       other_names: []
       type: Classification
       hyper_parameters:
         model_parameters:
            - name: split_quality
             kind_of_value: "{'gini', 'entropy'}"
              optional: 'True'
              description: The function to measure the quality of a split.
             default_value: "'gini'"
             path: criterion
            - name: splitting_strategy
             kind_of_value: "{'best', 'random'}"
              optional: 'True'
              description: The strategy used to choose the split at each node.
             default_value: "'best'"
             path: splitter
            - name: max_depth_tree
             kind_of_value: integer
             optional: 'True'
              description: The maximum depth of the tree.
             default_value: None
             path: max_depth
            - name: min_samples_split
             kind_of_value: "{integer, float}"
             optional: 'True'
             description: The minimum number of samples required to split an_
⇒internal node.
             default_value: '2'
             path: min_samples_split
            - name: min_samples_leaf
             kind_of_value: "{integer, float}"
              optional: 'True'
              description: The minimum number of samples required to be at a leaf.
⇔node.
             default_value: '1'
             path: min_samples_leaf
           - name: min_weight_fraction_leaf
             kind of value: float
              optional: 'True'
              description: The minimum weighted fraction of the sum total of weights,
→ (of all
               the input samples) required to be at a leaf node.
             default_value: '1'
             path: min_weight_fraction_leaf
             name: max_features
             kind_of_value: "{integer, float, 'auto', 'sqrt', 'log2', None}"
              optional: 'True'
              description: The number of features to consider when looking for the
⇒best split.
             default_value: None
             path: max_features
            - name: random state
             kind_of_value: "{integer, RandomState instance, None}"
              optional: 'True'
             description: The seed of the pseudo random number generator to use when,
                                                                          (continues on next page)
⇔shuffling
```

24 Chapter 3. PyPads

(continued from previous page)

```
the data. If int, random_state is the seed used by the random number.
⇔generator;
                If RandomState instance, random_state is the random number generator;
\hookrightarrow If None,
                the random number generator is the RandomState instance used by np.
\hookrightarrowrandom.
              default_value: None
              path: random_state
            - name: max_leaf_nodes
              kind_of_value: integer
              optional: 'True'
              description: Grow a tree with max_leaf_nodes in best-first fashion.
              default_value: None
              path: max_leaf_nodes
            - name: min_impurity_decrease
              kind of value: float
              optional: 'True'
              description: A node will be split if this split induces a decrease of_
\rightarrowthe impurity
                greater than or equal to this value.
              default_value: '0'
              path: min_impurity_decrease
            - name: class_weight
              kind_of_value: "{dict, list of dicts, 'balanced', None}"
              optional: 'False'
              description: Weights associated with classes.
              default_value: None
              path: class_weight
          optimisation_parameters:
            - name: presort
              kind_of_value: "{boolean, 'auto'}"
              optional: 'True'
              description: Whether to presort the data to speed up the finding of,
→best splits
                in fitting.
              default_value: "'auto'"
              path: presort
          execution_parameters: []
```

Metadata The metadata part contains information about the author, the mapping file version and the library information. The mapping file version is required so that a change in the tracking functionalities can be easily traced to the version of the mapping file. Even while having the same library version, a user can modify the mapping file to track additional functions of the library or remove some tracking functionalities. Such changes need to be handled to provide better experiment tracking and reproducibility. PyPads does this via versioning of the mapping file. Another tag called "library" contains information about the library which the mapping file addresses such as the name of the library and the version of the library. This metadata section helps PyPads track different versions of libraries without them having a conflict.

```
metadata:
   author: "Thomas Weißgerber"
   version: "0.1.0"
   library:
      name: "sklearn"
      version: "0.19.1"
```

Fragments Repeated patterns in the library can be included in the fragments section of the mappings file. Fragments allows users to link functions across classes. For example, in scikit-learn the fit function is a function for fitting

3.4. Mapping Files 25

the estimators. All classification/regression estimators will have a fit function. In such a scenario, the user does not have to write mappings for each and every estimator. Instead, the user can add the function to the fragments part and PyPads will automatically log those functions.

```
fragments:
    default_model:
        .__init__:
        events: "pypads_init"
        .{re: (fit|.fit_predict|fit_transform)$}:
        events: "pypads_fit"
```

Mappings This part in the mapping file gives information to PyPads about the functions to track. In the example, we use the sklearn base estimator to encompass all logging functionalities from a single point. The user can add other classes as shown with the Decision Tree Classifier. By doing this the user also has to provide all the hyperparameters so that PyPads knows what to track. For each hyperparameter the user also has to provide the name of the hyperparameter, whether it is optional or not, its description and so forth.

3.4.1 Concepts

PyPads mapping files contain keys called concepts. When creating a main key in the mappings file, it could be anything such as a metric, a dataset, splitting strategy, an algorithm and so forth. The concepts key present within the main key links the main key to previously determined categories such as metric, dataset or algorithm to name a few. This helps PyPads recognize what type the main key is and how to process it.

3.4.2 Notations

PyPads can accept different notations through the YAML parser. Users can use the power of regular expressions to specify function groups that should trigger specific events. Here in the below given example, we hook all functions in sklearn.metrics.classification to "pypads_metric". We also inform PyPads that all functions of this form are an instance of sklearn provided metrics using the concepts key.

```
mappings:
    sklearn:
    .metrics.classification.{re:.*}:
        data:
        concepts: ["Sklearn provided metric"]
        events: "pypads_metric"
```

3.4.3 Adding a new mapping file

When a user wants to add their own mapping file, they have to follow the following steps # Create a YAML mapping file in the path pypads/bindings/resources/mapping with the appropriate name and version number # Add a metadata part containing information about the author, version of the mapping file and library # Add fragments if a general function name is present. You can use regex to specify the patterns # Add mappings for metrics, datasets etc is they are present # PyPads will pick up the information when it is restarted.

CHAPTER 4

Extensions

• **PaDRe-Pads** is a tool that builds on PyPads and add some semantics to the tracked data of Machine learning experiments. See the padre-pads documentation.

4.1 Extensions and plugins

PyPads features a plugin system to extend its functionality. Currently following plugins are being developed.

pypads_padre Also called PadrePads introduces additional concepts of machine learning. While PyPads is fairly unopinionated about what it is logging PadrePads tries to impose some structure.

pypads_onto (unreleased) Also called OntoPads introduces ontology mappings to pypads. It is based on the other plugin PadrePads and will enable given concept unique references.

To enable an extension it just has to be installed into your active environment. If this fails due to some unexpected reason you can try to enable a plugin manually. In general this can look like this.

```
from pypads.app.base import PyPads
from pypads_padre import activate
activate()
tracker = PyPads(autostart=True)
```

If you don't want to use an installed plugin, you can add the disable_plugins parameter to PyPads.

```
from pypads.app.base import PyPads
tracker = PyPads(disable_plugins=["pypads_padre"], autostart=True)
```

4.1.1 PyPaDS-PaDRe

PyPaDS-PaDRe builds upon pypads when it comes to tracking, but it also adds a layer of loggers that tracks semantic information from experiments executions. The documentation for PyPaDS-PaDRe can be found here.

4.1.2 PyPaDS-Onto

PyPaDS-Onto introduces ontology mappings into PyPaDS. The documentation for PyPaDS-Onto can be found here.

CHAPTER 5

Related Projects

• **PyPadre** is the predecessor of PadrePads. Its development has been discontinued.

5.1 Related Projects

PyPads was developed of some related projects. One of which was its predecessor PyPadre.

5.1.1 PyPaDRE

PyPaDRE was the original experimental project developed on the context of padre-lab to track machine learning experiments. After identifying drawbacks in the basic architecture or pypadre the development on pypads was started. The documentation for PyPaDRE can be found here.

CHAPTER 6

Changelog

6.1 0.2.0 (2020-06-22)

• Bump version: $0.1.20 \rightarrow 0.2.0$. [Thomas Weißgerber]

6.2 0.1.20 (2020-05-19)

• Bump version: $0.1.19 \rightarrow 0.1.20$. [Thomas Weißgerber]

6.3 0.1.19 (2020-05-19)

• Bump version: $0.1.18 \rightarrow 0.1.19$. [Thomas Weißgerber]

6.4 0.1.18 (2020-05-19)

6.5 About Us

This work has been developed within the **Data Science Chair** of the University of Passau. It has been partially funded by the **Bavarian Ministry of Economic Affairs, Regional Development and Energy** by means of the funding programm "**Internetkompetenzzentrum Ostbayern**" as well as by the **German Federal Ministry of Education and Research** in the project "**Provenance Analytics**" with grant agreement number 03PSIPT5C.

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Python Module Index

D

pypads.utils.util, 22

34 Python Module Index

Index

call_wrapped()	Symbols	static method), 18
method), 22 _call () (pypads.app.injections.rum_loggers.PostRunFunction method), 21 _call () (pypads.app.injections.rum_loggers.PostRunFunction method), 21 _call () (pypads.app.injections.rum_loggers.PreRunFunction method), 21 _check_dependencies ()	call_wrapped() (py-	available_setup_functions() (py-
method), 22 _call () (pypads.app.injections.rum_loggers.PostRunFunction method), 21 _call () (pypads.app.injections.rum_loggers.PostRunFunction method), 21 _call () (pypads.app.injections.rum_loggers.PreRunFunction method), 21 _check_dependencies ()	$pads. injections. loggers. mlflow. mlflow_autolog. M$	IlflowAutologgerapp.base.PyPads static method), 18
method), 21 _call() (pypads.app.injections.run_loggers.PreRunFunction method), 21 _check_dependencies() pads.app.injections.run_loggers.PostRunFunction	method), 22	available_teardown_functions() (py-
_call() (pypads.app.injections.rum_loggers.PreRunFunction method), 21 _check_dependencies() pads.app.injections.rum_loggers.PostRunFunction method), 21 _check_dependencies() pads.app.injections.rum_loggers.PostRunFunction method), 21 _check_dependencies() pads.app.injections.rum_loggers.PreRunFunction ache (pypads.app.base.PyPads attribute), 18 method), 21 _needed_packages() pads.app.injections.rum_loggers.PostRunFunction static method), 21 _needed_packages() pads.app.injections.rum_loggers.PreRunFunction static method), 21 _needed_packages() pads.app.injections.rum_loggers.PostRunFunction cache (pypads.app.base.PyPads attribute), 18 static method), 21 _needed_packages() pads.app.injections.rum_loggers.PreRunFunction cache (pypads.app.base.PyPads attribute), 18 dall_tracker (pypads.app.base.PyPads attribute), 18 decorators(pypads.app.base.PyPads attribute), 18 decorators (pypads.app.base.PyPads attribute), 17 actuators (pypads.app.base.PyPads attribute), 17 actuators (pypads.app.base.PyPads static method), 18 available_actuators() pads.app.base.PyPads static method), 18 available_actuators() pads.app.base.PyPads static method), 18 available_decorators() pads.app.base.PyPads static method), 18 available_lo		icion
method), 21		
check_dependencies()		-
pads.app.injections.rum_loggers.PostRumFunction*backend (pypads.app.base.PyPads attribute), 18 method), 21 needed_packages()pads.app.injections.rum_loggers.PreRumFunction* astatic method), 21needed_packages()pads.app.injections.rum_loggers.PostRumFunction* astatic method), 21needed_packages()pads.app.injections.rum_loggers.PostRumFunction* astatic method), 21needed_packages()pads.app.injections.rum_loggers.PreRumFunction* astatic method), 18 available_actions.rum_loggers.PreRumFunction* astatic method), 18 available_actions.rum_loggers.PreRumFunction* astatic method), 18 available_actions.rum_loggers.PreRumFunction* astatic method), 18 available_decorators()pads.app.base.PyPads staticmethod), 18 available_decorators()pads.app.base.PyPads staticpads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads	check dependencies () (my-	
method), 21check_dependencies()	pads.app.iniections.run loggers.PostRunFunctio	mbackend (<i>pypads.app.base.PyPads attribute</i>), 18
check_dependencies() pads.app.injections.rum_loggers.PreRunFunction method), 21 needed_packages() pads.app.injections.rum_loggers.PostRunFunction static method), 21 needed_packages() pads.app.injections.rum_loggers.PostRunFunction static method), 21 needed_packages() pads.app.injections.rum_loggers.PreRunFunction deactivate_tracking() pads.app.injections.rum_loggers.PreRunFunction deactivate_tracking() pads.app.base.PyPads attribute), 18 decorators(pypads.app.base.PyPads attribute), 18 decorators(pypads.app.base.PyPads attribute), 18 decorators(pypads.app.base.PyPads attribute), 18 decorators(pypads.app.base.PyPads attribute), 17 actuators(pypads.app.base.PyPads attribute), 17 add_atexit_fn() pads.app.base.PyPads attribute), 17 available_actuators() pads.app.base.PyPads static method), 18 available_anchors() pads.app.base.PyPads static method), 18 available_cords() (pypads.app.base.PyPads static method), 18 available_decorators() pads.app.base.PyPads static method), 18 available_events() static method), 18 available_events() static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads static method), 18 (pypads.app.base.PyPads static) (pypads.app.base.	method), 21	<u> </u>
pads.app.injections.run_loggers.PreRunFunction method), 21 call_tracker (pypads.app.base.PyPads attribute), 18 call_tracker (pypads.app.base.PyPads attribute), 18 call_tracker (pypads.app.base.PyPads attribute), 18 static method), 21	check dependencies() (nv-	C
method), 21 _needed_packages()	pads.app.injections.run_loggers.PreRunFunction	n cache (pypads.app.base.PyPads attribute), 18
pads.app.injections.rum_loggers.PostRunFunction static method), 21 _needed_packages() pads.app.injections.rum_loggers.PreRunFunction static method), 21 A A A A A A A A A A A A A	method), 21	call_tracker (pypaas.app.base.PyPaas attribute),
needed_packages ()	_needed_packages() (py-	
needed_packages() (py- pads.app.injections.rum_loggers.PreRunFunction static method), 21 A activate_tracking() (pypads.app.base.PyPads method), 17 actuators (pypads.app.base.PyPads attribute), 17 add_atexit_fn() (pypads.app.base.PyPads method), 17 api (pypads.app.base.PyPads attribute), 17 api (pypads.app.base.PyPads attribute), 17 available_actuators() (py- pads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (py- pads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_levents() (pypads.app.base.PyPads static method),	pads.app.injections.run_loggers.PostRunFunctio	_m conrig (pypaas.app.base.FyFaas auribuie), 18
pads.app.injections.rum_loggers.PreRunFunction static method), 21 A activate_tracking() (pypads.app.base.PyPads method), 17 actuators (pypads.app.base.PyPads attribute), 17 add_atexit_fn() (pypads.app.base.PyPads method), 17 api (pypads.app.base.PyPads attribute), 17 available_actuators() (pypads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_levents() (pypads.app.base.PyPads static method), 18 available_levents() (pypads.app.base.PyPads attribute), 18 available_loggers() (pypads.app.base.PyPads attribute), 18 available_logge		D
dict_merge() (in module pypads.utils.util), 22 activate_tracking() (pypads.app.base.PyPads method), 17 actuators (pypads.app.base.PyPads attribute), 17 add_atexit_fn() (pypads.app.base.PyPads method), 17 api (pypads.app.base.PyPads attribute), 17 available_actuators() (pypads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_ovents() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 19 folder (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 19 hook_registry (pypads.app.b	pads.app.injections.run_loggers.PreRunFunction	pads.app.base.PyPads method), 18
activate_tracking() (pypads.app.base.PyPads method), 17 actuators (pypads.app.base.PyPads attribute), 17 add_atexit_fn() (pypads.app.base.PyPads method), 17 api (pypads.app.base.PyPads attribute), 17 api (pypads.app.base.PyPads attribute), 17 available_actuators() (pypads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads attribute), 18 av	A	
actuators (pypads.app.base.PyPads attribute), 17 add_atexit_fn() (pypads.app.base.PyPads method), 17 api (pypads.app.base.PyPads attribute), 17 available_actuators() (pypads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute), 18 H hook_registry (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 18	activate_tracking() (pypads.app.base.PyPads	dict_merge_caches() (in module py-
add_atexit_fn() (pypads.app.base.PyPads method), 17 api (pypads.app.base.PyPads attribute), 17 available_actuators() (pypads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 18 hook_registry (pypads.app.base.PyPads attribute), 18		F
api (pypads.app.base.PyPads attribute), 17 available_actuators() (pypads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute), hook_registry (pypads.app.base.PyPads attribute),		_
available_actuators() (py- pads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (py- pads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute), 18 folder (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 folder (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 folder (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18		
pads.app.base.PyPads static method), 18 available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute), 18 function_registry (pypads.app.base.PyPads attribute), 18 funct		F
available_anchors() (pypads.app.base.PyPads static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute), hook_registry (pypads.app.base.PyPads attribute), function_registry (pypads.app.base.PyPads attribute), get_class_that_defined_method() (in module pypads.utils.util), 22 H hook_registry (pypads.app.base.PyPads attribute),		folder (pypads.app.base.PyPads attribute), 18
static method), 18 available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),		
available_cmds() (pypads.app.base.PyPads static method), 18 available_decorators() (pypads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),		
method), 18 available_decorators() (py- pads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),		G
available_decorators() (py-pads.app.base.PyPads static method), 18 available_events() (pypads.app.base.PyPads static method), 18 available_loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),	*** **	<u>.</u>
available_events() (pypads.app.base.PyPads H static method), 18 available loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),	available_decorators() (py-	
static method), 18 available loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),		ule pypads.utils.util), 22
available loggers() (pypads.app.base.PyPads hook_registry (pypads.app.base.PyPads attribute),		Н
18		hook_registry (<i>pypads.app.base.PyPads attribute</i>),

```
hooks (pypads.app.base.PyPads attribute), 19
\verb|identity| (pypads.injections.loggers.mlflow.mlflow\_autolog.MlflowAutologger)| \\
        attribute), 22
inheritors() (in module pypads.utils.util), 22
is_affected_module() (pypads.app.base.PyPads
        method), 19
is_package_available()
                                      module
                                                py-
        pads.utils.util), 22
local_uri_to_path()
                              (in
                                     module
                                                py-
        pads.utils.util), 22
M
managed_git_factory
                            (pypads.app.base.PyPads
        attribute), 19
mapping_registry (pypads.app.base.PyPads at-
        tribute), 19
mappings (pypads.app.base.PyPads attribute), 19
mlf (pypads.app.base.PyPads attribute), 19
MlflowAutologger
                            (class
                                                py-
        pads.injections.loggers.mlflow.mlflow_autolog),
P
PostRunFunction
                           (class
                                       in
                                                py-
        pads.app.injections.run_loggers), 21
PreRunFunction
                          (class
                                                py-
        pads.app.injections.run_loggers), 21
PyPads (class in pypads.app.base), 17
pypads.utils.util (module), 22
S
sizeof_fmt() (in module pypads.utils.util), 22
start_track() (pypads.app.base.PyPads method),
        19
string_to_int() (in module pypads.utils.util), 22
U
uri (pypads.app.base.PyPads attribute), 19
validators (pypads.app.base.PyPads attribute), 19
W
wrap_manager (pypads.app.base.PyPads attribute),
         19
```

36 Index