

PyMVPA Developer Guidelines

Release 2.6.5.dev1

PyMVPA Authors

Apr 08, 2019

CONTENTS

1	Git Repository 1.1 Layout 1.2 Branches 1.3 Commits 1.4 Merges	1 1 1 2					
2	Code2.1Formatting2.2Docstrings2.3Classes2.4Function Arguments	3 3 4 4 4					
3	Documentation 3.1 Examples	5 5					
4	Tests	7					
5	Changelog	7 9 Dependency					
6	6 Extending PyMVPA 6.1 Adding an External Dependency 6.2 Adding a new Dataset type 6.3 Adding a new Classifier 6.4 Adding a new Measure 6.4.1 Classifier-independent Sensitivity Analyzers 6.4.2 Classifier-based Sensitivity Analyzers						
7	Developer-TODO7.1Things to implement for the next release (Release goals)7.2Long and medium term TODOs (aka stuff that has been here forever)	15 15 16					
8	8 Building a binary installer on MacOS X 10.5						
In	dex	21					

CHAPTER ONE

GIT REPOSITORY

1.1 Layout

The git repository is structured by a number of branches and clones (forks) at github. Anyone is welcome to fork the repository on github (just click on "Fork" button), and file a "Pull request" whenever he/she thinks that his changes are ready to be included (merged) into the main repository. Alternatively, if you just want quickly submit a patch – just email it to the mailing list. Concise accompanying description is a plus. You might take advantage of git format-patch command.

1.2 Branches

Any developer can have an infinite number of branches. If the number of branches causes gitk output to exceed a usual 19" screen, the respective developer has to spend some bucks (or euros) on new screens for all others ;-)

The main release branch is called *master*. This is a merge-only branch. Features finished or updated by some developer are merged from the corresponding branch into *master*. At a certain point the current state of *master* is tagged – a release is done.

Only usable feature should end-up in *master*. Ideally *master* should be releasable at all times. Something must not be merged into master if *any* unit test fails. Maintenance branches should be gone into *maint/epoch.major* branches (e.g. *maint/0.4*).

Additionally, there are packaging branches (prefixed with *dist/*). They are labeled after the package target (e.g. *debian* for a Debian package). Releases are merged into the packaging branches, packaging get updated if necessary and the branch gets tagged when a package version is released. Packaging maintenance (as well as backport) releases should be gone under *dist/target/flavor/codename* (e.g. *dist/debian/maint/lenny*, *dist/debian/security/lenny*). Branch *dist/debian/dev* is dedicated for Debian packages of development snapshots.

Besides master, maint/..., dist/... we are following the convention for additional prefixes for new branches:

_bf/...

Bugfix branches - should be simply deleted on remotes whenever accepted

_tent/...

Tentative new features which might be adopted or not. Whenever feature gets adopted (merged into some *master*), corresponding HEAD of *_tent/* branch should be tagged with a corresponding non-annotated +*tent/* tag

Please do not base your work on *_tent/* branches of the others since those could be forcefully rebased without further notice.

1.3 Commits

Please prefix all commit summaries with one (or more) of the following labels. This should help others to easily classify the commits into meaningful categories:

- *BF* : bug fix
- *RF* : refactoring
- *NF* : new feature
- ENH : enhancement of an existing feature/facility
- *BW* : addresses backward-compatibility
- **OPT** : optimization
- *BK* : breaks something and/or tests fail
- *PL* : making pylint happier
- DOC: for all kinds of documentation related commits

1.4 Merges

For easy tracking of what changes were absorbed during merge, we advice to enable automagic inclusion of their log entries into the commit message of the merge:

git config merge.log true

Note:

merge.log superseeds deprecated x'merge.summary'

CHAPTER TWO

CODE

2.1 Formatting

pylint

Code should be conformant with Pylint driven by config located at doc/misc/pylintrc. Previously we used camelBack notation, but since 0.5.0.dev we decided to mainly follow PEP8. Provided *pylintrc* file assures consistent coding style and also warns about obvious errors in the code. To engage, use 1 of 3 methods:

- place it in ~/.pylintrc for user-wide installation
- use within a call to pylint:

pylint --rcfile=\$PWD/doc/misc/pylintrc

• export environment variable from mvpa sources top directory:

export PYLINTRC=\$PWD/doc/misc/pylintrc

2 empty lines

According to original python style guidelines: single empty line to separate methods within class, and 2 empty lines between classes **BUT** we do 2 empty between methods, 3 empty between classes

module docstring

Each module should start with a docstring describing the module (which is not inside the hashed-comment of each file) look at mapper or neighbor for tentative organization if copyright/license has to be present in each file.

header

Each file should contain a header from doc/misc/header.py.

notes

Use following keywords will be caught by pylint to provide a summary of what yet to be done in the given file

FIXME

something which needs fixing (sooner than later)

TODO

future plan (i.e. later than sooner)

XXX

some concern/question

YYY

comment/answer to above mentioned XXX concern

WiP

Work in Progress: API and functionality might rapidly change

2.2 Docstrings

All documentation should be written using NumPy documentation conventions:

https://github.com/numpy/numpy/blob/master/doc/HOWTO_DOCUMENT.rst.txt

2.3 Classes

Classes should define:

__repr_

whenever possible, should be the string representation of the object which could be digested with func:eval if necessary.

__str_

most of the classes should provide meaningful and concise summary over their identity (name + parameters + some summary over results if any), not necessarily *eval*uable.

Note:

```
Classes derived from ClassWithCollections and using params and ca collections for their need of parametrization (e.g. Classifier) would obtain an acceptable definitions of __repr__ and __str__ automagically.
```

2.4 Function Arguments

dataset vs data

Ones which are supposed to be derived from Dataset class should have suffix (or whole name) dataset. In contrast, if argument is expected to be simply a NumPy array, suffix should be data. For example:

```
class Classifier(ClassWithCollections):
    ...
    def train(self, dataset):
    ...
    def predict(self, data):
    class FeatureSelection(ClassWithCollections):
    ...
    def __call__(self, dataset, testdataset):
```

Such convention should be enforced in all *train, *predict functions of classifiers.

CHAPTER THREE

DOCUMENTATION

3.1 Examples

Examples should be complete and stand-alone scripts located in doc/examples. If an example involves any kind of interactive step, it should honor the MVPA_EXAMPLES_INTERACTIVE setting, to allow for automatic testing of all examples. In case of a matplotlib-based visualization such snippet should be sufficient:

```
from mvpa2 import cfg
if cfg.getboolean('examples', 'interactive', True):
    pl.show()
```

All examples are automatically converted into RsT documents for inclusion in the manual. Each of them is preprocessed in the following way:

- Any header till the first docstring is stripped.
- Each top-level (non-assigned) docstring is taken as a text block in the generated RsT source file. Such a docstring might appear anywhere in the example, not just at the beginning. In this case, the code snippet is properly split and the text block is inserted at the corresponding location.
- All remaining lines are treated as code and inserted in the RsT source with appropriate markup.

The first docstring in each example must have a proper section heading (with '=' markup).

Finally, each example should be added to the appropriate toctree in doc/examples.rst and included into a test battery by adding it to testexamples rule within Makefile in the toplevel directory of the source tree.

CHAPTER FOUR

TESTS

We are slowly moving toward utilizing nose testing framework. It allows to carry out not only unit testing, but also verify correctness of the code snippets provided in the docstrings and the manual. All unit tests are stored in mvpa2.tests, and they make use of mvpa2.testing which provides

tools

basic tools (imported within __init__)

clfs

some additional classifiers to be used in the unittests

datasets

pre-crafted datasets warehouse to be used in the tests

```
sweepargs
```

defines a custom decorator to allow running the same unittest on a range of input values and later on nicely summarize the detected failures

While working on the project we adhere to the following rules:

- Every more or less "interesting" bugfix should be accompanied by a unittest which might help to prevent it in the future refactoring
- Every new feature should have a unittest
- Unit tests that might be non-deterministic (e.g. depending on classifier performance, which is turn is randomly initialized) should be made conditional like this:

```
>>> from mvpa2 import cfg
>>> if cfg.getboolean('tests', 'labile', default='yes'):
... pass
```

• Every additional unit test submodule (or a unittest method itself) requiring specific external being present should make use of skip_if_no_external(), e.g.

```
>>> from mvpa2.testing import *
>>> skip_if_no_external('numpy')
```

Furthermore we encourage detailed docstrings for the classes, including *Examples* section with the demonstration of most typical use cases and aspects of the classes. Those snippets are also part of the tests battery

CHAPTER FIVE

CHANGELOG

The PyMVPA changelog is located in the toplevel directory of the source tree in the Changelog file. The content of this file should be formated as restructured text to make it easy to put it into manual appendix and on the website.

This changelog should neither replicate the VCS commit log nor the distribution packaging changelogs (e.g. debian/changelog). It should be focused on the user perspective and is intended to list rather macroscopic and/or important changes to the module, like feature additions or bugfixes in the algorithms with implications to the performance or validity of results.

It may list references to 3rd party bug trackers, in case the reported bugs match the criteria listed above.

Changelog entries should be tagged with the name of the developer(s) (mainly) involved in the modification – initials are sufficient for people contributing regularly.

Changelog entries should be added whenever something is ready to be merged into the master branch, not necessarily with a release already approaching.

EXTENDING PYMVPA

This section shall provide a developer with the necessary pieces of information for writing extensions to PyMVPA. The guidelines given here, must be obeyed to ensure a maximum of compatibility and inter-operability. As a consequence, all modifications that introduce changes to the basic interfaces outlined below have to be documented here and also should be announced in the changelog.

6.1 Adding an External Dependency

Introducing new external dependencies should be done in a completely optional fashion. This includes both build-dependencies and runtime dependencies. With mvpa2.base.externals PyMVPA provides a simple framework to test the availability of certain external components and publish the results of the tests throughout PyMVPA.

6.2 Adding a new Dataset type

- Required interface for Mapper.
- only new subclasses of MappedDataset + new Mappers (all other as improvements into the Dataset base class)?

```
go into mvpa2/datasets/
```

6.3 Adding a new Classifier

To add a new classifier implementation it is sufficient to create a new sub-class of Classifier and add implementations of the following methods:

```
___init___(**kwargs)
```

Additional arguments and keyword arguments may be added, but the base-class contructor has to be called with **kwargs!

```
_train(dataset)
```

Has to train the classifier when it is called with a Dataset. Successive calls to this methods always have to train the classifier on the respective datasets. An eventually existing prior training status has to be cleared automatically. Nothing is returned.

```
_predict(data)
```

Unlike _train() the method is not called with a Dataset instance, but with any sequence of data samples (e.g. arrays). It has to return a sequence of predictions, one for each data sample.

With this minimal implementation the classifier provides some useful functionality, by automatically storing some relevant information upon request in conditional attributes.

Supported conditional attributes:

Name	Description	Default
feature_ids	Feature IDS which were used for the actual training.	Disabled
predicting_time	Time (in seconds) which took classifier to predict.	Enabled
predictions	Most recent set of predictions.	Enabled
trained_dataset	The dataset it has been trained on.	Disabled
trained_targets	Set of unique labels it has been trained on.	Enabled
training_stats	Confusion matrix of learning performance.	Disabled
training_time	Time (in seconds) which took classifier to train.	Enabled
values	Internal classifier values the most recent predictions are based on.	Disabled

If any intended functionality cannot be realized be implementing above methods. The Classifier class offers some additional methods that might be overridden by sub-classes. For all methods described below it is strongly recommended to call the base-class methods at the end of the implementation in the sub-class to preserve the full functionality.

```
_pretrain(dataset)
```

Called with the Dataset instance that shall be trained with, but before the actual training is performed.

```
_posttrain(dataset)
```

Called with the Dataset instance the classifier was trained on, just after training was performed.

```
_prepredict(data)
```

Called with the data samples the classifier should do a prediction with, just before the actual $_predict()$ call.

```
_postpredict(data,result)
```

Called with the data sample for which predictions were made and the resulting predictions themselves.

Source code files of all classifier implementations go into mvpa2/clfs/.

Outstanding Questions:

• when ca and when properties?

6.4 Adding a new Measure

There are few possible base-classes for new measures (former sensitivity analyzers). First, Measure can directly be sub-classed. It is a base class for any measure to be computed on a Dataset. This is the more generic approach. In the most of the cases, measures are to be reported per each feature, thus FeaturewiseMeasure should serve as a base class in those cases. Furthermore, for measures that make use of some classifier and extract the sensitivities from it, Sensitivity (derived from FeaturewiseMeasure) is a more appropriate base-class, as it provides some additional useful functionality for this use case (e.g. training a classifier if needed).

All measures (actually all objects based on Measure) support a transformer keyword argument to their constructor. The functor passed as its value is called with the to be returned results and its outcome is returned as the final results. By default no transformation is performed.

If a Measure computes a characteristic, were both large positive and large negative values indicate high relevance, it should nevertheless *not* return absolute sensitivities, but set a default transformer instead that takes the absolute (e.g. plain np.absolute or a convinience wrapper Absolute).

To add a new measure implementation it is sufficient to create a new sub-class of Measure (or FeaturewiseMeasure, or Sensitivity) and add an implementation of the _call(dataset) method. It will be called with an instance of Dataset. FeaturewiseMeasure (e.g. Sensitivity as well) has to return a vector of featurewise sensitivity scores.

Supported conditional attributes:

Name	Description	Default
null_prob	Conditional attribute.	Enabled
raw_results	Computed results before applying any transformation algorithm.	Disabled

Source code files of all sensitivity analyzer implementations go into mvpa2/measures/.

6.4.1 Classifier-independent Sensitivity Analyzers

Nothing special.

6.4.2 Classifier-based Sensitivity Analyzers

A Sensitivity behaves exactly like its classifier-independent sibling, but additionally provides support for embedding the necessary classifier and handles its training upon request (boolean force_train keyword argument of the constructor). Access to the embedded classifier object is provided via the clf property.

Supported conditional attributes:

Name	Description	Default
base_sensitivities	Stores basic sensitivities if the sensitivity relies on combining multiple ones.	Disabled
null_prob	Conditional attribute.	Enabled
raw_results	Computed results before applying any transformation algorithm.	Disabled

Outstanding Questions:

- What is a mvpa2.measures.base.ProxyClassifierSensitivityAnalyzer useful for?
- Shouldn't there be a sensitivities state?

6.5 Adding a new Algorithm

go into mvpa2/algorithms/

DEVELOPER-TODO

7.1 Things to implement for the next release (Release goals)

- A part of below restructuring TODO but is separate due to it importance: come up with cleaner hierarchy and tagging of classifiers and regressions now they are all Classifier
- Unify parameter naming across all classifiers and come up with a labeling guideline for future classifier implementations and wrappers:

```
Numeric parameters can be part of .params Collection now, so they are joined together.
```

• Restructure code base (incl. renaming and moving pieces)

Let's use the following list to come up with a nice structure for all logical components we have:

- Datasets
- Sensitivity analyzers (maybe: featurewise measures) * Classifier sensitivities (SVM, SMLR)
 respective classifiers * ANOVA -> mvpa2.measures.anova * Noise perturbation -> -> mvpa2.measures.noisepertrubation * meta-algorithms (splitting) -> mvpa2.measures

FeaturewiseMeasure?

- Mappers::

mvpa2.mappers (AKA mvpa2.projections mvpa2.transformers)

* Along with PCA/ICA mappers, we should add a PLS mapper:

```
PCA.train(learningdataset)
    .forward,
    .backward
Package pychem for Debian, see how to use from PyMVPA! ;-) Same for MDP
(i.e. use from pymvpa)
```

- Feature selection algorithms
 - * Simple thresholding
 - * RFE
 - * IFS
- .mapper conditional attribute

mvpa2.featsel (NB no featsel.featsel.featsel more than 4 times!) mvpa2.featsel.rfe mvpa2.featsel.ifs

- several base classes with framework infrastructure (ClassWithCollections, virtual properties, ...)
- Transfer error calculation

- Cross-validation support
- Monte-Carlo-based significance testing
- Dataset splitter
- Metrics and distance functions
- Functions operating on dataset for preprocessing or transformations
- Commandline interface support
- Functions to generate artificial datasets
- Error functions (i.e. for TransferError)
- Custom exception types
- Python 2.5 copy() aka external code shipped with PyMVPA
- Several helpers for data IO
- Left-over from the last attempt to establish a generic parameter interface
- Detrending (operating on Datasets)
- Result 'Transformers' to be used with 'transformer=' kwarg
- Debugging and verbosity infrastructure
- plus additional helpers, ranging from simple to complex scattered all over the place
- Resultant hierarchy:
 - mvpa
 - * datasets
 - * clfs
 - * measures
 - * featsel
- Add ability to add/modify custom attributes to a dataset.
- Possibly make NiftiDataset default to float32 when it sees that the data are ints.
- Add kernel methods as option to all classifiers, not just SVMs. For example, you should be able to run a predefined or custom kernel on the samples going into SMLR.
- TransferError needs to know what type of data to send to any specific ErrorFX. Right now there is only support for predictions and labels, but the area under the ROC and the correlation-based error functions expect to receive the "values" or "probabilities" from a classifier. Just to make this harder, every classifier is different. For example, a ridge regression's predictions are continuous values, whereas for a SVM you need to pass in the probabilities.

For binary: 1 value multiclass: 1 value, or N values

• In a related issue, the predictions and values ca of the classifiers need to have a consistent format. Currently, SVM returns a list of dictionaries for values and SMLR returns a NumPy ndarray.

7.2 Long and medium term TODOs (aka stuff that has been here forever)

• selected_ids -> implement via MaskMapper?

yoh:

it might be preferable to manipulate/expose MaskMapper instead of plain list of selected_ids within FeatureSelection classes

- unify naming of working/testing
 - transerror.py for instance uses testdata/trainingdata
 - rfe.py dataset, testdataset
- implement proper cloning of classifiers. untrain() doesn't work in some cases, since we can create somewhat convolved object definitions so it is hard, if not impossible, to get to all used classifiers. See for instance clfswh['SVM/Multiclass+RFE']. We can't get all the way into classifier-based sensitivity analyzer. Thus instead of tracking all the way down in hierarchy, we should finally create proper 'parametrization' handling of classifiers, so we could easily clone basic ones (which might have active SWIG bindings), and top-level ones should implement .clone() themselves. or may be some other way, but things should be done. Or may be via proper implementation of __reduce__ etc
- mvpa2.misc.warning may be should use stock python warnings module instead of custom one?
- ConfusionBasedError -> InternalError ?
- Renaming of the modules transerror.py -> errors.py
- SVM: get_sv and get_sv_coef return very 'packed' presentation whenever classifier is multiclass. Thus they have to be unpacked before proper use (unless it is simply a binary classifier).
- Regression tests: for instance using sample dataset which we have already, run doc/examples/searchlight.py and store output to validate against. Probably the best would be to create a regression test suite within unit tests which would load the dataset and run various algorithms on it a verify the results against previously obtained (and dumped to the disk)
- feature_selector may be we should return a tuple (selected_ids, discarded_ids)?

Michael:

Is there any use case for that? ElementSelector can 'select' and 'discard' already. DO we need both simultaneously?

- Non-linear SVM RFE
- ParameterOptimizer (might be also OptimizedClassifier which uses parameterOptimizer internally but as the result there is a classifier which automatically optimizes its parameters. It is close in idea to classifier based on RFE)

BUILDING A BINARY INSTALLER ON MACOS X 10.5

A simple way to build a binary installer for Mac OS is bdist_mpkg. This is a setuptools extension that uses the proper native parts of MacOS to build the installer. However, for PyMVPA there are two problems with bdist_mpkg: 1. PyMVPA uses distutils not setuptools and 2. current bdist_mpkg 0.4.3 does not work for MacOS X 10.5 (Leopard). But both can be solved.

Per 1) A simple wrapper script in tools/mpkg_wrapper.py will enable the use of setuptools on top of distutils, while keeping the distutils part in a usable state.

Per 2) The following patch (against 0.4.3.) makes bdist_mpkg compatible with MacOS 10.5. It basically changes the way bdist_mpkg determined the GID of the admin group. 10.5 removed the nidump command:

```
diff -rNu bdist_mpkg-0.4.3/bdist_mpkg/tools.py bdist_mpkg-0.4.3.leopard/bdist_mpkg/
→tools.py
--- bdist_mpkg-0.4.3/bdist_mpkg/tools.py
                                            2006-07-09 00:39:00.000000000 -0400
+++ bdist_mpkg-0.4.3.leopard/bdist_mpkg/tools.py 2008-08-21 07:43:35.
↔00000000 -0400
@@ -79,15 +79,12 @@
             yield os.path.join(root, fn)
def get_gid(name, _cache={}):
     if not _cache:
        for line in os.popen('/usr/bin/nidump group .'):
            fields = line.split(':')
             if len(fields) >= 3:
                 _cache[fields[0]] = int(fields[2])
    try:
        return _cache[name]
    except KeyError:
        raise ValueError('group %s not found' % (name,))
     for line in os.popen("dscl . -read /Groups/" + name + " PrimaryGroupID"):
+
         fields = [f.strip() for f in line.split(':')]
+
         if fields[0] == "PrimaryGroupID":
+
+
             return fields[1]
+
+
    raise ValueError('group %s not found' % (name,))
def find_root(path, base='/'):
     .....
```

INDEX

Е

environment variable MVPA_EXAMPLES_INTERACTIVE, 5

Μ

MVPA_EXAMPLES_INTERACTIVE, 5