pysubgroup Documentation

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pysubgroup is a Python package that enables subgroup discovery in Python+pandas (scipy stack) data analysis environment. It provides for a lightweight, easy-to-use, extensible and freely available implementation of state-of-the-art algorithms, interestingness measures and presentation options.

Start reading here: Overview

Prototype phase

This library is still in a prototype phase. It has, however, been already successfully employed in active application projects.

CHAPTER

ONE

CONTENTS

1.1 pysubgroup

pysubgroup is a Python package that enables subgroup discovery in Python+pandas (scipy stack) data analysis environment. It provides for a lightweight, easy-to-use, extensible and freely available implementation of state-of-the-art algorithms, interestingness measures and presentation options.

This library is still in a prototype phase. It has, however, been already successfully employed in active application projects.

1.1.1 Subgroup Discovery

Subgroup Discovery is a well established data mining technique that allows you to identify patterns in your data. More precisely, the goal of subgroup discovery is to identify descriptions of data subsets that show an interesting distribution with respect to a pre-specified target concept. For example, given a dataset of patients in a hospital, we could be interested in subgroups of patients, for which a certain treatment X was successful. One example result could then be stated as:

"While in general the operation is successful in only 60% of the cases", for the subgroup of female patients under 50 that also have been treated with drug d, the success rate was 82%."

Here, a variable *operation success* is the target concept, the identified subgroup has the interpretable description fe-male=True AND age<50 AND drug_D = True. We call these single conditions (such as female=True) selection expressions or short *selectors*. The interesting behavior for this subgroup is that the distribution of the target concept differs significantly from the distribution in the overall general dataset. A discovered subgroup could also be seen as a rule:

female=True AND age<50 AND drug_D = True ==> Operation_outcome=SUCCESS

Computationally, subgroup discovery is challenging since a large number of such conjunctive subgroup descriptions have to be considered. Of course, finding computable criteria, which subgroups are likely interesting to a user is also an eternal struggle. Therefore, a lot of literature has been devoted to the topic of subgroup discovery (including some of my own work). Recent overviews on the topic are for example:

- Herrera, Franciso, et al. "An overview on subgroup discovery: foundations and applications." Knowledge and information systems 29.3 (2011): 495-525.
- Atzmueller, Martin. "Subgroup discovery." Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery 5.1 (2015): 35-49.
- And of course, my point of view on the topic is summarized in my dissertation:

Prerequisites and Installation

pysubgroup is built to fit in the standard Python data analysis environment from the scipy-stack. Thus, it can be used just having pandas (including its dependencies numpy, scipy, and matplotlib) installed. Visualizations are carried out with the matplotlib library.

pysubgroup consists of pure Python code. Thus, you can simply download the code from the repository and copy it in your site-packages directory. pysubgroup is also on PyPI and should be installable using: pip install pysubgroup

Note: Some users complained about the **pip installation not working**. If, after the installation, it still doesn't find the package, then do the following steps:

- 1. Find where the directory site-packages is.
- 2. Copy the folder pysubgroup, which contains the source code, into the site-packages directory. (WARNING: This is not the main repository folder. The pysubgroup folder is inside the main repository folder, at the same level as doc)
- 3. Now you can import the module with import pysubgroup.

1.1.2 How to use:

A simple use case (here using the well known *titanic* data) can be created in just a few lines of code:

```
import pysubgroup as ps
# Load the example dataset
from pysubgroup.datasets import get_titanic_data
data = get_titanic_data()
target = ps.BinaryTarget ('Survived', True)
searchspace = ps.create_selectors(data, ignore=['Survived'])
task = ps.SubgroupDiscoveryTask (
    data,
    target,
    searchspace,
    result_set_size=5,
    depth=2,
    qf=ps.WRAccQF())
result = ps.DFS().execute(task)
```

The first line imports *pysubgroup* package. The following lines load an example dataset (the popular titanic dataset).

Therafter, we define a target, i.e., the property we are mainly interested in (_'survived'}. Then, we define the searchspace as a list of basic selectors. Descriptions are built from this searchspace. We can create this list manually, or use an utility function. Next, we create a SubgroupDiscoveryTask object that encapsulates what we want to find in our search. In particular, that comprises the target, the search space, the depth of the search (maximum numbers of selectors combined in a subgroup description), and the interestingness measure for candidate scoring (here, the Weighted Relative Accuracy measure).

The last line executes the defined task by performing a search with an algorithm—in this case beam search. The result of this algorithm execution is stored in a SubgroupDiscoveryResults object.

To just print the result, we could for example do:

print(result.to_dataframe())

to get:

1.1.3 Key classes

Here is an outline on the most important classes:

- Selector: A Selector represents an atomic condition over the data, e.g., *age* < 50. There several subtypes of Selectors, i.e., NominalSelector (color==BLUE), NumericSelector (age < 50) and NegatedSelector (a wrapper such as not selector1)
- SubgroupDiscoveryTask: As mentioned before, encapsulates the specification of how an algorithm should search for interesting subgroups
- SubgroupDicoveryResult: These are the main outcome of a subgroup disovery run. You can obtain a list of subgroups using the to_subgroups() or to a dataframe using to_dataframe()
- Conjunction: A conjunction is the most widely used SubgroupDescription, and indicates which data instances are covered by the subgroup. It can be seen as the left hand side of a rule.

1.1.4 License

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1.1.5 Warning

- Beam-Search is bugged at the moment and does not use beam width, see: https://github.com/flemmerich/ pysubgroup/issues/37
- GP-growth is in an experimental stage.

1.1.6 Cite

If you are using pysubgroup for your research, please consider citing our demo paper:

Lemmerich, F., & Becker, M. (2018, September). pysubgroup: Easy-to-use subgroup. →discovery in python. In Joint European Conference on Machine Learning and Knowledge. →Discovery in Databases (ECMLPKDD). pp. 658-662.

bibtex:

```
@inproceedings{lemmerich2018pysubgroup,
   title={pysubgroup: Easy-to-use subgroup discovery in python},
   author={Lemmerich, Florian and Becker, Martin},
   booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in_
   Databases},
   pages={658--662},
   year={2018}
}
```

1.1.7 Note

This project has been set up using PyScaffold 4.5. For details and usage information on PyScaffold see https: //pyscaffold.org/.

1.2 Components

1.2.1 GP-Growth

This tree based algorithm uses a condensed representation (a so called valuation basis) to find interesting subgroups. The main advantage of this approach is, that the (potentially large) database has to be scanned only twice and thereafter all the necessary information is represented as more compact pattern-tree. Gp-growth is a generalisation of the popular fp-growth algorithm. So refer to instructional material on fp-growth for more in depth knowledge on the workings of this tree based algorithm.

Contents
• GP-Growth
– Basic usage
– Create a custom target

Basic usage

The basic usage of the gp-growth algorithm is not very different from the usage of any other algorithm in this package.

But beware that gp-growth is using an exhaustive search strategy! This can greatly increase the runtime for high search depth. You can specify the mode argument in the constructor of GpGrowth to run gp-growth either bottom up (mode='b_u') or top down (mode='b_u'). As gp growth is a generalisation of fp-growth you can also perform standard fp-growth using gp_growth by using the CountQF (*Frequent Itemset Targets*) quality function.

Create a custom target

If you consider to use the gp-growth algorithm for your custom target that is totally possible if you find a valuation basis. We will now first introduce the concept of a valuation basis and thereafter outline the gp-growth interface that you have to support to use your quality function with our gp-growth implementation.

Valuation Basis

Think of a valuation basis as a codensed representation of a subgroup that allows to quickly compute the same representation for a union of two disjoint subgroups.

We call the function which takes the valuation basis of two disjoint sets and computes the valuation basis for the unified set merge. The function that compute the necessary statistics from a valuation basis stats_from_basis.

Now we can formulate: Given two disjoint sets A and B with $A \cap B = \emptyset$ and their valuation bases v(A) and v(B) with their functions stats_from_basis and merge as defined above, we can compute the properties of $A \cup B$ instead of from the union of the instances from the merged valuation basis. This can be summarized through the following equation:

 $props_from_instances(A \cup B) = props_from_basis(merge(v(A), v(B)))$

Required Methods

To make a target and quality function suitable for gp-growth you have to provide several methods (all methods start with gp_ to indicate that they are used in the gp-growth algorithm). In addition to the standard quality function methods (see *Custom Quality Function*) the following methods should be implemented to make a quality function usable with gp_growth.

```
class MyGpQualityFunction
    def gp_get_basis(self, row_index):
        """ returns the valuation basis of the element at this row_index """
```

```
pass
   def gp_get_null_vector(self):
   """ returns the zero element of the valuation basis """
       pass
   @staticmethod
   def gp_merge(v_l, v_r):
   """ merges the v_r valuation basis into the v_l valuation basis inplace! """
       pass
   def gp_get_statistics(self, cover_arr, v):
   """ computes the statistics for this quality function from the valuation basis v """
       pass
   @property
   def gp_requires_cover_arr(self) -> bool:
   """ returns a boolean value that indicates whether a cover array is required when.
→ calling the gp_get_statistics function
       usually this value is False
   .....
       pass
```

Saving a gp_tree

It is possible to save a gp tree to a txt file for e.g. debugging purpose. You therefor have to implement the gp_to_str function which takes a valuation basis and returns a string representation. It is an intentional choide to not call the str function on the valuation basis directly.

```
def gp_to_str(self, basis) -> str:
""" returns a string representation of the valuation basis """
    pass
```

1.2.2 Selectors

Selectors are objects that if applied to a dataset yield a set of instances. If an instance is retured from a selector we say that the selectors covers that instance. While the term selectors usually only refers to basic selectors, conjunctions and disjunctions as well as negated selectors are also in a general sense selectors. Broadly speaking anything that implements the code:*covers* function is a selector. We will first introduce the frequently used basic selectors and thereafter the more general selectors that are the conjunction and disjunction. We conclude the chapter by showing how to implement a selectors yourself.

Basic Selectors

The pysubgroup package provides two basic selectors: The EqualitySelector and the IntervalSelector. Lets start by exploring the EqualitySelector:

instances with First_name=='Alex' [True False True]
instances with age==22 [False False False]

The output indicates that the first and third instance in the dataset have a first name that is equal to 'Alex'. The second output shows that no instances in our dataset is of age 22. The EqualitySelector selector can be used on many different datatypes, but is most useful on binary, string and categorical data. In addition to the EqualitySelector the pysubgroup package also provides the IntervalSelector. The following codes selects all instances from the database, which are in the age range 18 (included) to 40 (excluded).

```
interval_selector = ps.IntervalSelector('age', 18, 40)
print(interval_selector.covers(df))
```

```
[False True True]
```

The outpu shows that the second and third instance in our dataset have an age within the interval [18, 40).

Selectors are the building block of all rules generated with the pysubgroup package. If you want to write your own custom selector that is not a problem see customselector for references.

Negations

The pysubgroup package also provides the NegatedSelector class that takes any selector (not just basic ones) and inverts it.

```
inverted_selector = ps.NegatedSelector(alex_selector)
print('instances with first name not equal to Alex', inverted_selector.covers(df))
```

instances with first name not equal to Alex [False True False]

The output is: instances with first name not equal to Alex [False, True, False].

Conjunctions

Most of the rules that are generated with the pysubgroup package use conjunctions to form more complex queries. Continuing the running example from above we can find all persons whose name is Alex *and* which have an age in the interval [18, 40) like so:

```
conj = ps.Conjunction([interval_selector, alex_selector])
print('instances with', str(conj), conj.covers(df))
```

instances with First_name=='Alex' AND age: [18:40[[False False True]

The output shows that only the last instance is covered by our conjunction.

Disjunctions

The pysubgroup package also provides disjunctions with the Disjunction class. Continuing the running example we can find all persons whose name is Alex or which have an age in the interval [18, 40) like so:

```
disj = ps.Disjunction([interval_selector, alex_selector])
print('instances with', str(disj), disj.covers(df))
```

instances with First_name=='Alex' OR age: [18:40[[True True True]

We can see that all instances are covered by our conjunction.

Implementing your own

As already mentioned in the introduction on selectors, anything that provides a cover function is a selector. In this case we will show how to implement a custom basic selector that checks whether a string contains a given substring:

```
class StrContainsSelector:
    def __init__(self, column, substr):
        self.column = column
        self.substr = substr
    def covers(self, df):
        return df[self.column].str.contains(self.substr).to_numpy()
    contains_selector = StrContainsSelector('Sur_name','m')
    print(contains_selector.covers(df))
```

```
[ True False True]
```

The output shows that only the first and last instance contain an m in their name. In addition to the covers function it is certainly advised to also implement the __str__ and __repr__ functions. This selector can now be added to the searchspace for any algorithm execution.

1.2.3 Targets and Quality Functions

To define the goal of our subgroup discovery task, we use targets and quality functions. Targets are used to define which attributes play a significant role and can provide common statistics for a subgroup in question. Quality functions assign a score to each subgroup. These scores are used by all the algorithms to determine the most interesting subgroups.

Frequent Itemset Targets

The most simple target is the *FITarget* with its associated quality functions *CountQF* and *AreaQf*. The CountQF simple counts the number of instances covered by the subgroup in question. The AreaQF multiplies the depth or length of the subgroup description with the number of instances covered by that description.

Binary Targets

For Boolean or Binary Targets we provide the *ChiSquaredQF* as well as the *StandardQF* quality functions. The *StandardQF* quality function uses a parameter α to weight the relative size $\frac{N_{SG}}{N}$ of a subgroup and multiplies it with the differences in relations of positive instances p to the number of instances N

$$\left(\frac{N_{SG}}{N}\right)^{\alpha} \left(\frac{p_{SG}}{N_{SG}} - \frac{p}{N}\right)$$

The *StandardQF* also supports an optimistic estimate.

The *ChiSquaredQF* is calculated based on the following contigency table which is then passed to the scipy $chi2_contigency$ function. The small *n* represents the number of negative instances and should not be confused with the capital *N* which represents the total number of instances.

p_{SG}	$p - p_{SG}$
n_{SG}	$n - n_{SG}$

Nominal Targets

Currently pysubgroup only supports nominal targets as binary targets. So you can look for deviations of one nominal value with respect to all othe nominal values.

Numeric Targets

For numeric targets pysubgroup offers the StandardQFNumeric which is defined similar to the StandardQF

$$\left(\frac{N_{SG}}{N}\right)^{\alpha}\left(\mu_{SG}-\mu\right)$$

where μ_{SG} and μ are the mean value for the subgroup and entire dataset respectively. For the *StandardQFNumeric* we offer three optimistic estimates: Average, Summation and Ordering. These are in detail described in Florian Lemmerich's dissertation. You can choose between the different optimistic estimates by using the keyword argument estimator the different options are 'sum', 'average', and 'order'

Custom Quality Function

To create a custom quality function that works will all algorithms except gp_growth.

```
class MyQualityFunction:
   def calculate_constant_statistics(self, task):
        """ calculate_constant_statistics
            This function is called once for every execution,
            it should do any preparation that is necessary prior to an execution.
        ......
       pass
   def calculate_statistics(self, subgroup, data=None):
        """ calculates necessary statistics
            this statistics object is passed on to the evaluate
            and optimistic_estimate functions
        ......
       pass
   def evaluate(self, subgroup, statistics_or_data=None):
        """ return the quality calculated from the statistics """
       pass
   def optimistic_estimate(self, subgroup, statistics=None):
        """ returns optimistic estimate
            if one is available return it otherwise infinity"""
       pass
```

1.3 Contributing

TODO: UPDATE THIS

Welcome to pysubgroup contributor's guide.

This document focuses on getting any potential contributor familiarized with the development processes, but other kinds of contributions are also appreciated.

If you are new to using git or have never collaborated in a project previously, please have a look at contributionguide.org. Other resources are also listed in the excellent guide created by FreeCodeCamp¹.

Please notice, all users and contributors are expected to be **open, considerate, reasonable, and respectful**. When in doubt, Python Software Foundation's Code of Conduct is a good reference in terms of behavior guidelines.

¹ Even though, these resources focus on open source projects and communities, the general ideas behind collaborating with other developers to collectively create software are general and can be applied to all sorts of environments, including private companies and proprietary code bases.

1.3.1 Issue Reports

If you experience bugs or general issues with pysubgroup, please have a look on the issue tracker. If you don't see anything useful there, please feel free to fire an issue report.

Tip: Please don't forget to include the closed issues in your search. Sometimes a solution was already reported, and the problem is considered **solved**.

New issue reports should include information about your programming environment (e.g., operating system, Python version) and steps to reproduce the problem. Please try also to simplify the reproduction steps to a very minimal example that still illustrates the problem you are facing. By removing other factors, you help us to identify the root cause of the issue.

1.3.2 Documentation Improvements

You can help improve pysubgroup docs by making them more readable and coherent, or by adding missing information and correcting mistakes.

pysubgroup documentation uses Sphinx as its main documentation compiler. This means that the docs are kept in the same repository as the project code, and that any documentation update is done in the same way as a code contribution. We are using CommonMark with MyST extensions as our markup language.

Tip: Please notice that the GitHub web interface provides a quick way of propose changes in pysubgroup's files. While this mechanism can be tricky for normal code contributions, it works perfectly fine for contributing to the docs, and can be quite handy.

If you are interested in trying this method out, please navigate to the docs folder in the source repository, find which file you would like to propose changes and click in the little pencil icon at the top, to open GitHub's code editor. Once you finish editing the file, please write a message in the form at the bottom of the page describing which changes have you made and what are the motivations behind them and submit your proposal.

When working on documentation changes in your local machine, you can compile them using tox :

```
tox -e docs
```

and use Python's built-in web server for a preview in your web browser (http://localhost:8000):

```
python3 -m http.server --directory 'docs/_build/html'
```

1.3.3 Code Contributions

Submit an issue

Before you work on any non-trivial code contribution it's best to first create a report in the issue tracker to start a discussion on the subject. This often provides additional considerations and avoids unnecessary work.

Create an environment

Before you start coding, we recommend creating an isolated virtual environment to avoid any problems with your installed Python packages. This can easily be done via either virtualenv:

```
virtualenv <PATH TO VENV>
source <PATH TO VENV>/bin/activate
```

or Miniconda:

```
conda create -n pysubgroup python=3 six virtualenv pytest pytest-cov
conda activate pysubgroup
```

Clone the repository

- 1. Create an user account on GitHub if you do not already have one.
- 2. Fork the project repository: click on the *Fork* button near the top of the page. This creates a copy of the code under your account on GitHub.
- 3. Clone this copy to your local disk:

```
git clone git@github.com:YourLogin/pysubgroup.git
cd pysubgroup
```

4. You should run:

```
pip install -U pip setuptools -e .
```

to be able to import the package under development in the Python REPL.

5. Install pre-commit:

```
pip install pre-commit
pre-commit install
```

pysubgroup comes with a lot of hooks configured to automatically help the developer to check the code being written.

Implement your changes

1. Create a branch to hold your changes:

```
git checkout -b my-feature
```

and start making changes. Never work on the main branch!

- 2. Start your work on this branch. Don't forget to add docstrings to new functions, modules and classes, especially if they are part of public APIs.
- 3. Add yourself to the list of contributors in AUTHORS.rst.
- 4. When you're done editing, do:

```
git add <MODIFIED FILES>
```

```
git commit
```

to record your changes in git.

Please make sure to see the validation messages from pre-commit and fix any eventual issues. This should automatically use flake8/black to check/fix the code style in a way that is compatible with the project.

Important: Don't forget to add unit tests and documentation in case your contribution adds an additional feature and is not just a bugfix.

Moreover, writing a descriptive commit message is highly recommended. In case of doubt, you can check the commit history with:

git log --graph --decorate --pretty=oneline --abbrev-commit --all

to look for recurring communication patterns.

5. Please check that your changes don't break any unit tests with:

tox

(after having installed tox with pip install tox or pipx).

You can also use tox to run several other pre-configured tasks in the repository. Try tox -av to see a list of the available checks.

Submit your contribution

1. If everything works fine, push your local branch to the remote server with:

```
git push -u origin my-feature
```

2. Go to the web page of your fork and click "Create pull request" to send your changes for review.

Troubleshooting

The following tips can be used when facing problems to build or test the package:

- 1. Make sure to fetch all the tags from the upstream repository. The command git describe --abbrev=0 --tags should return the version you are expecting. If you are trying to run CI scripts in a fork repository, make sure to push all the tags. You can also try to remove all the egg files or the complete egg folder, i.e., .eggs, as well as the *.egg-info folders in the src folder or potentially in the root of your project.
- 2. Sometimes tox misses out when new dependencies are added, especially to setup.cfg and docs/ requirements.txt. If you find any problems with missing dependencies when running a command with tox, try to recreate the tox environment using the -r flag. For example, instead of:

tox -e docs

Try running:

tox -r -e docs

3. Make sure to have a reliable tox installation that uses the correct Python version (e.g., 3.7+). When in doubt you can run:

```
tox --version
# OR
which tox
```

If you have trouble and are seeing weird errors upon running tox, you can also try to create a dedicated virtual environment with a tox binary freshly installed. For example:

```
virtualenv .venv
source .venv/bin/activate
.venv/bin/pip install tox
.venv/bin/tox -e all
```

4. Pytest can drop you in an interactive session in the case an error occurs. In order to do that you need to pass a --pdb option (for example by running tox -- -k <NAME OF THE FALLING TEST> --pdb). You can also setup breakpoints manually instead of using the --pdb option.

1.3.4 Maintainer tasks

Releases

If you are part of the group of maintainers and have correct user permissions on PyPI, the following steps can be used to release a new version for pysubgroup:

- 1. Make sure all unit tests are successful.
- 2. Tag the current commit on the main branch with a release tag, e.g., v1.2.3.
- 3. Push the new tag to the upstream repository, e.g., git push upstream v1.2.3
- 4. Clean up the dist and build folders with tox -e clean (or rm -rf dist build) to avoid confusion with old builds and Sphinx docs.
- 5. Run tox -e build and check that the files in dist have the correct version (no .dirty or git hash) according to the git tag. Also check the sizes of the distributions, if they are too big (e.g., > 500KB), unwanted clutter may have been accidentally included.
- 6. Run tox -e publish -- -- repository pypi and check that everything was uploaded to PyPI correctly.

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1.5 Contributors

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1.6 Changelog

1.6.1 [0.7.6] - 2020-05-20

Some internal changes to the continuous integration pipeline on top of version 0.7.6.

1.6.2 [0.7.5] - 2020-05-20

Moved to pyscaffold, src/test structure and GitHub Actions.

1.6.3 [0.7.1] - 2020-05-20

Added

• you can now additionally provide constraints to SubgroupDiscovery

- MinSupportConstraint added

- you can now run the slow tests py passing --runslow to pytest
- Conjunction, Disjunction and Selectors now all have the public property .selectors that provides all basic selectors involved

Removed

• support for weights has been removed, it will probably be added in the future as seperate targets and Quality functions.

Changed

• create_numeric_selector_for_attribute has been renamed to create_numeric_selectors_for_attribute (inserting an s) This brings it in lign with the corresponding name shema for nominal.

Changed internally

- statistics are now also store along with score and description
- The function ps.get_cover_array_and_size was added, it allows for a consistent way to acces a cover array (a.k.a. sth to be thrown into a dataframe or a numpy array)
- algorithm tests now also call the to_subgroups and to_dataframe methods to check they work with that algorithm
- the order of calculate_statistics and get_base_statistics are now in lign with that of quality functions (first subgroup then data)
- the size of a subgroup specified in a statistics object is now called size_sg uniformly. This avoids confusion with the size attribute of numpy arrays etc.

1.6.4 [0.7.0] - 2020-04-24

This update prepares pysubgroup for a better future. To do so we had to break backwards compatibility. Many of the classes that you know and love have been renamed so as to make their purpose more clear.

Changed:

- SubgroupDescription is now called Conjunction
- NominalTarget is now called BinaryTarget
- algorithms now return a SubgroupDiscoveryResult object
- the structure of quality functions changed (see documentation for more info)

Added

- pysubgroup now has a bunch of tests
- some algorithms and quality functions support numba for just in time compilation
- ModelTarget
- gp-growth
- 3 types of Representations (bitset, set, numpy-set)
- Refinement operator
- Disjunction
- New algorithms

1.6.5 [0.6.2.1] - 2019-20-11

Added

- Apriori now has the option to disable numba using the use_numba flag
- SimpleSrach now has a progressbar (enabled via the show_progress=True flag)
- The number of quality function evaluations can now be tracked using the CountCallsInterestingMeasure as a wrapper
- · StandardQfNumeric now offers three different options to calculate the optimistic estimate
 - 'sum' (default) sums the values larger then the dataset mean (cf. Lemmerich 2014 p. 81 top)
 - 'average' uses the maximum target values as estimate (cf. Lemmerich 2014 p. 82 center)
 - 'order' uses ordering based bounds (cf. Lemmerich 2014 p. 89 bottom)

Bugfix

- Apriori now calculates the constant statistics before using representation
- DFS now properly works with any quality function

Improvements

- Apriori now reuses the compiled numba function
- Nominal target now uses subgroup.size to access the size of a subgroup representation
- · StaticSpecializationOperator now avoids checking refinements of the same attribute
- test_algorithms_numeric now checks more algorithms

1.6.6 [0.6.2] - 2019-31-10

Changed

- SubgroupDescription has been replaced with Conjunction
- Selector .covers function returns a numpy array instead of a pandas Series (speedup on dense data)
- Conjunction .selectors is renamed to Conjunction._selectors
- quality functions have a different interface
 - calculate_constant_statistics(self, task) caches necessary precomputation
 - calculate_statistics(self, subgroup, data=None) returns a namedtuple with necessary statistics
 - evaluate(self, subgroup, statistics=None) computes quality from provided statistics
 - optimistic_estimate(self, subgroup, statistics=None) computes optimistic estimate from provided statistics

•

Added

- Conjunction (replaces SubgroupDescription)
- Disjunction
- DNF (Disjunctive Normal Form)
- representations (given a dataset selectors are queried only once)
 - BitsetRepresentation
 - SetRepresentation
 - NumpySetRepresentation
- SimpleSearch algorithm
- DFS (Depth first search) using a representation for StandardQF
- tests
 - access to datasets for testing is provided through DataSets class
 - tests for selector classes (NominalSelector, NumericSelector)

- * ___eq___
- * __lt__
- * __hash__ similarity
- * uniqueness of selectors
- * cover function for NominalSelector
- tests for Conjunction, Disjuntion

* ___eq___

- * __lt__
- * __hash__ similarity
- * cover
- tests for algorithms with nominal target concept on the creditg dataset (StandardQF(1) + NominalSearchSpace, StandardQF(1)+Nominal&Numeric Searchspace, StandardQF(0.5)+Nominal&Numeric Searchspace)
 - * Apriori
 - * SimpleDFS
 - * BeamSearch
 - * DFS_bitset
 - * DFS_set
 - * DFS_numpy_sets
 - * SimpleSearch
- tests for algorithms with numeric target concept (StandardQFNumeric)
 - * Apriori
 - * SimpleDFS
 - * DFSNumeric
- tests for algorithm with fi target (CountQF)
 - * Apriori
 - * DFS
- tests for algorithms to find the best Disjunctions
 - * Apriori
 - * Generalising BFS

Improvements

• Apriori algorithm now runs significantly faster due to precomputing and usage of list comprehension

1.7 pysubgroup

1.7.1 pysubgroup package

Submodules

pysubgroup.algorithms module

Created on 29.04.2016

@author: lemmerfn

Bases: object

execute(task)

get_next_level(promising_candidates)

get_next_level_candidates(task, result, next_level_candidates)

get_next_level_candidates_vectorized(task, result, next_level_candidates)

get_next_level_numba(promising_candidates)

class pysubgroup.algorithms.BeamSearch(beam_width=20, beam_width_adaptive=False)
Bases: object

Implements the BeamSearch algorithm. Its a basic implementation

execute(task)

class pysubgroup.algorithms.BestFirstSearch

Bases: object

execute(task)

class pysubgroup.algorithms.DFS(apply_representation)

Bases: object

Implementation of a depth-first-search with look-ahead using a provided datastructure.

execute(task)

search_internal(task, result, sg)

class pysubgroup.algorithms.DFSNumeric

Bases: object

execute(task)

search_internal(task, prefix, modification_set, result, bitset)

tpl

alias of size_mean_parameters

class pysubgroup.algorithms.GeneralisingBFS

Bases: object

execute(task)

```
class pysubgroup.algorithms.SimpleDFS
```

Bases: object

execute(task, use_optimistic_estimates=True)

search_internal(task, prefix, modification_set, result, use_optimistic_estimates)

class pysubgroup.algorithms.SimpleSearch(show_progress=True)

Bases: object

execute(task)

Bases: object

Capsulates all parameters required to perform standard subgroup discovery

pysubgroup.algorithms.constraints_satisfied(constraints, subgroup, statistics=None, data=None)

pysubgroup.binary_target module

Created on 29.09.2017

@author: lemmerfn

Bases: BaseTarget

```
calculate_statistics(subgroup, data, cached_statistics=None)
```

covers(instance)

get_attributes()

get_base_statistics(subgroup, data)

```
statistic_types = ('size_sg', 'size_dataset', 'positives_sg', 'positives_dataset',
'size_complement', 'relative_size_sg', 'relative_size_complement', 'coverage_sg',
'coverage_complement', 'target_share_sg', 'target_share_complement',
'target_share_dataset', 'lift')
```

```
class pysubgroup.binary_target.ChiSquaredQF(direction='both', min_instances=5, stat='chi2')
Bases: SimplePositivesQF
```

ChiSquaredQF which test for statistical independence of a subgroup against it's complement

•••

Performs chi2 test of statistical independence

Test whether a subgroup is statistically independent from it's complement (see scipy.stats.chi2_contingency).

Parameters

instances_dataset -

positives_dataset, instances_subgroup, positives_subgroup : int

counts of subgroup and dataset

:param

[positives_dataset,]

instances_subgroup, positives_subgroup : int

counts of subgroup and dataset

Parameters

- **min_instances** (*int*, *optional*) number of required instances, if less -inf is returned for that subgroup
- **bidirect** (*bool*, *optional*) If true both directions are considered interesting else direction_positive decides which direction is interesting
- **direction_positive** (*bool*, *optional*) Only used if bidirect=False; specifies whether you are interested in positive (True) or negative deviations
- **index** ({0, 1}, optional) decides whether the test statistic (0) or the p-value (1) should be used

evaluate(subgroup, target, data, statistics=None)

class pysubgroup.binary_target.GeneralizationAware_StandardQF(a)

Bases: GeneralizationAwareQF_stats

evaluate(subgroup, target, data, statistics=None)

get_max(*args)

class pysubgroup.binary_target.LiftQF

Bases: StandardQF

Lift Quality Function

LiftQF is a StandardQF with a=0. Thus it treats the difference in ratios as the quality without caring about the relative size of a subgroup.

class pysubgroup.binary_target.SimpleBinomialQF

Bases: StandardQF

Simple Binomial Quality Function

SimpleBinomialQF is a StandardQF with a=0.5. It is an order equivalent approximation of the full binomial test if the subgroup size is much smaller than the size of the entire dataset.

class pysubgroup.binary_target.SimplePositivesQF

Bases: AbstractInterestingnessMeasure

calculate_constant_statistics(data, target)

calculate_statistics(subgroup, target, data, statistics=None)

gp_get_null_vector()

gp_get_params(_cover_arr, v)

gp_get_stats(row_index)

gp_merge(left, right)

property gp_requires_cover_arr

gp_size_sg(stats)

gp_to_str(stats)

tpl

alias of PositivesQF_parameters

class pysubgroup.binary_target.StandardQF(a)

Bases: SimplePositivesQF, BoundedInterestingnessMeasure

StandardQF which weights the relative size against the difference in averages

The StandardQF is a general form of quality function which for different values of a is order equivalen to many popular quality measures.

a

used as an exponent to scale the relative size to the difference in averages

Type float

evaluate(subgroup, target, data, statistics=None)

optimistic_estimate(subgroup, target, data, statistics=None)

optimistic_generalisation(subgroup, target, data, statistics=None)

static standard_qf(a, instances_dataset, positives_dataset, instances_subgroup, positives_subgroup)

class pysubgroup.binary_target.WRAccQF

Bases: StandardQF

Weighted Relative Accuracy Quality Function

WRAccQF is a StandardQF with a=1. It is order equivalent to the difference in the observed and expected number of positive instances.

pysubgroup.constraints module

class pysubgroup.constraints.MinSupportConstraint(min_support)

Bases: object

gp_is_satisfied(node)

gp_prepare(qf)

property is_monotone

is_satisfied(subgroup, statistics=None, data=None)

pysubgroup.datasets module

pysubgroup.datasets.get_credit_data()

pysubgroup.datasets.get_titanic_data()

pysubgroup.fi_target module

Created on 29.09.2017

@author: lemmerfn

class pysubgroup.fi_target.AreaQF

Bases: SimpleCountQF

evaluate(subgroup, target, data, statistics=None)

class pysubgroup.fi_target.CountQF

 $Bases: \ Simple Count QF, \ Bounded Interesting ness Measure$

evaluate(subgroup, target, data, statistics=None)

optimistic_estimate(subgroup, target, data, statistics=None)

class pysubgroup.fi_target.FITarget

Bases: BaseTarget

calculate_statistics(subgroup_description, data, cached_statistics=None)

get_attributes()

get_base_statistics(subgroup, data)

statistic_types = ('size_sg', 'size_dataset')

class pysubgroup.fi_target.SimpleCountQF

Bases: AbstractInterestingnessMeasure

calculate_constant_statistics(data, target)

calculate_statistics(subgroup_description, target, data, statistics=None)

gp_get_null_vector()

```
gp_get_params(_cover_arr, v)
     gp_get_stats(_)
     gp_merge(left, right)
     gp_requires_cover_arr = False
     gp_size_sg(stats)
     gp_to_str(stats)
     tpl
          alias of CountQF_parameters
pysubgroup.gp_growth module
class pysubgroup.gp_growth.GpGrowth(mode='b_u')
     Bases: object
     add_if_required(prefix, gp_stats)
     calculate_quality_function_for_patterns(task, results, arrs)
     check_constraints(node)
     check_tree_is_ordered(root, prefix=None)
          Verify that the nodes of a tree are sorted in ascending order
     convert_results_to_subgroups(results, selectors_sorted)
     create_copy_of_path(nodes, new nodes, stats)
     create_copy_of_tree_top_down(from_root, nodes=None, parent=None, is_valid_class=None)
     create_initial_tree(arrs)
     create_new_tree_from_nodes(nodes)
     execute(task)
     get_nodes_upwards(node)
     get_stats_for_class(cls_nodes)
     get_top_down_tree_for_class(cls_nodes, cls, is_valid_class)
     merge_trees_top_down(nodes, mutable_root, from_root, is_valid_class)
     nodes_to_cls_nodes(nodes)
     normal_insert(root, nodes, new_stats, classes)
     prepare_selectors(search_space, data)
     recurse(cls_nodes, prefix, is_single_path=False)
     recurse_top_down(cls_nodes, root, depth_in=0)
```

```
remove_selectors_with_low_optimistic_estimate(s, search_space_size)
```

setup(task)

```
setup_constraints(constraints, qf)
```

setup_from_quality_function(qf)

to_file(task, path)

pysubgroup.gp_growth.identity(x, *args, **kwargs)

pysubgroup.measures module

Created on 28.04.2016

@author: lemmerfn

class pysubgroup.measures.AbstractInterestingnessMeasure
 Bases: ABC

ensure_statistics(subgroup, target, data, statistics=None)

- class pysubgroup.measures.BoundedInterestingnessMeasure
 Bases: AbstractInterestingnessMeasure
- class pysubgroup.measures.CombinedInterestingnessMeasure(measures, weights=None)
 Bases: BoundedInterestingnessMeasure

calculate_constant_statistics(data, target)

calculate_statistics(subgroup, target, data, cached_statistics=None)

evaluate(subgroup, target, data, statistics=None)

optimistic_estimate(subgroup, target, data, statistics=None)

class pysubgroup.measures.CountCallsInterestingMeasure(qf)
 Bases: BoundedInterestingnessMeasure

calculate_statistics(sg, target, data, statistics=None)

```
class pysubgroup.measures.GeneralizationAwareQF(qf)
```

Bases: AbstractInterestingnessMeasure

calculate_constant_statistics(data, target)

calculate_statistics(subgroup, target, data, statistics=None)

evaluate(subgroup, target, data, statistics=None)

class ga_tuple(subgroup_quality, generalisation_quality)
Bases: tuple

generalisation_quality

Alias for field number 1

subgroup_guality Alias for field number 0 get_qual_and_previous_qual(subgroup, target, data) class pysubgroup.measures.GeneralizationAwareQF_stats(qf) Bases: AbstractInterestingnessMeasure calculate_constant_statistics(data, target) calculate_statistics(subgroup, target, data, statistics=None) evaluate(subgroup, target, data, statistics=None) ga_tuple alias of ga_stats_tuple get_max(*args) get_stats_and_previous_stats(subgroup, target, data) pysubgroup.measures.maximum_statistic_filter(result_set, statistic, maximum) pysubgroup.measures.minimum_quality_filter(result_set, minimum) pysubgroup.measures.minimum_statistic_filter(result_set, statistic, minimum, data) pysubgroup.measures.overlap_filter(result_set, data, similarity_level=0.9) pysubgroup.measures.overlaps_list(sg, list_of_sgs, data, similarity_level=0.9) pysubgroup.measures.unique_attributes(result_set, data)

pysubgroup.model_target module

class pysubgroup.model_target.EMM_Likelihood(model)
Bases: AbstractInterestingnessMeasure
calculate_constant_statistics(data, target)
calculate_statistics(subgroup, target, data, statistics=None)
evaluate(subgroup, target, data, statistics=None)
get_tuple(sg_size, params, cover_arr)
gp_get_params(cover_arr, v)
property gp_requires_cover_arr
tpl
alias of EMM_Likelihood

class pysubgroup.model_target.PolyRegression_ModelClass(x_name='x', y_name='y', degree=1)
Bases: object

calculate_constant_statistics(data, target)

fit(subgroup, data=None)

gp_get_null_vector()

gp_get_params(v)

gp_get_stats(row_index)

static gp_merge(u, v)

property gp_requires_cover_arr

gp_size_sg(stats)

gp_to_str(stats)

likelihood(stats, sg)

loglikelihood(stats, sg)

class pysubgroup.model_target.beta_tuple(beta, size_sg)

Bases: tuple

beta

Alias for field number 0

size_sg

Alias for field number 1

pysubgroup.numeric_target module

Created on 29.09.2017

@author: lemmerfn

class pysubgroup.numeric_target.NumericTarget(target_variable)

Bases: object

```
calculate_statistics(subgroup, data, cached_statistics=None)
```

get_attributes()

get_base_statistics(subgroup, data)

```
statistic_types = ('size_sg', 'size_dataset', 'mean_sg', 'mean_dataset', 'std_sg',
'std_dataset', 'median_sg', 'median_dataset', 'max_sg', 'max_dataset', 'min_sg',
'min_dataset', 'mean_lift', 'median_lift')
```

class pysubgroup.numeric_target.StandardQFNumeric(a, invert=False, estimator='sum')
Bases: BoundedInterestingnessMeasure

```
class Average_Estimator(qf)
Bases: object
calculate_constant_statistics(data, target)
get_data(data, target)
```

get_estimate(subgroup, sg_size, sg_mean, cover_arr, _)

```
class Ordering_Estimator(af)
          Bases: object
          calculate_constant_statistics(data, target)
          get_data(data, target)
          get_estimate(subgroup, sg_size, sg_mean, cover_arr, target_values_sg)
          get_estimate_numpy(values_sg, _, mean_dataset)
     class Summation_Estimator(qf)
          Bases: object
          calculate_constant_statistics(data, target)
          get_data(data, target)
          get_estimate(subgroup, sg_size, sg_mean, cover_arr, _)
     calculate_constant_statistics(data, target)
     calculate_statistics(subgroup, target, data, statistics=None)
     evaluate(subgroup, target, data, statistics=None)
     optimistic_estimate(subgroup, target, data, statistics=None)
     static standard_qf_numeric(a, _, mean_dataset, instances_subgroup, mean_sg)
     tpl
          alias of StandardQFNumeric_parameters
class pysubgroup.numeric_target.StandardQFNumericMedian(a, invert=False, estimator='sum')
     Bases: BoundedInterestingnessMeasure
     class Average_Estimator(qf)
          Bases: object
          calculate_constant_statistics(data, target)
          get_data(data, target)
          get_estimate(subgroup, sg_size, sg_mean, cover_arr, _)
     class Ordering_Estimator(qf)
          Bases: object
          calculate_constant_statistics(data, target)
          get_data(data, target)
          get_estimate(subgroup, sg_size, sg_mean, cover_arr, target_values_sg)
          get_estimate_numpy(values_sg, _, mean_dataset)
```

class Summation_Estimator(qf)

Bases: object

calculate_constant_statistics(data, target)

get_data(data, target)

get_estimate(subgroup, sg_size, sg_median, cover_arr, _)

calculate_constant_statistics(data, target)

calculate_statistics(subgroup, target, data, statistics=None)

evaluate(subgroup, target, data, statistics=None)

optimistic_estimate(subgroup, target, data, statistics=None)

static standard_qf_numeric(a, _, median_dataset, instances_subgroup, median_sg)

tpl

alias of StandardQFNumericMedian_parameters

class pysubgroup.numeric_target.StandardQFNumericTscore(a, invert=False, estimator='sum')
Bases: BoundedInterestingnessMeasure

class Average_Estimator(qf)

Bases: object

calculate_constant_statistics(data, target)

get_data(data, target)

get_estimate(subgroup, sg_size, sg_mean, cover_arr, _)

class Ordering_Estimator(qf)

Bases: object

calculate_constant_statistics(data, target)

get_data(data, target)

get_estimate(subgroup, sg_size, sg_mean, cover_arr, target_values_sg)

get_estimate_numpy(values_sg, _, mean_dataset)

class Summation_Estimator(qf)

Bases: object

calculate_constant_statistics(data, target)

get_data(data, target)

get_estimate(subgroup, sg_size, sg_mean, cover_arr, _)

calculate_constant_statistics(data, target)

calculate_statistics(subgroup, target, data, statistics=None)

evaluate(subgroup, target, data, statistics=None)

optimistic_estimate(subgroup, target, data, statistics=None)

static standard_qf_numeric(*a*, _, *mean_dataset*, *instances_subgroup*, *mean_sg*, *std_sg*)

tpl

alias of StandardQFNumericTscore_parameters

pysubgroup.refinement_operator module

class pysubgroup.refinement_operator.RefinementOperator

Bases: object

class pysubgroup.refinement_operator.StaticGeneralizationOperator(selectors)
 Bases: object

refinements(sG)

class pysubgroup.refinement_operator.StaticSpecializationOperator(selectors) Bases: object

refinements(subgroup)

pysubgroup.representations module

class pysubgroup.representations.BitSetRepresentation(df, selectors_to_patch)

Bases: RepresentationBase

Conjunction

alias of BitSet_Conjunction

Disjunction

alias of BitSet_Disjunction

patch_classes()

patch_selector(sel)

class pysubgroup.representations.BitSet_Conjunction(*args, **kwargs)

Bases: Conjunction

append_and(to_append)

compute_representation()

n_instances = 0

property size_sg

class pysubgroup.representations.BitSet_Disjunction(*args, **kwargs)

Bases: Disjunction

append_or(to_append)

compute_representation()

property size_sg

class pysubgroup.representations.NumpySetRepresentation(df, selectors_to_patch) Bases: RepresentationBase

Conjunction

alias of NumpySet_Conjunction

patch_classes()

patch_selector(sel)

class pysubgroup.representations.NumpySet_Conjunction(*args, **kwargs)

Bases: Conjunction

all_set = None

append_and(to_append)

compute_representation()

property size_sg

class pysubgroup.representations.RepresentationBase(new_conjunction, selectors_to_patch)
Bases: object

patch_all_selectors()

patch_classes()

patch_selector(sel)

undo_patch_classes()

class pysubgroup.representations.SetRepresentation(df, selectors_to_patch)
Bases: RepresentationBase

Conjunction

alias of Set_Conjunction

patch_classes()

patch_selector(sel)

class pysubgroup.representations.Set_Conjunction(*args, **kwargs)

Bases: Conjunction

all_set = {}

append_and(to_append)

compute_representation()

property size_sg

pysubgroup.subgroup_description module

Created on 28.04.2016 @author: lemmerfn class pysubgroup.subgroup_description.BooleanExpressionBase Bases: ABC abstract append_and(to_append) abstract append_or(to_append)

class pysubgroup.subgroup_description.Conjunction(selectors)

Bases: BooleanExpressionBase

append_and(to_append)

append_or(to_append)

covers(instance)

property depth

static from_str(s)

pop_and()

pop_or()

property selectors

class pysubgroup.subgroup_description.DNF(selectors=None)

Bases: Disjunction

append_and(to_append)

append_or(to_append)

pop_and()

class pysubgroup.subgroup_description.Disjunction(selectors=None)

Bases: BooleanExpressionBase

append_and(to_append)

append_or(to_append)

covers(instance)

property selectors

class pysubgroup.subgroup_description.EqualitySelector(*args, **kwargs)

Bases: SelectorBase

property attribute_name

property attribute_value

classmethod compute_descriptions(attribute_name, attribute_value, selector_name)

covers(data)

static from_str(s)

property selectors

set_descriptions(attribute_name, attribute_value, selector_name=None)

class pysubgroup.subgroup_description.IntervalSelector(*args, **kwargs)

Bases: SelectorBase

property attribute_name

classmethod compute_string(attribute_name, lower_bound, upper_bound, rounding_digits)

covers(data_instance)

static from_str(s)

property lower_bound

property selectors

set_descriptions(attribute_name, lower_bound, upper_bound, selector_name=None)

property upper_bound

class pysubgroup.subgroup_description.NegatedSelector(*args, **kwargs)

Bases: SelectorBase

property attribute_name

covers(data_instance)

property selectors

set_descriptions(selector)

class pysubgroup.subgroup_description.SelectorBase(*args, **kwargs)
Bases: ABC

abstract set_descriptions(*args, **kwargs)

pysubgroup.subgroup_description.create_nominal_selectors(data, ignore=None)

intervals_only=True, weighting_attribute=None)

pysubgroup_description.create_selectors(*data*, *nbins*=5, *intervals_only=True*, *ignore=None*)

pysubgroup.subgroup_description.get_cover_array_and_size(subgroup, data_len=None, data=None)

pysubgroup.subgroup_description.get_size(subgroup, data_len=None, data=None)

pysubgroup.subgroup_description.remove_target_attributes(selectors, target)

pysubgroup.utils module

Created on 02.05.2016

@author: lemmerfn

class pysubgroup.utils.BaseTarget

Bases: object

all_statistics_present(cached_statistics)

class pysubgroup.utils.SubgroupDiscoveryResult(results, task)

Bases: object

to_dataframe(statistics_to_show=None, autoround=False, include_target=False)

to_descriptions(include_stats=False)

to_latex(statistics_to_show=None)

to_table(statistics_to_show=None, print_header=True, include_target=False)

Important: Only add/remove subgroups from *result* by using *heappop* and *heappush* to ensure order of subgroups by quality.

pysubgroup.utils.conditional_invert(val, invert)

pysubgroup.utils.count_bits(bitset_as_int)

pysubgroup.utils.derive_effective_sample_size(weights)

pysubgroup.utils.find_set_bits(bitset_as_int)

pysubgroup.utils.float_formatter(x, digits=2)

pysubgroup.utils.intersect_of_ordered_list(list_1, list_2)

pysubgroup.utils.is_categorical_attribute(data, attribute_name)

pysubgroup.utils.is_numerical_attribute(data, attribute_name)

pysubgroup.utils.minimum_required_quality(result, task)

pysubgroup.utils.overlap(sg, another_sg, data)

pysubgroup.utils.perc_formatter(x)

pysubgroup.utils.powerset([1,2,3]) --> () (1,) (2,) (3,) (1,2) (1,3) (2,3) (1,2,3)

pysubgroup.utils.prepare_subgroup_discovery_result(result, task)

pysubgroup.utils.remove_selectors_with_attributes(selector_list, attribute_list)

pysubgroup.utils.results_df_autoround(df)

pysubgroup.utils.to_bits(list_of_ints)

pysubgroup.visualization module

pysubgroup.visualization.compare_distributions_numeric(sgs, data, bins)

pysubgroup.visualization.plot_distribution_numeric(sg, data, bins)

pysubgroup.visualization.plot_npspace(result_df, data, annotate=True, fixed_limits=False)

pysubgroup.visualization.similarity_dendrogram(result, data)

pysubgroup.visualization.similarity_sgs(sgd_results, data, color=True)

pysubgroup.visualization.supportSetVisualization(result, in_order=True, drop_empty=True)

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