caspo Documentation

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Contents

CHAPTER 1

Install

In what follows we describe three alternative ways to install **caspo**:

- *Using Docker*
- *Using Anaconda*
- *Using pip*

Note that using pip requires the user to install all dependencies manually. Since installing such dependecies requires basic skills on how to compile and deploy third-party python packages it is only recommended for experienced users. Therefore, we recommend less experienced users to use either Docker or Anaconda.

1.1 Using Docker

Follow the instructions to install Docker at http://docs.docker.com. Once you have installed Docker on your computer, you can use the **caspo** docker image as follows. First you need to pull the image with:

```
$ docker pull bioasp/caspo
```

That's it. Now, you should be able to run **caspo** with docker. Usually, **caspo** will need to read and writes files to do their work. A possible way to this using docker is as follows. For safety, we recommend to use an empty directory:

```
$ mkdir caspo-wd && cd caspo-wd
```

Next, let's take a look to the command needed to run docker, mount the current directory (*caspo-wd*) into the docker container, and use it as the working directory for running **caspo**:

```
$ docker run --rm -v $PWD:/caspo-wd -w /caspo-wd bioasp/caspo
```

If you don't want to write the full docker command every time you run **caspo**, you may want to create a shell script or alias as a shortcut. For example, you may want to create a file in your working directory named *caspo* and with the following content:

```
#!/bin/sh
docker run --rm -v $PWD:/caspo-wd -w /caspo-wd bioasp/caspo $@
```

Next, make the file executable:

```
$ chmod a+x caspo
```

Now you can run **caspo** with just:

```
$ ./caspo
```

Next, go to *Testing your installation*.

1.2 Using Anaconda

NOTE: In order for this method to work, the standard C/C++ libraries must be installed in your system. In Linux you need to have gcc >= 4.9 while in OS X 10.9+ you need to install Xcode and the command line tools.

Follow the instructions to install Anaconda at https://www.continuum.io/downloads. Next, download the file `environment.yml` and use it to create a conda environment where **caspo** will be installed:

```
$ conda env create --file environment.yml
Using Anaconda Cloud api site https://api.anaconda.org
Fetching package metadata ...............
Solving package specifications: ..........
...
Linking packages ...
[      COMPLETE      ]|##################################################| 100%
#
# To activate this environment, use:
# $ source activate caspo-env
#
# To deactivate this environment, use:
# $ source deactivate
#
```

That's it. Now, you should be able to run **caspo** within the created environment. Note that you need to *activate* the environment every time you open a new terminal.

Next, go to *Testing your installation*.

1.3 Using pip

NOTE: Depending on your platform and whether you decide to use the system's python or a virtual environment, this method may require you to install additional compilers and libraries beforehand.

Essentially, you will need to have python 3.x and some of the standard scientific python packages installed. Download the file `requirements.txt` and install **caspo** by running:

```
$ pip install -r requirements.txt
```

Alternatively, you could download **caspo** sources and after unpacking run:

```
$ python setup.py install
```

Note that installing **caspo** in this way **does not** force the installation of any of the runtime dependencies. In other words, you take full responsibility of installing all required packages to run **caspo** successfully.

Also, the python module of the answer set programming solver clingo must be available in the PYTHONPATH. After unpacking clingo sources, you will find detailed instructions about how to compile and build the python module in the INSTALL file.

Next, go to *Testing your installation*.

1.4 Testing your installation

Once **caspo** is installed you can test the installation as follows. To start with, you can ask for help:

```
$ caspo --help
usage: caspo [-h] [--quiet] [--out O] [--version]
             {learn,classify,predict,design,control,visualize,test} ...

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optional arguments:
  -h, --help            show this help message and exit
  --quiet               do not print anything to standard output
  --out O               output directory path (Default to './out')
  --version             show program's version number and exit

caspo subcommands:
  for specific help on each subcommand use: caspo {cmd} --help

  {learn,classify,predict,design,control,visualize,test}
```

A more interesting test is to run **caspo test** to make sure all subcommands are working:

```
$ caspo test --help
usage: caspo test [-h] [--threads T] [--conf C]
                  [--testcase {Toy,LiverToy,LiverDREAM,ExtLiver}]

optional arguments:
  -h, --help            show this help message and exit
  --threads T           run clingo with given number of threads
  --conf C              threads configurations (Default to many)
  --testcase {Toy,LiverToy,LiverDREAM,ExtLiver}
                        testcase name
```

This subcommand will run all subcommands in **caspo** using different testcases (see `--testcase` argument):

```
$ caspo test

Testing caspo subcommands using test case Toy.

Copying files for running tests:
  Prior knowledge network: pkn.sif
  Phospho-proteomics dataset: dataset.csv
  Experimental setup: setup.json
```

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```
  Intervention scenarios: scenarios.csv

$ caspo --out out learn out/pkn.sif out/dataset.csv 10 --fit 0.1 --size 5

Optimum logical network learned in 0.0183s
Optimum logical networks has MSE 0.1100 and size 7
5 (nearly) optimal logical networks learned in 0.0082s
Weighted MSE: 0.1100

$ caspo --out out classify out/networks.csv out/setup.json out/dataset.csv 10

Classifying 5 logical networks...
3 input-output logical behaviors found in 0.2029s
Weighted MSE: 0.1100

$ caspo --out out design out/behaviors.csv out/setup.json

1 optimal experimental designs in 0.0043s

$ caspo --out out predict out/behaviors.csv out/setup.json

Computing all predictions and their variance for 3 logical networks...

$ caspo --out out control out/networks.csv out/scenarios.csv

3 optimal intervention strategies found in 0.0047s

$ caspo --out out visualize --pkn out/pkn.sif --setup out/setup.json
        --networks out/networks.csv --midas out/dataset.csv 10
        --stats-networks=out/stats-networks.csv --behaviors out/behaviors.csv
        --designs=out/designs.csv --predictions=out/predictions.csv
        --strategies=out/strategies.csv --stats-strategies=out/stats-strategies.csv
```

If everything works as expected, you should find a directory named *out* in the current directory having all the output files generated by **caspo**.

CHAPTER 2

Usage

2.1 Input/Output files

Input and output files in **caspo** are mostly comma separated values (csv) files. Next, we describe all files either consumed or produced when running **caspo** subcommands.

2.1.1 Prior knowledge network

A prior knowledge network (PKN) is given using the simple interaction format (SIF). Lines in the SIF file must specify a source node, an edge sign (1 or -1), and one target node. Note that SIF format specification also consider several target nodes per line but this is not supported in **caspo** at the moment. In the example shown below we would say that *a* and *b* have a positive influence over *d* while *c* has a negative influence over *d*.

a	1	d
b	1	d
c	-1	d
b	1	e
c	1	e

2.1.2 Experimental setup

An experimental setup is given using the JSON format. The JSON file must specify three list of node names, namely, *stimuli*, *inhibitors*, and *readouts*. In the following example, *a*, *b*, and *c* are stimuli, *d* is an inhibitor while *f* and *g* are readouts.

```
{
  "stimuli": ["a", "b", "c"],
  "inhibitors": ["d"],
  "readouts": ["f", "g"]
}
```

2.1.3 Experimental dataset

A phospho-proteomics dataset is given using the MIDAS format. Notably, MIDAS format considers time-series data but as we will see later, **caspo** always requires the user to define the time-point of interest when reading a MIDAS file (see *Learn*). Different time-points of *data acquisition* are specified in columns with prefix DA:.

In the example shown below, looking at the third row we would say that, when *a* and *c* are present, i.e. stimulated, and *d* is not inhibited, i.e., the inhibitor of *d* is not present, readouts for *f* and *g* at time-point 10 are 0.9 and 0, respectively. Meanwhile, looking at the four row we would say that when *a* and *c* are present and *d* is inhibited (the inhibitor of *d* it is present), readouts for *f* and *g* at time-point 10 are 0.1 and 0.9, respectively.

TR:Toy:CellLine	TR:a	TR:b	TR:c	TR:di	DA:f	DA:g	DV:f	DV:g
1	1	0	1	0	0	0	0	0
1	1	0	1	1	0	0	0	0
1	1	0	1	0	10	10	0.9	0
1	1	0	1	1	10	10	0.1	0.9

2.1.4 Logical networks

Logical networks are given using a csv file as follows. We assume that every logical mapping in a given network is in disjunctive normal form (DNF). Thus, columns header specify all possible conjunctions targeting any given node, e.g. *d<-a+!c* (*d equals a AND NOT c*). Then, each row describes a logical network by specifying which conjunctions are present (1) in the network or not (0). Whenever, two conjunctions targeting the same node are present in a given network they are connected using OR. For example, if we look at the first row in the example below, since *d<-a* and *d<-b+!c* are both present, the complete logical mapping for *d* would be: *d equals a OR (b AND NOT c)*.

Additional columns could be included to give more details related to each network, e.g., MSE, size, or the number of networks having the same input-output behavior. See the output csv files in subcommands *Learn* (*networks.csv*) or *Classify* (*behaviors.csv*). However, when parsing a csv file of logical networks, **caspo** ignores columns that cannot be parsed as logical mappings except for a column named *networks* which is interpreted as the number of networks exhibiting the same input-output behavior (including the representative network being parsed). In particular, such a column will be relevant when computing weighted average predictions (see *Predict*).

e<-c	e<-b	d<-a	d<-!c	d<-b	d<-a+!c	d<-b+!c	f<-d+e
1	1	1	0	0	0	1	0
1	1	1	1	0	0	0	0
1	1	1	0	1	0	1	0
1	1	1	1	1	0	0	0
1	1	1	0	0	0	1	0

Basic statistics over a family of logical networks are described using a csv file as follows. For each logical mapping conjunction we compute its frequency of occurrence over all logical networks in the family. Also, mutually exclusive/inclusive pairs of mapping conjunctions are identified.

mapping	frequency	exclusive	inclusive
e<-c	1.0000		
e<-b	1.0000		
d<-a	1.0000		
d<-b+!c	0.6000	d<-!c	
d<-!c	0.4000	d<-b+!c	
d<-b	0.4000		

2.1.5 Experimental designs

An experimental design is essentially a set of experimental perturbations, i.e., various combinations of stimuli and inhibitors. But also, we describe an experimental design by how its perturbations discriminate the family of input-output behaviors (see *Design* for an example visualization). Experimental designs are given using a csv file as shown below. A column named *id* is used to identify rows corresponding to the same experimental design. Next, columns with prefix TR: correspond to experimental perturbations in the same way as in MIDAS format. Finally, for each combination of stimuli and inhibitors in a given experimental design, we count pairwise differences generated over specific readouts (columns with prefix DIF:) and pairs of behaviors being discriminated by at least one readout (column named *pairs*).

In the example below we show one experimental design made of two experimental perturbations. The first perturbation requires *b* and *c* to be stimulated, it generates 2 pairwise differences over *f*, and it discriminates 2 pairs of behaviors. The second perturbation requires *b* to be stimulated and *d* to be inhibited, it generates 1 pairwise difference over *f*, 1 pairwise difference over *g*, and it discriminates 1 pair of behaviors.

id	TR:a	TR:b	TR:c	TR:di	DIF:f	DIF:g	pairs
0	0	1	1	0	2	0	2
0	0	1	0	1	1	1	1

2.1.6 Logical predictions

Based on the input-output classification (see *Classify*), we can compute the response of the system for every possible perturbation by combining the ensemble of predictions from all input-output behaviors. Thus, predictions of a logical networks family are given using a csv file as the (incomplete) example below. For each possible combination of stimuli and inhibitors (columns with prefix TR:), the prediction for any readout node will be the weighted average (columns with prefix AVG:) over the predictions from all input-output behaviors and where each weight corresponds to the number of networks exhibiting the corresponding behavior. Also, the mean variance over all predictions is computed (columns with prefix VAR:). See *Predict* for an example visualization of readout mean variances.

TR:a	TR:c	TR:b	TR:di	AVG:g	AVG:f	VAR:g	VAR:f
1	0	0	0	0.0	0.0	0.0	0.0
0	1	0	0	0.0	0.0	0.0	0.0
0	0	1	0	1.0	0.8	0.0	0.16
0	1	1	0	0.0	0.4	0.0	0.24

2.1.7 Intervention scenarios

An intervention scenario is simply a pair of constraints and goals over nodes in a logical network. Thus, intervention scenarios are given using a csv file as shown below. Each column specifies either a *scenario constraint* (SC:) or a *scenario goal* (SG:) over any node in the network. Next, each row in the file describes a different intervention scenario. Values can be either 1 for active, -1 for inactive, or 0 for neither active nor inactive. That is, a 0 means there are no constraint nor expectation over that node in the corresponding scenario.

In the example below, we show two intervention scenarios. The first scenario requires that both, *f* and *g* to reach the inactive state under the constraint of *a* being active. The second scenario required only *f* to reach the active state under no constraints.

SC:a	SG:f	SG:g
1	-1	-1
0	1	0

2.1.8 Intervention strategies

An intervention strategy is a set of Boolean interventions over nodes in a logical network. Thus, intervention strategies are given using a csv file as shown below. Each column specifies a Boolean intervention over a given node (prefix TR: is used for consistency with MIDAS and other csv files). Next, each row in the file describes a different intervention strategy. Values can be either 1 for active, -1 for inactive, or 0 for neither active nor inactive. That is, a 0 means there is no intervention over that node in the corresponding strategy.

TR:c	TR:b	TR:e	TR:d
0	0	-1	0
-1	-1	0	0
1	0	0	-1

Basic statistics over a set of intervention strategies are described using a csv file as follows. For each Boolean intervention we compute its frequency of occurrence over all strategies in the set. Also, mutually exclusive/inclusive pairs of interventions are identified.

intervention	frequency	exclusive	inclusive
c=-1	0.3333		b=-1
c=1	0.3333		d=-1
b=-1	0.3333		c=-1
e=-1	0.3333		
d=-1	0.3333		c=1

2.2 Command Line Interface

The command line interface (CLI) of **caspo** offers various subcommands:

- *learn*: for learning a family of (nearly) optimal logical networks
- *classify*: for classifying a family of networks wrt their I/O behaviors
- *design*: for designing experiments to discriminate a family of I/O behaviors
- *predict*: for predicting based on a family of networks and I/O behaviors
- *control*: for controlling a family of logical networks in several intervention scenarios
- *visualize*: for basic visualization of the subcommands outputs
- *test*: for running all subcommands using various examples

Next, we will see how to run each subcommand and describe their outputs.

If you haven't done it yet, start by asking **caspo** for help:

```
$ caspo --help
usage: caspo [-h] [--quiet] [--out O] [--version]
             {learn,classify,predict,design,control,visualize,test} ...

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optional arguments:
  -h, --help            show this help message and exit
  --quiet               do not print anything to standard output
  --out O               output directory path (Default to './out')
```

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```
  --version             show program's version number and exit

caspo subcommands:
  for specific help on each subcommand use: caspo {cmd} --help

  {learn,classify,predict,design,control,visualize,test}
```

2.2.1 Learn

This subcommand implements the learning of logical networks given a prior knowledge network and a phospho-proteomics dataset [1, 2]. In order to account for the noise in experimental data, a percentage of tolerance with respect to the maximum fitness can be used, e.g., we use 4% in the example below. Analogously, in order to relax the parsimonious principle a tolerance with respect to the minimum size (networks complexity) can be used as well. Further, other arguments allow for controlling the data discretization or the maximum number of inputs per AND gate.

Help on **caspo learn**:

```
$ caspo learn --help
usage: caspo learn [-h] [--threads T] [--conf C] [--fit F] [--size S]
                   [--factor D] [--discretization T] [--length L]
                   pkn midas time

positional arguments:
  pkn                 prior knowledge network in SIF format
  midas               experimental dataset in MIDAS file
  time                time-point to be used in MIDAS

optional arguments:
  -h, --help          show this help message and exit
  --threads T         run clingo with given number of threads
  --conf C            threads configurations (Default to many)
  --optimum O         logical network in CSV format. If many networks are
                      given, the first network is used (If given, avoids
                      learning the optimum and go directly to enumeration)
  --fit F             tolerance over fitness (Default to 0)
  --size S            tolerance over size (Default to 0)
  --factor D          discretization over [0,D] (Default to 100)
  --discretization T  discretization function: round, floor, ceil (Default to
                      round)
  --length L          max conjunctions length (sources per hyperedges)
                      (Default to 0; unbounded)
```

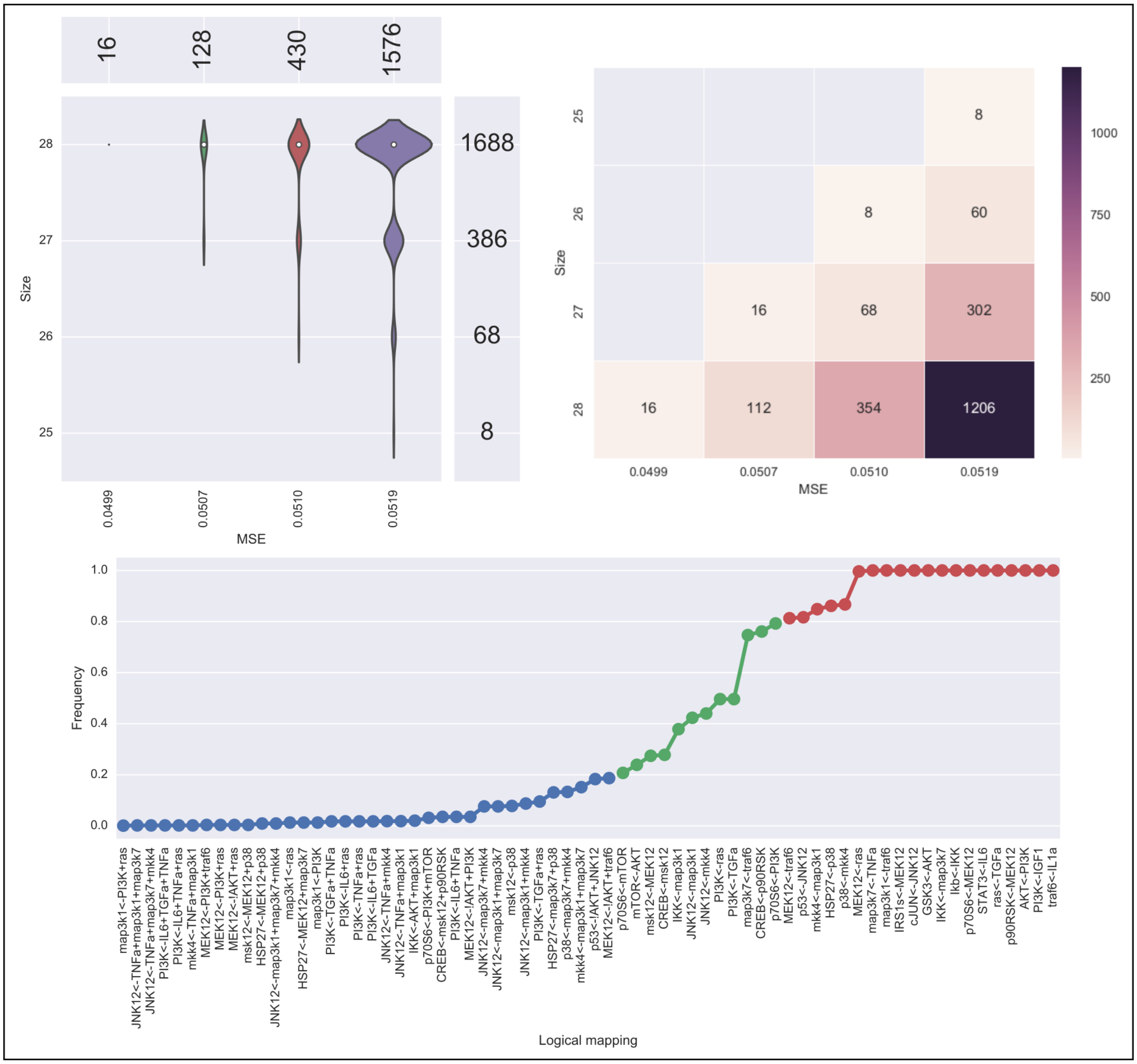
Run **caspo learn**:

```
$ caspo learn pkn.sif dataset.csv 30 --fit 0.04

Running caspo learn...
Number of hyperedges (possible logical mappings) derived from the compressed PKN: 130
Optimum logical network learned in 1.0537s
Optimum logical networks has MSE 0.0499 and size 28
2150 (nearly) optimal logical networks learned in 2.6850s
Weighted MSE: 0.0513
```

The output of **caspo learn** will be two csv files, namely, *networks.csv* and *stats-networks.csv*. The file *networks.csv* describes all logical networks found with their corresponding MSE and size. The file *stats-networks.csv* describes the frequency of each logical mapping conjunction over all networks together with pairs of mutually inclusive/exclusive mappings. The weighted MSE combining all networks is also computed and printed in the standard output.

In addition, the following default visualizations are provided describing the family of logical networks. At the top, we show two alternative ways of describing the distribution of logical networks with respect to MSE and size. At the bottom, we show the (sorted) frequencies for all logical mapping conjunctions.



2.2.2 Classify

This subcommand implements the classification of a given family of logical networks with respect to their input-output behaviors [1]. Notably, the list of networks generated by **caspo learn** can be used directly as the input for **caspo classify**.

Help on **caspo classify**:

```
$ caspo classify --help
usage: caspo classify [-h] [--threads T] [--conf C] [--midas M T]
                      networks setup
```

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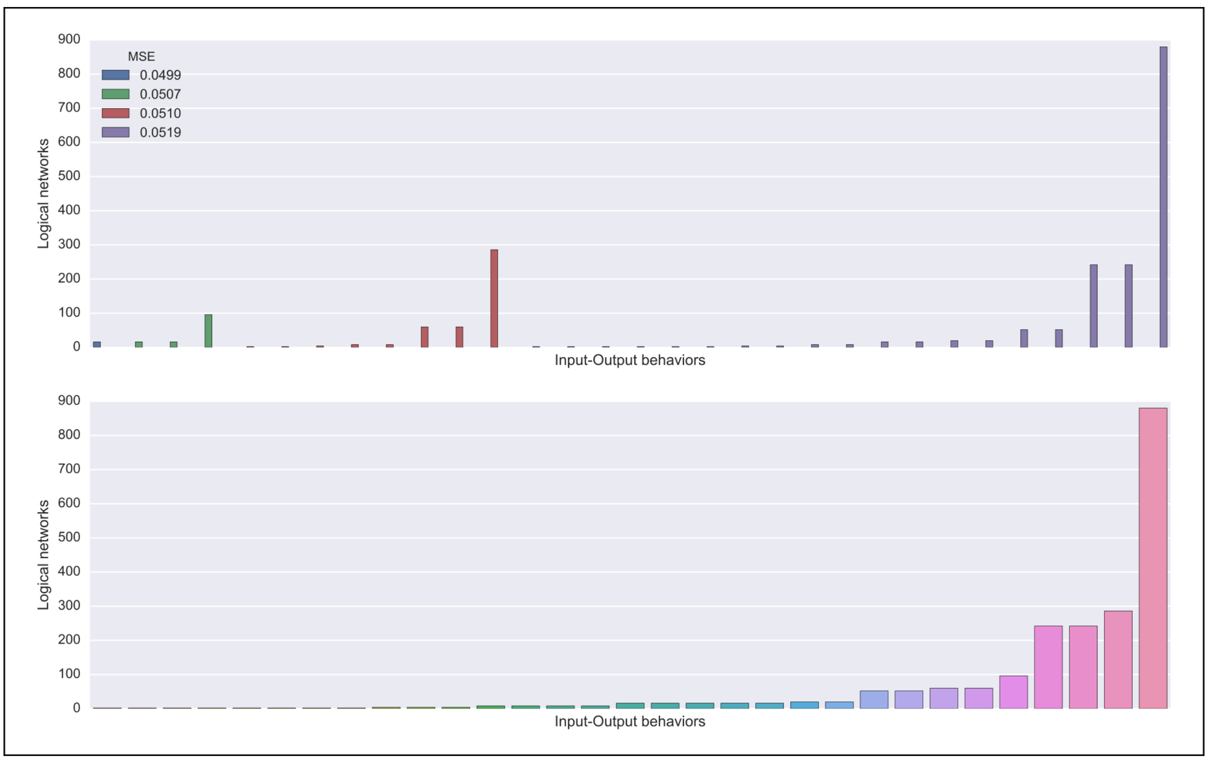
```
positional arguments:
  networks      logical networks in CSV format
  setup         experimental setup in JSON format

optional arguments:
  -h, --help    show this help message and exit
  --threads T   run clingo with given number of threads
  --conf C      threads configurations (Default to many)
  --midas M T   experimental dataset in MIDAS file and time-point to be used
```

Run **caspo classify**:

```
$ caspo classify networks.csv setup.json --midas dataset.csv 30

Running caspo classify...
Classifying 2150 logical networks...
31 input-output logical behaviors found in 156.9032s
Weighted MSE: 0.0513
```

The output of **caspo classify** will be a csv file named *behaviors.csv* describing one representative logical network for each input-output behavior found among given networks. For each representative network, the number of networks having the same behavior is also given. Further, if a dataset is given, the weighted MSE is computed.

Also, one of the following visualizations is provided depending on whether the dataset was given as an argument or not. If the a dataset is given, the figure at the top is generated where I/O behaviors are grouped by MSE to the given dataset. Otherwise, the figure at the bottom is generated.



2.2.3 Design

This subcommands implements the design of novel experiments in order discriminate a given family of input-output behaviors [3]. Notably, the list of input-output behaviors generated by **caspo classify** can be used directly as the input for **caspo design**. Further, other arguments allow for controlling the maximum number of stimuli and inhibitors used per experimental condition, or the maximum number of experiments allowed.

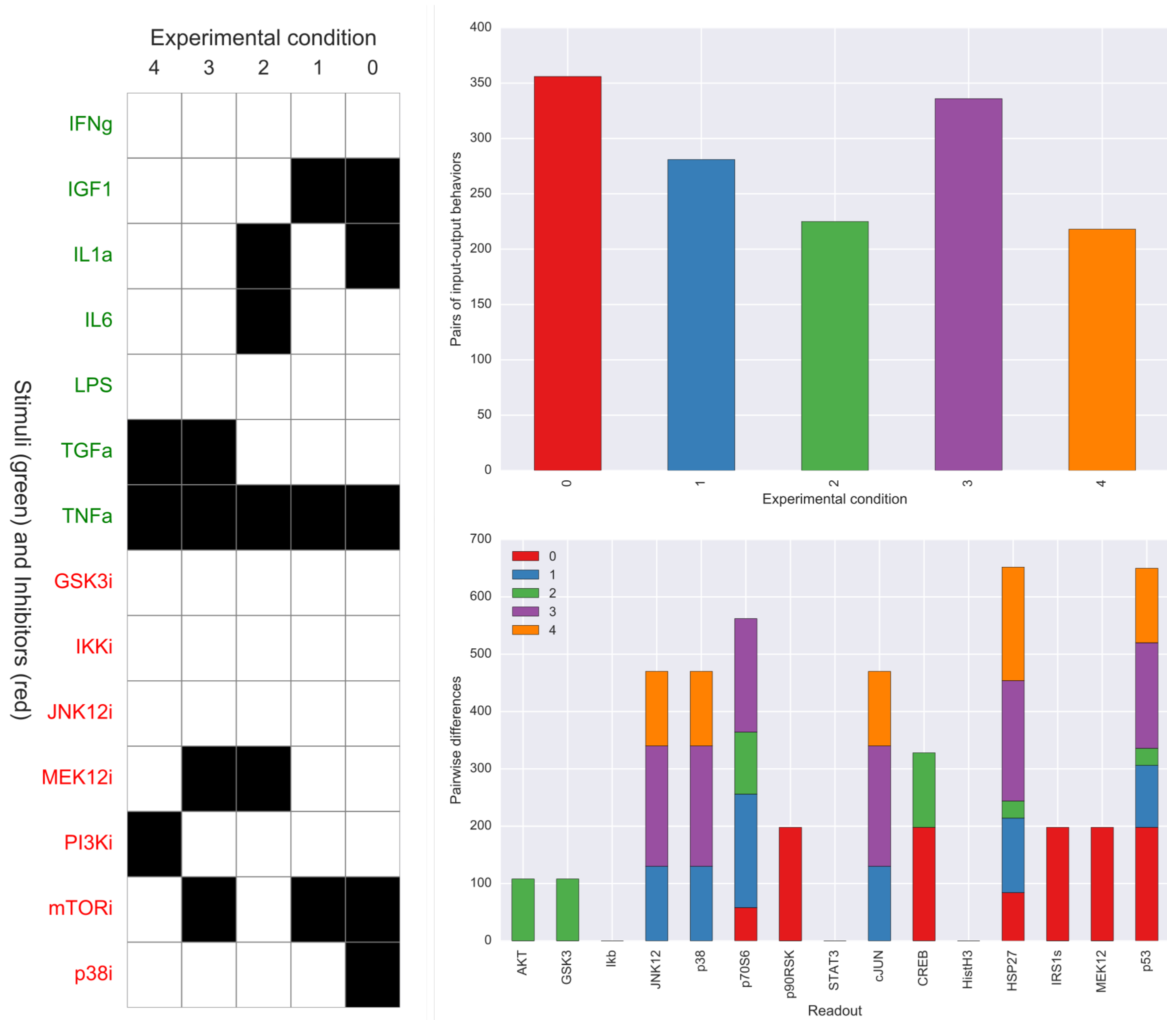
Help on **caspo design**:

```
$ caspo design --help
usage: caspo design [-h] [--threads T] [--conf C] [--stimuli S]
                    [--inhibitors I] [--nexp E] [--list L] [--relax]
                    networks setup

positional arguments:
  networks        logical networks in CSV format
  setup           experimental setup in JSON format

optional arguments:
  -h, --help      show this help message and exit
  --threads T     run clingo with given number of threads
  --conf C        threads configurations (Default to many)
  --stimuli S     maximum number of stimuli per experiment
  --inhibitors I  maximum number of inhibitors per experiment
  --nexp E        maximum number of experiments (Default to 10)
  --list L        list of possible experiments
  --relax         relax full pairwise discrimination (Default to False)
```

Run **caspo design**:

```
$ caspo design behaviors.csv setup.json

Running caspo design...
1 optimal experimental designs found in 219.5648s
```

The output of **caspo design** will be one csv file, namely, *designs.csv*, describing all optimal experimental designs. In addition, the following visualizations are provided for each experimental design in such a file. At the left we show all experimental conditions for each experimental design. At the top right we show the number of pairs of I/O behaviors discriminated by each experimental condition. At the bottom right we show the number of pairwise differences over specific readouts by each experimental condition.



2.2.4 Predict

This subcommands implements the prediction of all possible experimental condition using the ensemble of predictions from a given family of logical networks. Since predictions are based on a weighted average, a variance can also be computed to investigate the variability on every prediction. Again, the list of input-output behaviors generated by **caspo classify** can be used directly as the input for **caspo predict**. In fact, any list of logical networks could be used. However, it is recommended to use a list of representative logical networks (with their corresponding number of represented networks) for better performance.

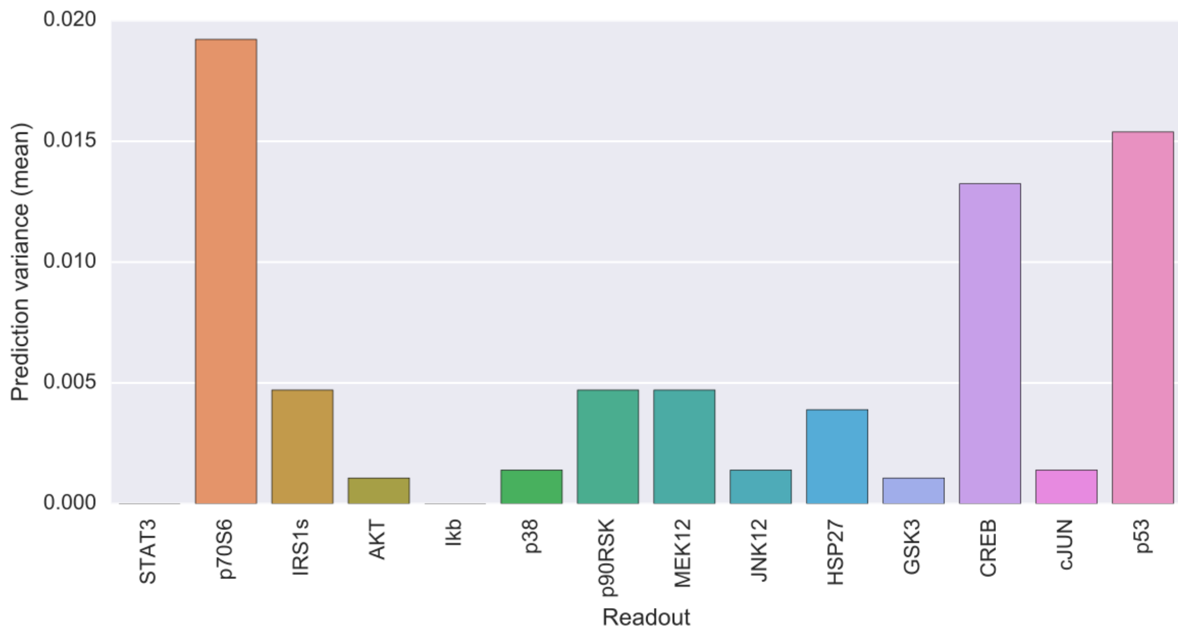
Help on **caspo predict**:

```
$ caspo predict --help
usage: caspo predict [-h] networks setup

positional arguments:
  networks    logical networks in CSV format.
  setup       experimental setup in JSON format

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

Run **caspo predict**:

```
$ caspo predict behaviors.csv setup.json

Running caspo predict...
Computing all predictions and their variance for 31 logical networks...
```

The output of **caspo predict** will be a csv file named *predictions.csv* describing for each possible experimental perturbation, the corresponding weighted average prediction and its variance for each readout. Also, the following visualization is provided showing the mean prediction variance for each readout over all possible experimental perturbations.



2.2.5 Control

This subcommand implements the control of a family of logical networks in terms of satisfying several intervention scenarios [4]. That is, it will find all intervention strategies for the given scenarios which are valid in every logical network in the family. Notably, the list of logical networks generated by **caspo learn** can be used directly as the input for **caspo control**. Further, other arguments allow for controlling the maximum number of interventions per strategy or whether interventions are allowed over constraints or goals.

Help on **caspo control**:

```
$ caspo control -h
usage: caspo control [-h] [--threads T] [--conf C] [--size M]
                     [--allow-constraints] [--allow-goals]
                     networks scenarios

positional arguments:
  networks              logical networks in CSV format
  scenarios             intervention scenarios in CSV format

optional arguments:
  -h, --help            show this help message and exit
  --threads T           run clingo with given number of threads
```

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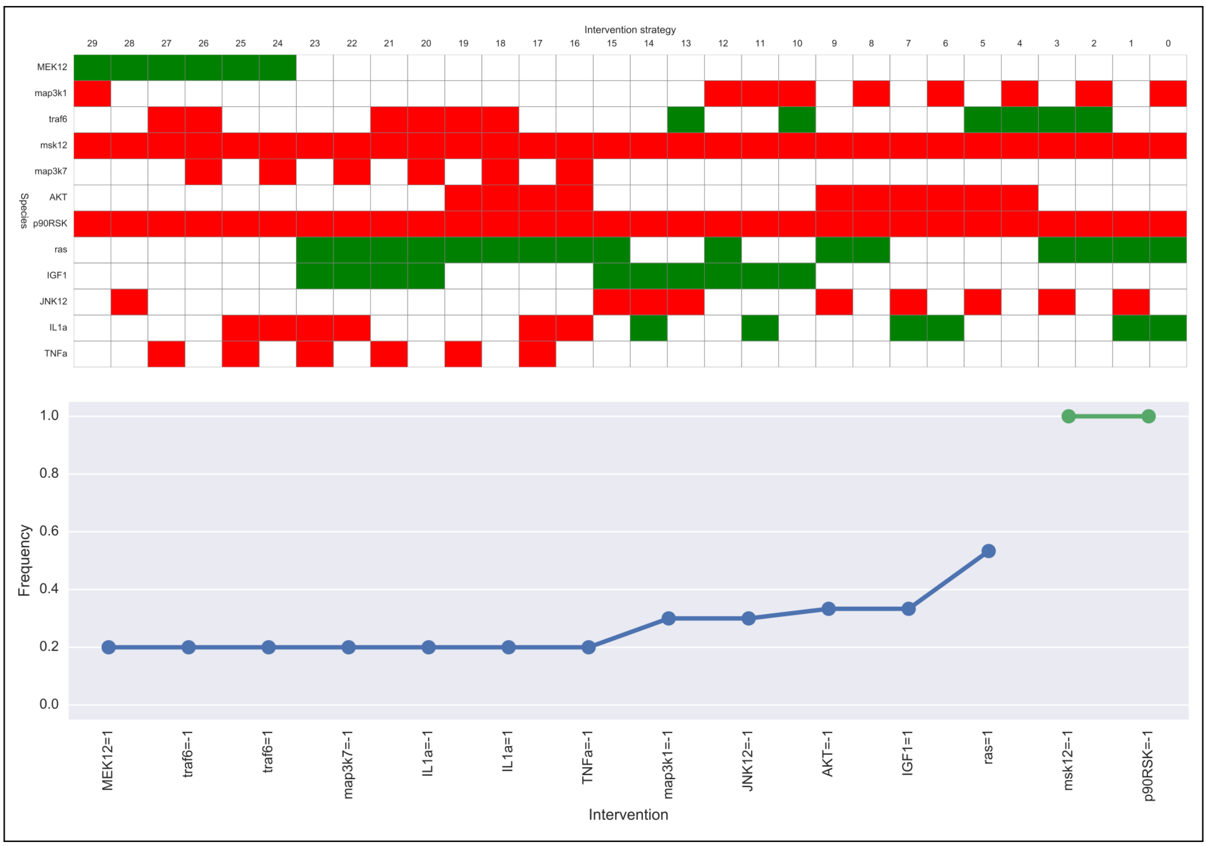
```
  --conf C              threads configurations (Default to many)
  --size M              maximum size for interventions strategies (Default to 0
                        (no limit))
  --allow-constraints   allow intervention over side constraints (Default to
                        False)
  --allow-goals         allow intervention over goals (Default to False)
```

Run **caspo control**:

```
$ caspo control networks.csv scenarios.csv

Running caspo control...
30 optimal intervention strategies found in 9.2413s
```

The output of **caspo control** will be two csv files, namely, *strategies.csv* and *stats-strategies.csv*. The file *strategies.csv* describes all intervention strategies found. The file *stats-strategies.csv* describes the frequency of each intervention over all strategies together with pairs of mutually inclusive/exclusive interventions. In addition, the following default visualizations are provided describing all intervention strategies:



2.2.6 Visualize

This subcommand implements all visualizations generated in other subcommands but to be run independently from the subcommand generating the data. This could be useful to visualize logical networks, experimental designs or intervention strategies not necessarily generated by **caspo**.

Help on **caspo visualize**:

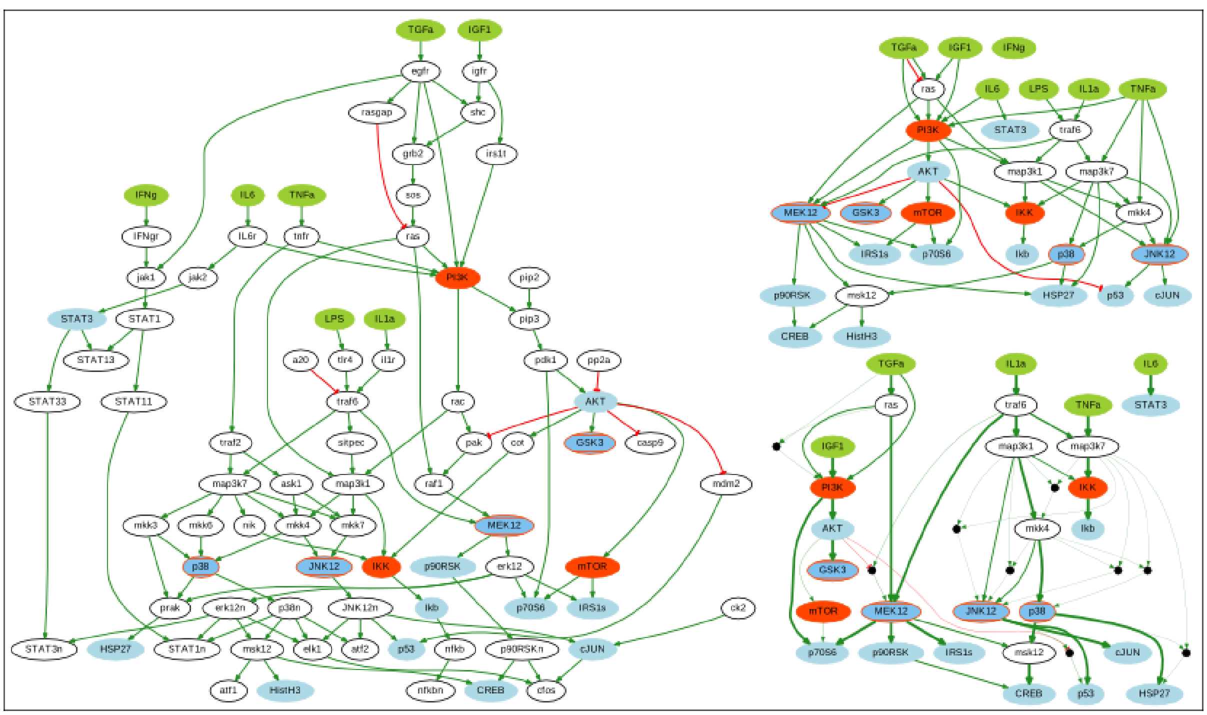
```
$ caspo visualize --help
usage: caspo visualize [-h] [--pkn P] [--setup S] [--networks N] [--midas M T]
                       [--sample R] [--stats-networks F] [--behaviors B]
                       [--designs D] [--predictions P] [--strategies S]
                       [--stats-strategies F]

optional arguments:
  -h, --help            show this help message and exit
  --pkn P               prior knowledge network in SIF format
  --setup S             experimental setup in JSON format
  --networks N          logical networks in CSV format
  --midas M T           experimental dataset in MIDAS file and time-point
  --sample R            visualize a sample of R logical networks or 0 for all
                        (Default to -1 (none))
  --stats-networks F    logical mappings frequencies in CSV format
  --behaviors B         logical networks in CSV format
  --designs D           experimental designs in CSV format
  --predictions P       logical predictions in CSV format
  --strategies S        intervention strategies in CSV format
  --stats-strategies F  intervention frequencies in CSV format
```

Run **caspo visualize**:

```
$ caspo visualize --pkn pkn.sif --networks networks.csv --setup setup.json
```

The output of **caspo visualize** will depend on the given arguments. Apart from the visualizations already shown when we described previous subcommands, it also provides visualization for a given PKN or a list of logical networks. Below we show an original PKN in the left, a compressed PKN in the top right, and the union of logical networks in the bottom right. Either all or a sample of logical networks can also be visualized individually using the `--sample` argument.



Note that PKNs and logical networks visualizations are generated as DOT files which can be either opened using a dot viewer or converted to different formats (pdf, ps, png, among others) using Graphviz. For example, you can convert from dot to pdf by running:

```
$ dot pkn.dot -Tpdf -o pkn.pdf
```

2.2.7 Test

Help on **caspo test**:

```
$ caspo test --help
usage: caspo test [-h] [--threads T] [--conf C]
                  [--testcase {Toy,LiverToy,LiverDREAM,ExtLiver}]

optional arguments:
  -h, --help            show this help message and exit
  --threads T           run clingo with given number of threads
  --conf C              threads configurations (Default to many)
  --testcase {Toy,LiverToy,LiverDREAM,ExtLiver}
                        testcase name
```

Run **caspo test**:

```
$ caspo test

Testing caspo subcommands using test case Toy.

Copying files for running tests:
    Prior knowledge network: pkn.sif
    Phospho-proteomics dataset: dataset.csv
    Experimental setup: setup.json
    Intervention scenarios: scenarios.csv

$ caspo --out out learn out/pkn.sif out/dataset.csv 10 --fit 0.1 --size 5

Optimum logical network learned in 0.0066s
Optimum logical networks has MSE 0.1100 and size 7
5 (nearly) optimal logical networks learned in 0.0075s
Weighted MSE: 0.1100

$ caspo --out out classify out/networks.csv out/setup.json out/dataset.csv 10

Classifying 5 logical networks...
3 input-output logical behaviors found in 0.2029s
Weighted MSE: 0.1100

$ caspo --out out design out/behaviors.csv out/setup.json

1 optimal experimental designs found in 0.0047s

$ caspo --out out predict out/behaviors.csv out/setup.json

Computing all predictions and their variance for 3 logical networks...

$ caspo --out out control out/networks.csv out/scenarios.csv

3 optimal intervention strategies found in 0.0043s
```

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```
$ caspo --out out visualize --pkn out/pkn.sif --setup out/setup.json \
        --networks out/networks.csv --midas out/dataset.csv 10 \
        --stats-networks=out/stats-networks.csv --behaviors out/behaviors.csv \
        --designs=out/designs.csv --predictions=out/predictions.csv \
        --strategies=out/strategies.csv --stats-strategies=out/stats-strategies.csv
```

2.3 References

- [1] Exhaustively characterizing feasible logic models of a signaling network using Answer Set Programming. (2013). Bioinformatics.
- [2] Learning Boolean logic models of signaling networks with ASP. (2015). Theoretical Computer Science.
- [3] Designing experiments to discriminate families of logic models. (2015). Frontiers in Bioengineering and Biotechnology 3:131.
- [4] Minimal intervention strategies in logical signaling networks with ASP. (2013). Theory and Practice of Logic Programming.

CHAPTER 3

API Reference

3.1 Core

3.1.1 caspo.core.setup

3.1.2 caspo.core.literal

3.1.3 caspo.core.clamping

3.1.4 caspo.core.dataset

3.1.5 caspo.core.graph

3.1.6 caspo.core.hypergraph

3.1.7 caspo.core.mapping

3.1.8 caspo.core.clause

3.1.9 caspo.core.logicalnetwork

3.2 Modules

3.2.1 Learn

3.2.2 Classify

3.2.3 Design

3.2.4 Predict

class caspo.predict.**Predictor**(*networks*, *setup*)

Predictor of all possible experimental conditions over a given experimental setup using a given list of logical networks.

Parameters

- **networks** (caspo.core.logicalnetwork.LogicalNetworkList) – The list of logical networks used to generate the ensemble of predictions
- **setup** (caspo.core.setup.Setup) – The experimental setup to generate possible experimental conditions

networks

Type caspo.core.logicalnetwork.LogicalNetworkList

setup

Type caspo.core.setup.Setup

predict()

Computes all possible weighted average predictions and their variances

Example:

```
>>> from caspo import core, predict

>>> networks = core.LogicalNetworkList.from_csv('behaviors.csv')
>>> setup = core.Setup.from_json('setup.json')

>>> predictor = predict.Predictor(networks, setup)
>>> df = predictor.predict()

>>> df.to_csv('predictions.csv'), index=False)
```

Returns DataFrame with the weighted average predictions and variance of all readouts for each possible clamping

Return type pandas.DataFrame

3.2.5 Control

3.2.6 Visualize

caspo.visualize.**behaviors_distribution**(*df*, *filepath=None*)

Plots the distribution of logical networks across input-output behaviors. Optionally, input-output behaviors can be grouped by MSE.

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns *networks* and optionally *mse*
- **filepath** (*str*) – Absolute path to a folder where to write the plot

Returns Generated plot

Return type plot

caspo.visualize.**coloured_network**(*network*, *setup*, *filename*)

Plots a coloured (hyper-)graph to a dot file

Parameters

- **network** (*object*) – An object implementing a method *__plot__* which must return the networkx.MultiDiGraph instance to be coloured. Typically, it will be an instance of either `caspo.core.graph.Graph`, `caspo.core.logicalnetwork.LogicalNetwork` or `caspo.core.logicalnetwork.LogicalNetworkList`
- **setup** (`caspo.core.setup.Setup`) – Experimental setup to be coloured in the network

`caspo.visualize.`**`differences_distribution`**(*df*, *filepath=None*)
For each experimental design it plot all the corresponding generated differences in different plots

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns *id*, *pairs*, and starting with *DIF:*
- **filepath** (*str*) – Absolute path to a folder where to write the plots

Returns Generated plots

Return type list

`caspo.visualize.`**`experimental_designs`**(*df*, *filepath=None*)
For each experimental design it plot all the corresponding experimental conditions in a different plot

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns *id* and starting with *TR:*
- **filepath** (*str*) – Absolute path to a folder where to write the plot

Returns Generated plots

Return type list

`caspo.visualize.`**`intervention_strategies`**(*df*, *filepath=None*)
Plots all intervention strategies

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns starting with *TR:*
- **filepath** (*str*) – Absolute path to a folder where to write the plot

Returns Generated plot

Return type plot

`caspo.visualize.`**`interventions_frequency`**(*df*, *filepath=None*)
Plots the frequency of occurrence for each intervention

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns *frequency* and *intervention*
- **filepath** (*str*) – Absolute path to a folder where to write the plot

Returns Generated plot

Return type plot

`caspo.visualize.`**`mappings_frequency`**(*df*, *filepath=None*)
Plots the frequency of logical conjunction mappings

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns *frequency* and *mapping*
- **filepath** (*str*) – Absolute path to a folder where to write the plot

Returns Generated plot

Return type plot

`caspo.visualize.networks_distribution`(*df*, *filepath=None*)

Generates two alternative plots describing the distribution of variables *mse* and *size*. It is intended to be used over a list of logical networks.

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns *mse* and *size*
- **filepath** (*str*) – Absolute path to a folder where to write the plots

Returns Generated plots

Return type tuple

`caspo.visualize.predictions_variance`(*df*, *filepath=None*)

Plots the mean variance prediction for each readout

Parameters

- **df** (pandas.DataFrame) – DataFrame with columns starting with *VAR:*
- **filepath** (*str*) – Absolute path to a folder where to write the plots

Returns Generated plot

Return type plot

CHAPTER 4

Indices and tables

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