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# **AlgoRun Documentation**

***Release 2.0***

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AlgoRun is a docker-based software container template designed to package computational algorithms. These pages show steps of how to create an AlgoRun container of an implemented algorithm.



# CHAPTER 1

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## Packaged Algorithms with AlgoRun before?

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Don't forget to use **docker pull algorun/algorun** before you start packaging algorithms, in order to get the latest update of AlgoRun Docker image.





## 2.1 Packaging Algorithms

AlgoRun is a docker-based software container template designed to package computational algorithms. These pages show steps of how to create an AlgoRun container of your implemented algorithm.

### 2.1.1 Packaged Algorithms with AlgoRun before?

Don't forget to use **docker pull algorun/algorun** before you start packaging algorithms, in order to get the latest update of AlgoRun Docker image.

### 2.1.2 1. Download and Install Docker

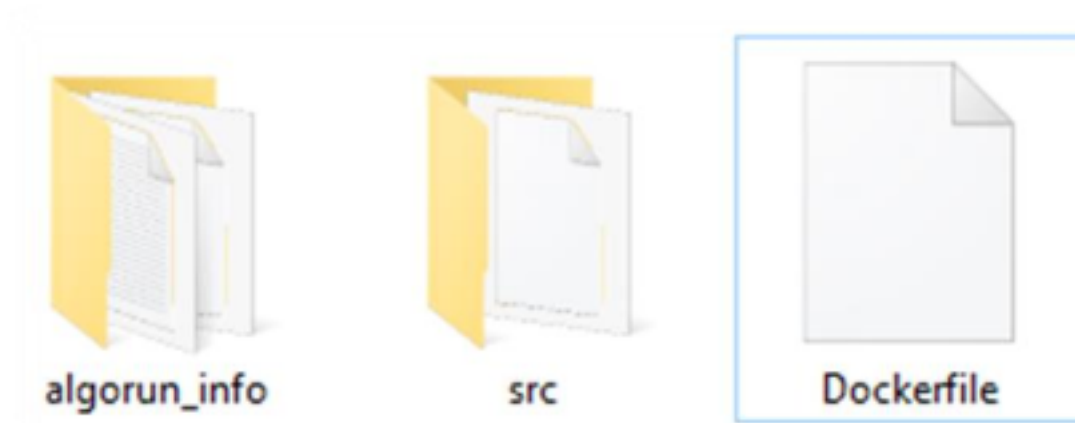
Before starting, download and install Docker on your local machine. Docker can be installed on Mac OS, Linux as well as Windows. Follow the instructions on: <https://docs.docker.com/v1.8/installation/>

### 2.1.3 2. Download AlgoRun

Download AlgoRun from: <https://github.com/algorun/skeleton>

### 2.1.4 3. Create an AlgoRun-based Docker Image

Unzip the downloaded skeleton-master.zip file. The resulting folder has the following structure:



- A Dockerfile is a text document that contains all commands needed to build the software container. Docker builds a software container automatically by reading the instructions from the Dockerfile.
- AlgoRun template container uses the *src* and *algorun\_info* folders to deposit all your source code and to describe the implemented algorithm in a standard format.

**STEP 1:** Add all source code files of your algorithms in to the *src* folder

**STEP 2:** Edit the *Dockerfile* to make sure your algorithm dependencies will get installed in the container. AlgoRun is based on Ubuntu 15.10 Linux system so you can leverage Ubuntu packaging system to get your dependencies installed

For more information about Dockerfile, please refer to the Docker documentation (<https://docs.docker.com/v1.8/reference/builder/>)

**STEP 3:** Edit the *manifest.json* file inside the *algorun\_info* folder. Below is an example of the manifest file.

```

1  {
2      "manifest_version": "2.0",
3      "algo_name": "BLAST",
4      "algo_version": "2.3.0",
5      "algo_summary": "Compares a nucleotide query sequence against a nucleotide sequence database",
6      "algo_description": "BLAST for Basic Local Alignment Search Tool is an algorithm for comparing primary biological sequences",
7      "algo_website": "http://blast.ncbi.nlm.nih.gov/Blast.cgi",
8      "algo_keywords": ["similarity", "biological", "sequences"],
9      "published_paper": {
10         "title": "Basic local alignment search tool",
11         "url": "http://www.sciencedirect.com/science/article/pii/S0022283605803602"
12     },
13     "algo_authors": [
14         {
15             "name": "Stephen Frank",
16             "email": "",
17             "profile_picture": "stephan.jpeg",
18             "personal_website": "https://scholar.google.com/citations?user=VRccPlQAAAAJ&hl=en&oi=sra",
19             "organization": "NCBI, NLM, NIH",
20             "org_website": "http://www.nih.gov/"
21         }
22     ],
23     "algo_packager": {
24         "name": "Abdelrahman Hosny",
25         "email": "abdelrahman.hosny@hotmail.com",
26         "personal_website": "http://www.abdelrahmanhosny.me",
27         "profile_picture": "",
28         "organization": "University of Connecticut",
29         "org_website": "http://cse.uconn.edu"
30     },
31     "algo_exec": "sh run_blast.sh $input",
32     "algo_input": [
33         { "name": "input", "src": "file", "type": "text/plain", "accepted_format": "FASTA" }
34     ],
35     "algo_output": [
36         { "name": "output", "src": "output.txt", "type": "text/plain", "format": "BLAST" }
37     ],
38     "algo_parameters": {
39         "caching": "on"
40     },
41     "algo_image": "algorun:blast"
42 }

```

In addition to adding algorithm's information, the following fields are necessary for AlgoRun to correctly execute the algorithm source code:

- “algo\_exec”: is the command used to start algorithm executed.
- “algo\_input”: is how the algorithm reads the input data.
- “algo\_output”: is the path of the file where the algorithm outputs its result or stdout if the algorithm prints the result to the standard output stream.

Command line options can be exposed in the “algo\_parameters” field (Refer to examples tab for a detailed example using parameters). AlgoRun website uses “input\_type” and “output\_type” to easily identify algorithms that can communicate together. Please refer to <http://algorun.org/input-output-types> to see what input and output types you should use. Users can also download and use the algorithm Docker image locally from Docker Hub if the value “algo\_image” is provided.

**STEP 4:** Provide input and output examples in the input\_example and output\_example folders respectively.

**STEP 5:** Build the algorithm container from the command line using docker build command: *docker build -t <algorithm\_name> .*

## 2.1.5 4. Run the algorithm

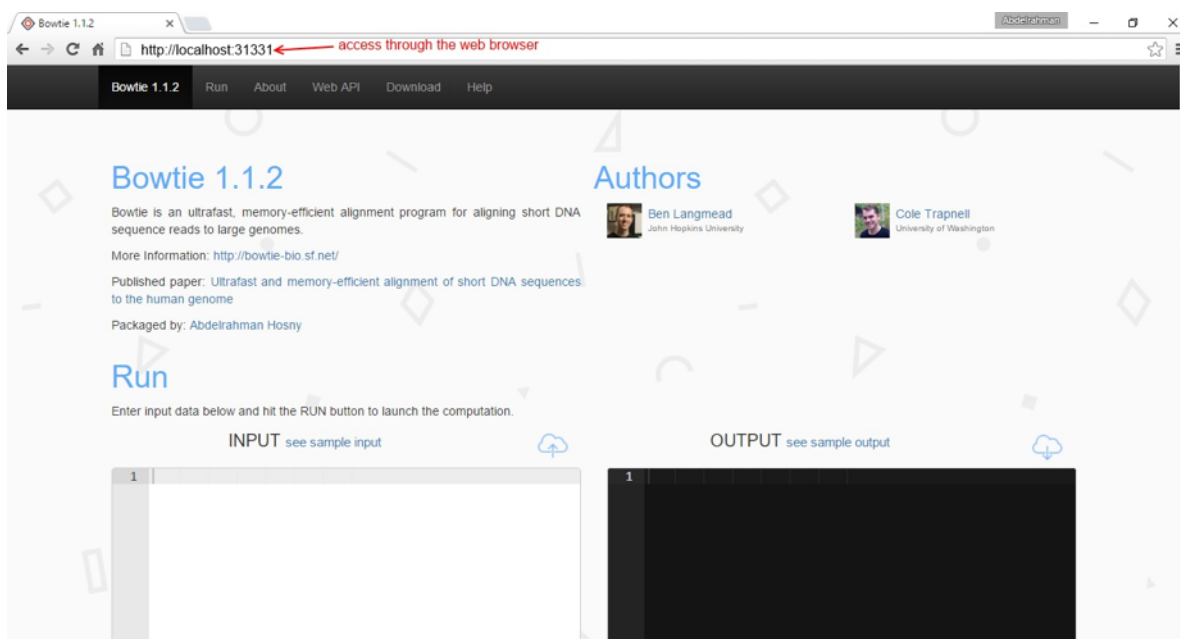
Once the algorithm container has been created, it must first be deployed before the user can start using the packaged algorithm. The container can be deployed with the following command:

```
docker run -p 31331:8765 --name <container_name> <algorithm_name>
```

Now that the algorithm container has been deployed on your local machine (localhost), AlgoRun provides the user with three different ways to run the algorithm.

### 4.1 Web User Interface

The easiest and quickest way to run the packaged algorithm is to open the web browser and type <http://localhost:31331>

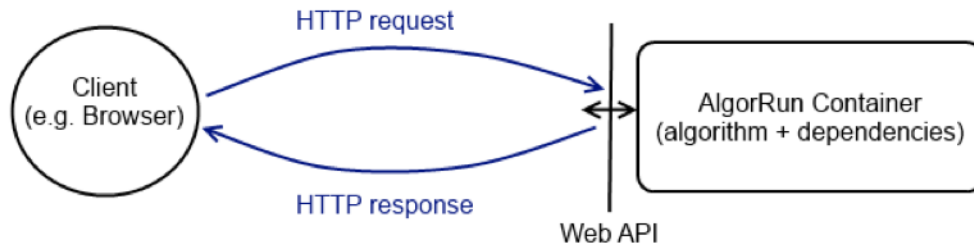


The web user interface of an algorithm packaged with AlgoRun. Type in the address <http://localhost:31331> in a web browser to open the web page of the running algorithm container.

### 4.2 Web API

A web API is an Application Programming Interface (API) used to offer programmatic access to remote resources or services (in our case “computations from an algorithm”) that can be accessed by clients such as web browsers or any http-enabled third-party applications. AlgoRun containers are pre-included with a RESTful API<sup>1</sup> that allows access to the computation through the traditional HTTP POST request. Clients communicate to web APIs through a request/response protocol. To ask the web service to perform a computation, a client sends an HTTP request. The body of the request includes necessary input data for the algorithm behind the web service to start. The response of the web service includes the result of the computation.

<sup>1</sup> REpresentational State Transfer (REST) APIs uses Hyper Text Transfer Protocol (HTTP) requests as the main scheme of communication.



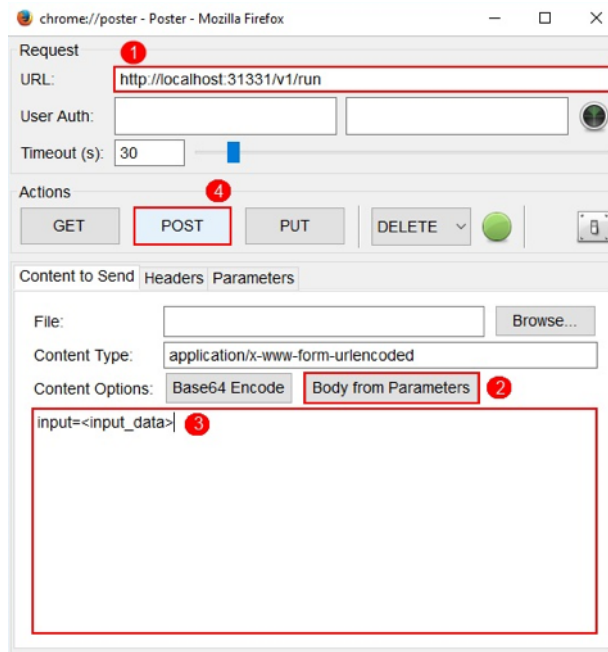
AlgoRun Web API Communication Scheme.

The HTTP request should be sent to a specific address, which is called an endpoint. The two main endpoints exposed by AlgoRun containers are shown below.

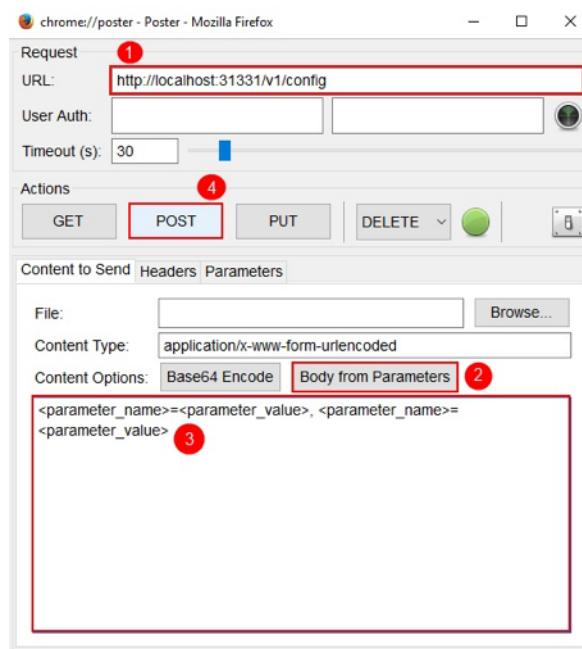
Endpoint	Usage	Request Parameters	Response
<b>HTTP POST /v1/run</b>	used to run the algorithm on a given input data	input: <input_data>	The result of the computation in the body of the response
<b>HTTP POST /v1/config</b>	used to dynamically change the parameters values	<parameter_name>: <parameter_value>	The result of changing the parameter value

By offering standardized input and output, Web APIs are particularly useful when it comes to building complex software applications as they make it easy to integrate different algorithms that usually run on different programming environments. It enhances the modularity of the software, hence increases its robustness and makes troubleshooting problems easier. You can embed computations in large software programs in just a few lines of code, removing the hassle of installing the whole algorithm environment locally.

To test a web API, Firefox Poster Plugin is a graphical user interface tool used to easily send and troubleshoot HTTP requests. See below for examples on using the above AlgoRun endpoints.



Calling Web API using Firefox Poster Plugin: (1) Type the URL of the endpoint `http://localhost:31331/v1/run` (2) Select Body from Parameters. (3) Type `input=<paste_your_input_data_here>`. (4) Click Post to initiate the request



Configuring Parameters using Web API: (1) Type the URL of the endpoint <http://localhost:31331/v1/config> (2) Select Body from Parameters. (3) Type `<parameter_name>=<parameter_value>`. (4) Click Post to initiate the request.

### 4.3 Command Line

The traditional command line execution is still available as well.

```
docker exec -i <container_name> /bin/algorun < sample_input.txt
```

## 2.1.6 5. Publish your algorithm to the AlgoRun website

If you packaged your algorithm with AlgoRun and want to give your algorithm more visibility, we encourage you to submit it for listing on the AlgoRun website. The AlgoRun website serves as a repository for all computational algorithms that were packaged using AlgoRun: <http://algorun.org>

To submit your algorithm for listing, fill the form located at <http://algorun.org/submit-algorithm>

## 2.2 Examples

In this section, we show the process of creating AlgoRun containers for 3 different examples of published software:<sup>1</sup> the popular bioinformatics software Bowtie (Langmead, 2009),<sup>2</sup> REACT (Vera-Licona, 2014), a systems biology software to infer gene regulatory networks and,<sup>3</sup> the KS algorithm to solve the transversal hypergraph generation problem (Kavvadias, 2005). For the first example, Bowtie, we show how to create an AlgoRun container, how to run the Bowtie AlgoRun container using AlgoRun web interface, how to expose command line options as parameters,

<sup>1</sup> Langmead, B. et al. (2009). Ultrafast and memory-efficient alignment of short DNA sequences to the human genome. *Genome Biology*, 10:R25.

<sup>2</sup> Vera-Licona, P., Jarrah, A.S., Garcia, LD., McGee, J., Laubenbacher, R. (2014): An Algebra-Based Method for Inferring Gene Regulatory Networks. *BMC Systems Biology*, 8:37.

<sup>3</sup> Kavvadias D. and Stavropoulos E. (2005): An Efficient Algorithm for the Transversal Hypergraph Generation. *J. of Graph Alg & App*, 9:2, 239-264.

some input examples to highlight the use of command line options vs. parameters and finally, how to access the tool deployed with AlgoRun via a RESTful API interface. For the other two examples we show how to create the AlgoRun containers and provide the users with the appropriate links to allow users to deploy and use all the AlgoRun features as presented in the first example.

### 2.2.1 Packaging Bowtie Software with AlgoRun

Bowtie (Langmead, 2009) is an ultra-fast memory-efficient short read aligner. The source code is written in C++ and is available under the Artistic License. Download it from <http://sourceforge.net/projects/bowtie-bio/files/bowtie/1.1.2/>

Unzip the downloaded file. This unzipped file will contain all the source code of Bowtie.

**STEP 1:** Add all Bowtie source files inside the src folder.

**STEP 2:** Add the instructions to install the C++ dependencies as well as the instructions to build Bowtie source code to the Dockerfile. Below is how the Dockerfile of Bowtie looks like.

```
1 FROM algorun/algorun
2
3 ADD ./algorun_info /home/algorithm/web/algorun_info/
4 ADD ./src /home/algorithm/src/
5
6 # Install any algorithm dependencies here
7 RUN apt-get update && apt-get install -y build-essential
8 RUN cd /home/algorithm/src && make
```

Source code: Dockerfile of Bowtie software

#### Hints:

1. Dockerfile syntax requires preceding all commands with RUN keyword.
2. To ensure successful installation, always use apt-get update before installing packages and use -y option in the install command.
3. Change to /home/algorithm/src directory before running any command that operates on the source files inside src folder.

**STEP 3:** *manifest.json* file is required to describe the computational algorithm. Comments in the file will guide you to fill the correct values. Below is how the manifest of Bowtie looks like.

```

1 {
2   "manifest_version": "1.2",
3   "algo_name": "Bowtie 1.1.2",
4   "algo_summary": "Bowtie is an ultrafast, memory-efficient alignment program for aligning short DNA sequence reads to large genomes.",
5   "algo_description": "Bowtie is an ultrafast, memory-efficient short read aligner geared toward quickly aligning large sets of short DNA sequences (reads) to large genomes. Check <a href
6   \"http://bowtie-bio.sourceforge.net/\" target='_blank'>our website</a> for detailed explanation. This interface is meant to provide a quick and easy access to the computation without having to install
7   Bowtie packages. Command line options are exposed as parameters, which you can configure from the above window.",
8   "algo_website": "http://bowtie-bio.sourceforge.net/",
9   "algo_keywords": ["bowtie", "DNA", "genome", "sequencing", "alignment", "Burrows-Wheeler", "indexing"],
10  "algo_authors": [
11    {
12      "name": "Ben Langmead",
13      "email": "langmead@cs.umd.edu",
14      "profile_picture": "ben.jpg",
15      "personal_website": "http://www.cs.jhu.edu/~langmea/",
16      "organization": "John Hopkins University",
17      "org_website": "https://www.jhu.edu/"
18    },
19    {
20      "name": "Cole Trapnell",
21      "email": "colettrap@uw.edu",
22      "profile_picture": "cole.png",
23      "personal_website": "http://cole-trapnell-lab.github.io/team/cole-trapnell/",
24      "organization": "University of Washington",
25      "org_website": "http://www.uw.edu/"
26    }
27  ],
28  "algo_exec": "ruby bowtie.rb",
29  "algo_input_stream": "direct",
30  "algo_output_stream": "stdout",
31  "algo_parameters": {},
32  "input_type": "algorun:dna-sequence",
33  "output_type": "algorun:aligned-dna-sequence",
34  "algo_image": "algorun/bowtie"
35 }

```

Source Code: manifest.json of Bowtie software (comments-skimmed)

#### STEP 4:

- `input_example.txt` file includes a sample input data for users to quickly try the algorithm. Enter ATGCATCAT-GCGCCAT as an example.
- `output_example.txt` file includes a sample of the expected output for the same input. It makes it easier for users to expect the output.
 

```
0 - g|110640213|reflNC_008253.1| 148810 ATGGCGCATGATGCAT IIIIIIIIIIIII 0 10:A>G,13:C>G
```

#### Notes:

- Bowtie source code comes with `e_coli` index packaged by default. So, use it in the `algo_exec`. If you included other indexes, it's ok to use them as well.
- Use `direct` in `algo_input_stream` to accept input directly from the command line. Bowtie has other options to read the input from a file. However, AlgoRun will automatically present an option to upload a file to the input area in the web interface.
- Use `stdout` in `algo_output_stream` to let AlgoRun get the result from the terminal. Bowtie has other options to write the output to a file. However, AlgoRun will automatically present an option to download the result to a file from the web interface.

#### STEP 5:

- **From the directory where the Dockerfile exists, build Bowtie container using:** `docker build -t bowtie .`
- You should see a success message as in the following picture.

```

---> 0788ef071b7e
Removing intermediate container e6d52cdf612c
Step 6 : MAINTAINER Abdelrahman Hosny <abdelrahman.hosny@hotmail.com>
---> Running in 5c9d49c5c70f
---> 6e1bfa3d638f
Removing intermediate container 5c9d49c5c70f
Successfully built 6e1bfa3d638f
abdelrahman@abdelrahman-laptop:~/uchc/algorun/examples/bowtie-1.1.2$

```

Bowtie container build success message

## User Interface

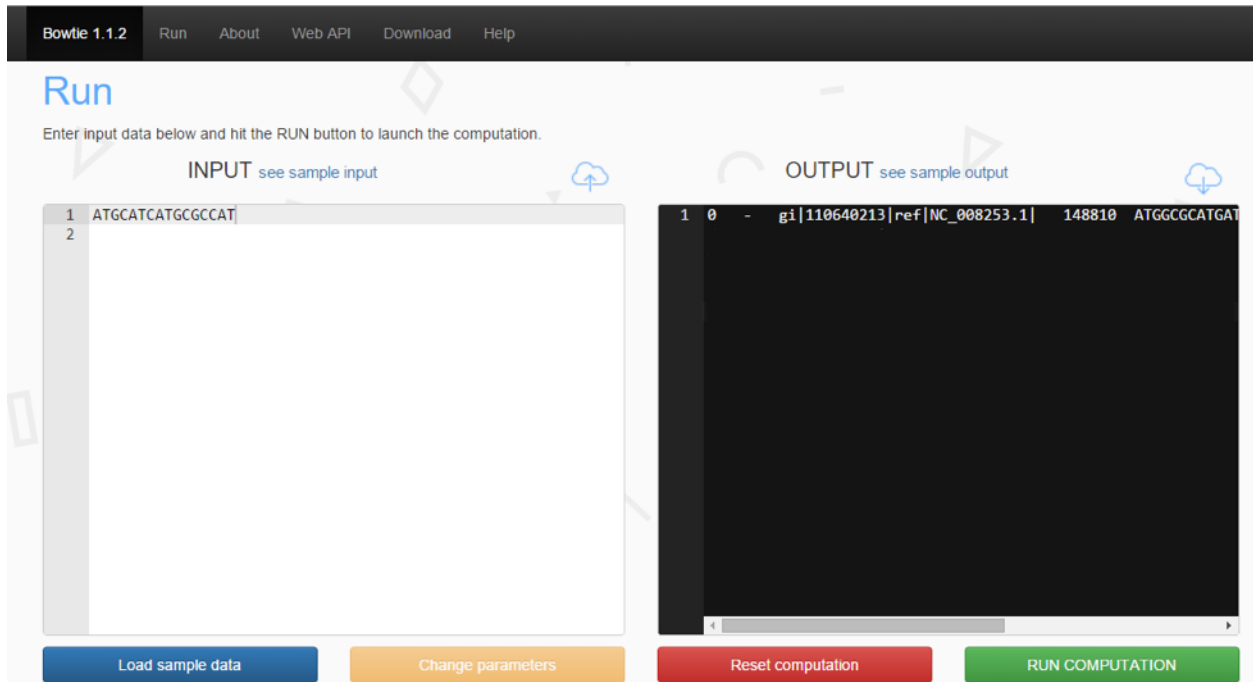
Run Bowtie container using:



```
docker run -p 31331:8765 bowtie
```

Open the web browser and type <http://localhost:31331>

**Hint:** You can use any available port other than 31331. Yet, you must bind it to 8765 port as it is the gateway to AlgoRun.



### [OPTIONAL] Expose Command Line Options as Parameters

To give flexibility to an implemented algorithm, AlgoRun allows exposing parameters that can be easily changed from the web interface. These parameters will be available as environment variables in the source code.

The power of Bowtie as a very fast DNA sequences aligner comes from the available command line options. So, you can make use of AlgoRun parameters to expose these command line options. You have two options: either to manipulate the source code of Bowtie so that it reads options from environment variables (instead of command line) or to develop a wrapper around Bowtie main executable that will internally translate environment variables to command line options. To do so, follow the below steps:

```

28 ▾ "algo_parameters": {
29     "Skip": "0",
30     "Only-Align": "all",
31     "Trim-Left": "0",
32     "Trim-Right": "0",
33     "Phred-Quality": "33",
34     "Solexa": "off",
35     "Align-v": "0",
36     "Align-n": "2",
37     "Align-e": "70",
38     "Align-l": "28",
39     "Align-I": "0",
40     "Align-X": "250",
41     "Report-k": "1",
42     "Report-all": "off",
43     "Report-m": "no-limit",
44     "Report-best": "off",
45     "Report-strata": "off",
46     "suppress": "0"
47 },

```

1. Specify parameters and their default values in the manifest file. The adjacent picture shows some parameters.
2. Read the input data. The input data is passed as the first command line argument.
3. Read the environment variables (of the same names you specified in the manifest) and form the options string. Call the executable file and to print the output to the standard output.

Modify the Dockerfile to install ruby dependency:

```
RUN apt-get update && apt-get install -y ruby build-essential
```

Modify `algo_exec` value in the manifest file to:

```
"algo_exec": "ruby bowtie.rb",
```

Rebuild Bowtie container using:

```
`docker build -t bowtie .`
```

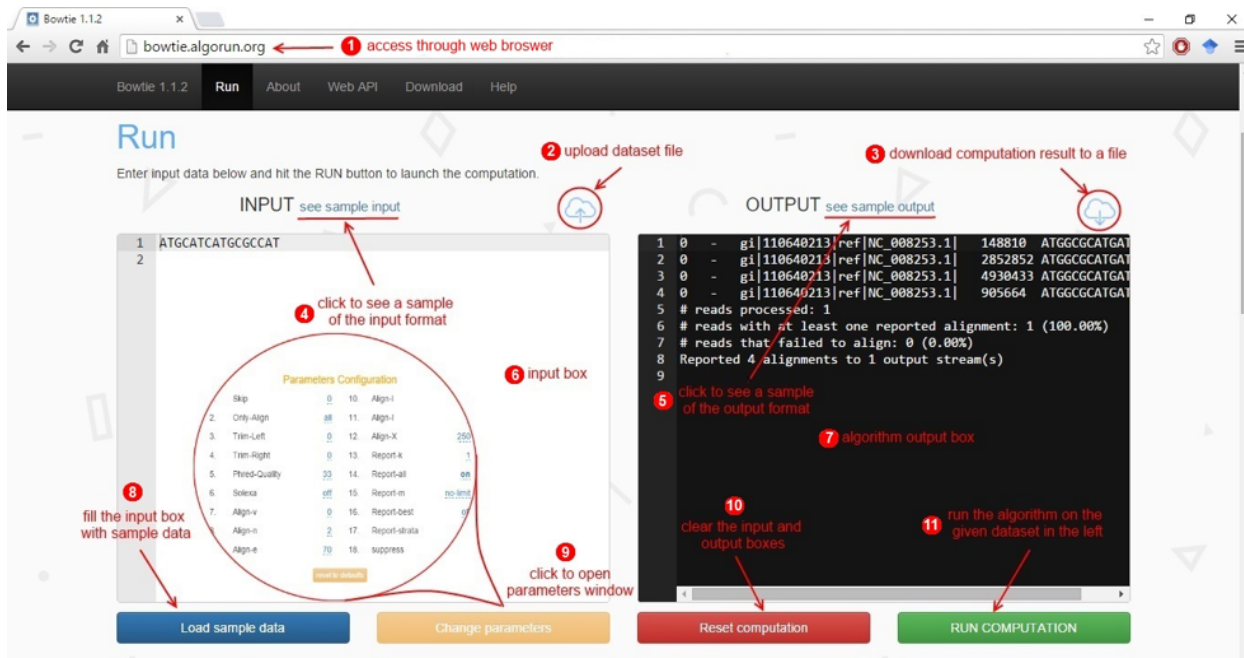
At this point, options available from Bowtie can be changed by clicking on “Change Parameters” button from the web interface. Visit <http://bowtie.algorun.org> for the final version of Bowtie running inside AlgoRun standard container. Find the complete example on AlgoRun GitHub repository (<https://github.com/algorun/algorun/tree/master/examples/bowtie-1.1.2>).

```

1 require 'open3'
2
3 # read input data that is passed directly
4 input_data=ARGV[0].strip
5
6 # form the options string by reading environment variables
7 options = ""
8
9 options += " -s " + ENV["Skip"].strip
10 options += " -u " + ENV["Only-Align"].strip unless ENV["Only-Align"] == "all"
11 options += " -5 " + ENV["Trim-Left"].strip
12 options += " -3 " + ENV["Trim-Right"].strip
13 options += " --phred64-quals" if ENV["Phred-Quality"] == "64"
14 options += " --solexa-quals" if ENV["Solexa"] == "on"
15 options += " -n " + ENV["Align-n"].strip
16 options += " -v " + ENV["Align-v"].strip
17 options += " -n " + ENV["Align-n"].strip
18 options += " -e " + ENV["Align-e"].strip
19 options += " -l " + ENV["Align-l"].strip
20 options += " -I " + ENV["Align-I"].strip
21 options += " -X " + ENV["Align-X"].strip
22 options += " -k " + ENV["Report-k"].strip
23 options += " --all" if ENV["Report-all"] == "on"
24 options += " -m " + ENV["Report-m"].strip unless ENV["Report-m"] == "no-limit"
25 options += " --best" if ENV["Report-best"] == "on"
26 options += " --strata" if ENV["Report-strata"] == "on"
27 options += " --suppress " + ENV["suppress"].delete(' ') unless ENV["suppress"] == "0"
28 options.strip!
29
30 # run the algorithm with the options injected
31 command = "/bowtie " + options + " e_coli -c " + input_data
32 stdin, stdout, stderr, wait_thr = Open3.popen3(command)
33
34 # print the output to the standard output stream
35 puts stdout.read
36 puts stderr.read

```

Source Code: bowtie.rb wrapper code



Bowtie web interface

## Input Examples (Command Line Options vs. Parameters)

- Example Link: <http://bowtie-bio.sourceforge.net/manual.shtml#example-1-a>

Command line: `./bowtie -a -v 2 e_coli --suppress 1,5,6,7 -c ATGCATCATGCGCCAT`

With AlgoRun: Change Report-all to on, Align-v to 2 and suppress to 1,5,6,7

2. Example Link: <http://bowtie-bio.sourceforge.net/manual.shtml#example-2-k-3>

Command line: `./bowtie -k 3 -v 2 e_coli -suppress 1,5,6,7 -c ATGCATCATGCGCCAT`

With AlgoRun: Change Report-k to 3, Align-v to 2 and suppress to 1,5,6,7

3. Example Link: <http://bowtie-bio.sourceforge.net/manual.shtml#example-3-k-6>

Command line: `./bowtie -k 6 -v 2 e_coli -suppress 1,5,6,7 -c ATGCATCATGCGCCAT`

With AlgoRun: Change Report-k to 6, Align-v to 2 and suppress to 1,5,6,7

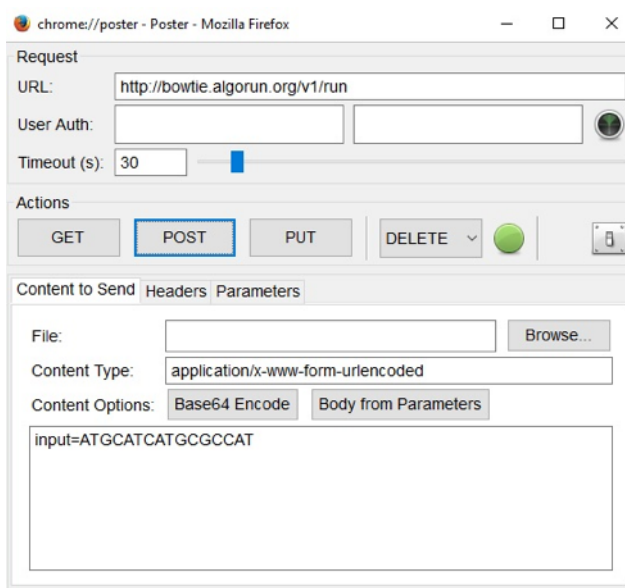
4. Example Link: <http://bowtie-bio.sourceforge.net/manual.shtml#example-9-a-m-3—best—strata>

Command line: `./bowtie -a -m 3 -best -strata -v 2 e_coli -suppress 1,5,6,7 -c ATGCATCATGCGC-CAT`

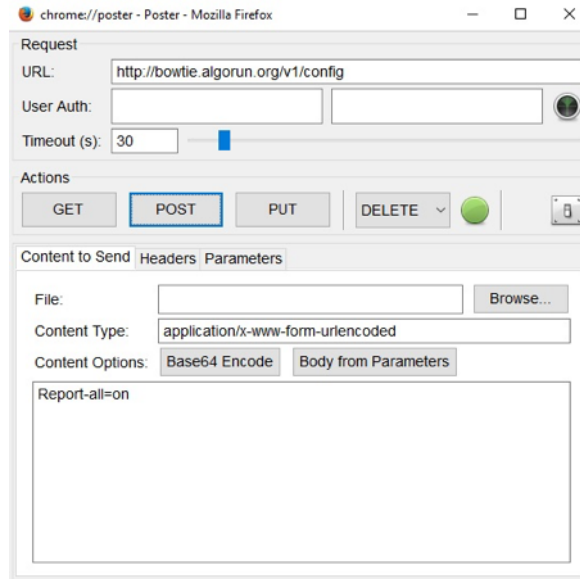
With AlgoRun: Change Report-all to on, Report-m to 3, Report-best to on, Report-strata to on, Align-v to 2 and suppress to 1,5,6,7.

## Running Bowtie through AlgoRun's Web API

In addition to the web user interface available at <http://bowtie.algorun.org>, you can run Bowtie using the web API. Using the web API is useful to perform the computation from different client applications. As an example of running Bowtie through the web API, see the Firefox Poster plugin examples below. Refer to supplementary file 1 for a detailed illustration on web APIs.



Run Bowtie Computation: (1) Type the URL of the endpoint <http://bowtie.algorun.org/v1/run> (2) Select Body from Parameters. (3) Type input=ATGCATCATGCGCCAT. (4) Click Post to initiate the request



Configure Bowtie Parameters: (1) Type the URL of the endpoint <http://bowtie.algorun.org/v1/config> (2) Select Body from Parameters. (3) Type Report-all=on. (4) Click Post to initiate the request.

## 2.2.2 Packaging REACT Algorithm with AlgoRun

REACT<sup>2</sup> (Vera-Licona, 2014), is a software tool to reverse engineer gene regulatory networks from time series data. The source code is written in C++ and is available on GitHub at: <https://github.com/veralicona/REACT/tree/master/src>. In addition, the source code includes ruby files as a helper to run the algorithm.

**STEP 1:** Add all REACT source files inside the src folder.

**STEP 2:** Add the instructions to install the C++ and ruby dependencies as well as the instructions to build REACT source code to the Dockerfile. Use the helper *ruby file ruby /home/algorithm/src/run.rb make*

```
1 FROM algorun/algorun
2 ADD ./algorun_info /home/algorithm/web/algorun_info/
3 ADD ./src /home/algorithm/src/
4
5 # Install any algorithm dependencies here
6 RUN apt-get update && \
7 apt-get install -y build-essential ruby
8 RUN ruby /home/algorithm/src/run.rb make
```

Source code: Dockerfile of REACT algorithm

**STEP 3:** manifest.json describes REACT algorithm. Below is how the manifest of REACT looks like.

```

1 {
2   "manifest_version": "1.2",
3   "algo_name": "REACT",
4   "algo_summary": "Evolutionary Algorithm for Discrete Dynamical System Optimization",
5   "algo_description": "The inference of gene regulatory networks (GRNs) from system-level experimental observations is at the heart of systems
6   biology due to its centrality in gaining insight into the complex regulatory mechanisms in cellular systems. This includes the inference of both
7   the network topology and dynamic mathematical models.",
8   "algo_website": "http://compsysmed.org/Software/EAREvEng/REACT.html",
9   "algo_keywords": ["reverse engineering", "cell biology"],
10  "algo_authors": [
11    {
12      "name": "Paola Vera-Licona",
13      "email": "veralicona@uchc.edu",
14      "profile_picture": "",
15      "personal_website": "http://compsysmed.org",
16      "organization": "Center for Quantitative Medicine, UConn Health",
17      "org_website": "http://cqm.uchc.edu/"
18    },
19    {
20      "name": "John J. McGee",
21      "email": "",
22      "profile_picture": "",
23      "personal_website": "",
24      "organization": "Wolfram Alpha",
25      "org_website": "http://www.wolframalpha.com/"
26    }
27  ],
28  "algo_exec": "ruby React.rb",
29  "algo_input_stream": "file",
30  "algo_output_stream": "output.txt",
31  "algo_parameters": {},
32  "input_type": "[superAdam:TimeSeriesSet,superAdam:PolynomialDynamicalSystemSet,(superAdam:DirectedGraph)]",
33  "output_type": "SuperAdam:PolynomialDynamicalSystemSet",
34  "algo_image": "algorun/react"
35 }

```

Source Code: manifest.json of REACT algorithm (comments-skimmed)

#### STEP 4:

- input\_example.txt file includes a sample input data for users to quickly try the algorithm. Copy and paste an example from: [http://react.algorun.org/algorun\\_info/input\\_example.txt](http://react.algorun.org/algorun_info/input_example.txt)
- output\_example.txt file includes a sample of the expected output for the same input. The above input produces an output of the format: [http://react.algorun.org/algorun\\_info/output\\_example.txt](http://react.algorun.org/algorun_info/output_example.txt)

#### STEP 5:

- From the directory where the Dockerfile exists, build REACT container using:

[EXTRA STEP] Expose REACT Parameters:

REACT algorithm uses default values for different parameters. To expose these parameters to the user, include them in the manifest file in the “algo\_parameter” key as in the below picture.

```

29 {
30   "algo_parameters": {
31     "HammingPolyWeight": "0.5",
32     "ComplexityWeight": "0.2",
33     "RevEngWeight": "0",
34     "BioProbWeight": "0",
35     "HammingModelWeight": "0.35",
36     "PolyScoreWeight": "0.65",
37     "GenePoolSize": "100",
38     "NumCandidates": "55",
39     "NumParentsToPreserve": "5",
40     "MaxGenerations": "100",
41     "StableGenerationLimit": "50",
42     "MutateProbability": "0.5"
43   },

```

REACT parameters in the manifest file

Parameters can be changed by clicking on “Change Parameters” button from the web interface. Visit <http://react.algorun.org> for the final version of REACT running inside AlgoRun standard container.

Find the complete example on AlgoRun GitHub repository (<https://github.com/algorun/algorun/tree/master/examples/REACT>).

## 2.2.3 Packaging KS Algorithm with AlgoRun

KS<sup>3</sup> Kavvadias-Stavropoulos algorithm (Kavvadias, 2005) generates all minimal hitting sets (traversals) of a hypergraph. The source code is written in Pascal and is available on Murakami and Uno's repository.

As the source code is using a dialect of Pascal that is not compatible with the modern compiler, download a helper executable that has been written to come over that problem: <https://github.com/algorun/algorun/tree/master/examples/ks> For your convenience, the repository above includes KS algorithm source code as well.

**STEP 1:** Add KS thg.pas source file with the helper mhs file inside the src folder. The helper

**STEP 2:** Add the instructions to install the C++ dependencies and Pascal compiler to the Dockerfile. As the helper is written in python, add the instructions to install the python dependencies as well. After that, navigate to the src directory and compile the source code file pc thg.pas

Adding the instructions to install *python-pip* dependency helps in installing other python packages as simplejson in a much easier way.

```
1 FROM algorun/algorun:latest
2 ADD ./src /home/algorithm/src/
3 ADD ./algorun_info /home/algorithm/web/algorun_info/
4
5 # Install any algorithm dependencies here
6 RUN apt-get update && \
7     apt-get install -y --no-install-recommends \
8     build-essential \
9     fp-compiler \
10    python-pip \
11    && rm -rf /var/lib/apt/lists/
12 RUN pip install \
13     simplejson
14 WORKDIR /home/algorithm/src/alg
15 RUN pc thg.pas
```

Source Code: Dockerfile of KS algorithm

**STEP 3:** manifest.json describes KS algorithm. Below is how the manifest of KS looks like.

```

1- {
2   "manifest_version": "1.2",
3   "algo_name": "KS",
4   "algo_summary": "KS algorithm for minimal hitting set computations",
5   "algo_description": "Introduced in <a href='\"//doi.org/10.7155/jgaa.00107\">An efficient algorithm for the transversal hypergraph generation</a>
by Kavvadias and Stavropoulos. Container sources available at the CompSysMed group <a href='\"//github.com/VeraLiconaResearchGroup/\"MHSGenerationAlgorit
hms/tree/master/containers/ks\">github page</a>.",
6   "algo_website": "http://lca.ceid.upatras.gr/~estavrop/transversal/",
7   "algo_keywords": ["minimum hitting set", "hypergraph transversal", "MHS"],
8-  "algo_authors": [
9-    {
10     "name": "Elias C. Stavropoulos",
11     "email": "estavrop@ceid.upatras.gr",
12     "organization": "Department of Computer Engineering and Informatics, University of Patras",
13     "org_website": "www.ceid.upatras.gr"
14    },
15-    {
16     "name": "Dimitris J. Kavvadias",
17     "email": "kavvadias@ceid.upatras.gr",
18     "organization": "Department of Computer Engineering and Informatics, University of Patras",
19     "org_website": "www.ceid.upatras.gr"
20    }
21  ],
22  "algo_exec": "./mhs",
23  "algo_input_stream": "file",
24  "algo_output_stream": "out.dat",
25  "input_type": "algorun:mhs-in",
26  "output_type": "algorun:mhs-out",
27  "algo_image": "compsysmed/ks"
28 }

```

Source Code: manifest.json of KS algorithm (comments-skimmed)

#### STEP 4:

- input\_example.txt: Copy and paste the following sample input:

```

{
  "sets": [
    [1, 2, 5],
    [3, 2, 4],
    [1, 3]
  ]
}

```

- output\_example.txt: Copy and paste the following sample output:

```

{"transversals": [[2], [3, 4], [4, 5]], "timeTaken": 0.002045721, "sets": [[1, 2, 5],
↪ [3, 2, 4], [1, 3]]}

```

#### STEP 5:

- From the directory where the Dockerfile exists, build KS container using:

```
docker build -t ks .
```

## References

## 2.3 Input/Output Types

### 2.3.1 algorun:DNASequence

Usage: A Short DNA Sequence

Example:

```
ATGCATCATGCGCCAT
```





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```

    }
  ],
  "target": "x4"
}
]
}
```

### 2.3.4 superadam:DiscreteDynamicalSystemSet

**Usage:** a set of discrete dynamical systems

**Example:**

```

{
  "type": "DiscreteDynamicalSystemSet",
  "description": "a description",
  "simulationName": "a name",
  "updateRules": [
    {
      "target": "CAP",
      "functions": [
        {
          "inputVariables": ["CAP"],
          "transitionTable": [
            [[0],0],
            [[1],1]
          ]
        }
      ]
    },
    {
      "target": "mRNA",
      "functions": [
        {
          "inputVariables": ["CAP", "LacI", "mRNA"],
          "transitionTable": [
            [[0,0,0],0],
            [[0,0,1],1],
            [[0,1,0],0],
            [[0,1,1],0],
            [[0,2,0],0],
            [[0,2,1],0],
            [[1,0,0],1],
            [[1,0,1],0],
            [[1,1,0],0],
            [[1,1,1],0],
            [[1,2,0],0],
            [[1,2,1],0]
          ]
        }
      ]
    }
  ],
  {
    "target": "LacY",
    "functions": [
```

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```

        {
            "inputVariables": ["mRNA", "LacY"],
            "transitionTable": [
                [[0,0],0],
                [[0,1],1],
                [[1,0],1],
                [[1,1],1]
            ]
        }
    ],
    {
        "target": "LacZ",
        "functions": [
            {
                "inputVariables": ["mRNA", "LacZ"],
                "transitionTable": [
                    [[0,0],0],
                    [[0,1],1],
                    [[1,0],1],
                    [[1,1],1]
                ]
            }
        ]
    },
    {
        "target": "LacI",
        "functions": [
            {
                "inputVariables": ["LacI"],
                "transitionTable": [
                    [[0],0],
                    [[1],1],
                    [[2],2]
                ]
            }
        ]
    }
],
"variables": [
    {
        "id": "CAP",
        "states": [0,1],
        "speed": 1
    },
    {
        "id": "mRNA",
        "states": [0,1],
        "speed": 1
    },
    {
        "id": "LacY",
        "states": [0,1],
        "speed": 1
    },
    {
        "id": "LacZ",

```

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```

        "states": [0,1],
        "speed": 1
    },
    {
        "id": "LacI",
        "states": [0,1,2],
        "speed": 1
    }
]
}

```

### 2.3.5 superadam:BooleanDynamicalSystemSet

**Usage:** a set of boolean dynamical systems

**Example:**

```

{
  "type": "BooleanDynamicalSystemSet",
  "description": "Sample Boolean Network",
  "parameters": [
    {
      "id": "k1",
      "states": [0,1]
    },
    {
      "id": "k2",
      "states": [0,1]
    }
  ],
  "updateRules": [
    {
      "target": "x1",
      "functions": [
        {
          "inputVariables": ["k1", "x3"],
          "booleanFunction": "k1 & x3"
        }
      ]
    },
    {
      "target": "x2",
      "functions": [
        {
          "inputVariables": ["x1", "k2"],
          "booleanFunction": "x1 | k2"
        }
      ]
    },
    {
      "target": "x3",
      "functions": [
        {
          "inputVariables": ["x4", "x2"],
          "booleanFunction": "x2 & !x4"
        }
      ]
    }
  ]
}

```

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```

    }
  ]
},
{
  "target": "x4",
  "functions": [
    {
      "inputVariables": ["x2", "k2"],
      "booleanFunction": "x2 & k2"
    }
  ]
}
],
"variables": [
  {
    "id": "x1",
    "states": [0,1]
  },
  {
    "id": "x2",
    "states": [0,1]
  },
  {
    "id": "x3",
    "states": [0,1]
  },
  {
    "id": "x4",
    "states": [0,1]
  }
]
}

```

### 2.3.6 superadam:TimeSeriesSet

**Usage:** A set of time series

**Example:**

```

{
  "type": "timeSeriesSet",
  "timeSeriesData": [
    {
      "index": [],
      "matrix": [
        [1,0,0,0],
        [0,1,0,1],
        [1,1,0,0]
      ],
      "name": "wildtype experiment 1"
    },
    {
      "index": [],
      "matrix": [

```

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```

        [1,1,0,0],
        [0,0,0,1],
        [1,0,0,0]
    ],
    "name": "wildtype experiment 2"
  },
  {
    "index": [1],
    "matrix": [
      [0,0,0,0],
      [0,0,0,1],
      [0,1,0,0],
      [0,0,0,1]
    ],
    "name": "knockout experiment 1"
  },
  {
    "index": [3],
    "matrix": [
      [0,1,0,0],
      [0,1,0,1],
      [0,1,0,1],
      [0,0,0,0]
    ],
    "name": "knockout experiment 2"
  },
  {
    "index": [2],
    "matrix": [
      [1,0,0,0],
      [0,0,0,1],
      [1,0,0,1],
      [0,0,0,0]
    ],
    "name": "knockout experiment 3"
  }
]
}

```

## 2.3.7 superadam:DirectedGraph

**Usage:** a directed graph representation

**Example:**

```

{
  "description": "",
  "fieldCardinality": 2,
  "name": "priorReverseEngineeringNetwork",
  "type": "directedGraph",
  "edges": [
    {
      "sources": [
        { "score": 0.5, "source": "x1" },
        { "score": 1, "source": "x2" },

```

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```

        { "score": 1, "source": "x3" },
        { "score": 1, "source": "x4" }
    ],
    "target": "x1"
},
{
    "sources": [
        { "score": 1, "source": "x2" },
        { "score": 1, "source": "x4" }
    ],
    "target": "x2"
},
{
    "sources": [
        { "score": 0.5, "source": "x1" },
        { "score": 0.5, "source": "x2" }
    ],
    "target": "x3"
},
{
    "sources": [
        { "score": 0.33, "source": "x2" },
        { "score": 0.66, "source": "x3" }
    ],
    "target": "x4"
}
]
}
```

## 2.3.8 superadam:AnnotatedGraph

**Usage:** an annotated graph representation

**Example:**

```

{
    "type": "AnnotatedGraph",
    "description": "Sample Annotated Graph",
    "node": [
        {
            "id" : "node0",
            "label": " 0 0 0 0 0"
        },
        {
            "id" : "node1",
            "label": " 0 0 0 0 1"
        },
        {
            "id" : "node2",
            "label": " 0 0 0 0 2"
        },
        {
            "id" : "node3",
            "label": " 0 0 0 1 0"
        }
    ],
}
```

(continues on next page)

(continued from previous page)

```
{
  "id" : "node4",
  "label": " 0 0 0 1 1"
},
{
  "id" : "node5",
  "label": " 0 0 0 1 2"
},
{
  "id" : "node6",
  "label": " 0 0 1 0 0"
},
{
  "id" : "node7",
  "label": " 0 0 1 0 1"
},
{
  "id" : "node8",
  "label": " 0 0 1 0 2"
},
{
  "id" : "node9",
  "label": " 0 0 1 1 0"
},
{
  "id" : "node10",
  "label": " 0 0 1 1 1"
},
{
  "id" : "node11",
  "label": " 0 0 1 1 2"
},
{
  "id" : "node12",
  "label": " 0 1 0 0 0"
},
{
  "id" : "node13",
  "label": " 0 1 0 0 1"
},
{
  "id" : "node14",
  "label": " 0 1 0 0 2"
},
{
  "id" : "node15",
  "label": " 0 1 0 1 0"
},
{
  "id" : "node16",
  "label": " 0 1 0 1 1"
},
{
  "id" : "node17",
  "label": " 0 1 0 1 2"
},
{
```

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```

    "id" : "node18",
    "label": " 0 1 1 0 0"
  },
  {
    "id" : "node19",
    "label": " 0 1 1 0 1"
  },
  {
    "id" : "node20",
    "label": " 0 1 1 0 2"
  },
  {
    "id" : "node21",
    "label": " 0 1 1 1 0"
  },
  {
    "id" : "node22",
    "label": " 0 1 1 1 1"
  },
  {
    "id" : "node23",
    "label": " 0 1 1 1 2"
  },
  {
    "id" : "node24",
    "label": " 1 0 0 0 0"
  },
  {
    "id" : "node25",
    "label": " 1 0 0 0 1"
  },
  {
    "id" : "node26",
    "label": " 1 0 0 0 2"
  },
  {
    "id" : "node27",
    "label": " 1 0 0 1 0"
  },
  {
    "id" : "node28",
    "label": " 1 0 0 1 1"
  },
  {
    "id" : "node29",
    "label": " 1 0 0 1 2"
  },
  {
    "id" : "node30",
    "label": " 1 0 1 0 0"
  },
  {
    "id" : "node31",
    "label": " 1 0 1 0 1"
  },
  {
    "id" : "node32",

```

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```

    "label": " 1 0 1 0 2"
  },
  {
    "id" : "node33",
    "label": " 1 0 1 1 0"
  },
  {
    "id" : "node34",
    "label": " 1 0 1 1 1"
  },
  {
    "id" : "node35",
    "label": " 1 0 1 1 2"
  },
  {
    "id" : "node36",
    "label": " 1 1 0 0 0"
  },
  {
    "id" : "node37",
    "label": " 1 1 0 0 1"
  },
  {
    "id" : "node38",
    "label": " 1 1 0 0 2"
  },
  {
    "id" : "node39",
    "label": " 1 1 0 1 0"
  },
  {
    "id" : "node40",
    "label": " 1 1 0 1 1"
  },
  {
    "id" : "node41",
    "label": " 1 1 0 1 2"
  },
  {
    "id" : "node42",
    "label": " 1 1 1 0 0"
  },
  {
    "id" : "node43",
    "label": " 1 1 1 0 1"
  },
  {
    "id" : "node44",
    "label": " 1 1 1 0 2"
  },
  {
    "id" : "node45",
    "label": " 1 1 1 1 0"
  },
  {
    "id" : "node46",
    "label": " 1 1 1 1 1"
  }

```

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(continued from previous page)

```

    },
    {
      "id" : "node47",
      "label": " 1 1 1 1 2"
    }
  ],
  "connection": [
    ["node0", "node0"],
    ["node1", "node1"],
    ["node2", "node2"],
    ["node3", "node3"],
    ["node4", "node4"],
    ["node5", "node5"],
    ["node6", "node6"],
    ["node7", "node7"],
    ["node8", "node8"],
    ["node9", "node9"],
    ["node10", "node10"],
    ["node11", "node11"],
    ["node12", "node21"],
    ["node13", "node10"],
    ["node14", "node11"],
    ["node15", "node21"],
    ["node16", "node10"],
    ["node17", "node11"],
    ["node18", "node21"],
    ["node19", "node10"],
    ["node20", "node11"],
    ["node21", "node21"],
    ["node22", "node10"],
    ["node23", "node11"],
    ["node24", "node36"],
    ["node25", "node25"],
    ["node26", "node26"],
    ["node27", "node39"],
    ["node28", "node28"],
    ["node29", "node29"],
    ["node30", "node42"],
    ["node31", "node31"],
    ["node32", "node32"],
    ["node33", "node45"],
    ["node34", "node34"],
    ["node35", "node35"],
    ["node36", "node33"],
    ["node37", "node34"],
    ["node38", "node35"],
    ["node39", "node33"],
    ["node40", "node34"],
    ["node41", "node35"],
    ["node42", "node33"],
    ["node43", "node34"],
    ["node44", "node35"],
    ["node45", "node33"],
    ["node46", "node34"],
    ["node47", "node35"]
  ]
}

```

### 2.3.9 superadam:SteadyStates

**Usage:** steady states of boolean dynamical system set

**Example:**

```
{
  "type": "SteadyStates",
  "description": "steady states of boolean dynamical system set",
  "steadystates": {
    "idorder": ["x1", "x2", "x3", "x4"],
    "value": [
      [0, 0, 0, 0],
      [1, 1, 1, 0]
    ]
  }
}
```

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## 2.5 Help

Please contact Abdelrahman Hosny at [abdelrahman.hosny@hotmail.com](mailto:abdelrahman.hosny@hotmail.com)



## CHAPTER 3

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## CHAPTER 4

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### Authors

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