Executable / code issues

Acyclic

Module 2 - Fail

Missing sample input files `ha_fv4_plus.csv` and `ha_target_data.csv`.

Module 3 - Fail

Module 2 failed, thus no usable `rt_desc.csv`, `rt_weights.txt` and `rt_biases.txt`.

Module 4 - Pass

Sample input file `ha_tv3500_n15_dia10_dmax3_k2_bn2_bh1.txt` not present in `instances` folder.

The required argument "*3. an integer of vector size bound per iteration*" is not given in the manual.

Tested with the following commands:

```
citrus@citrus-MS-7C94:~/lab/mol-infer/Acyclic/Module_4/2-branches$ ./main ./inst
ances/ha_tv6700.0_n31_dia20_k2_dmax3_bn3_bh1_solver1.txt 10 10000 2 output.sdf
Number of feasible pairs = 984
A lower bound on the number of graphs = 24310
Number of generated graphs = 2
Time : 0.193056s.
citrus@citrus-MS-7C94:~/lab/mol-infer/Acyclic/Module_4/2-branches$ ./main ./inst
ances/ha_tv3500.0_n15_dia10_k2_dmax3_bn3_bh1_solver1.txt 10 50 2 output.sdf
Number of feasible pairs = 33
A lower bound on the number of graphs = 39
Number of generated graphs = 2
Time : 0.0015746s.
```

Cyclic

Pass

Cyclic_improved

Module 3 - Fail

Seems fail to write the result to file.

```
citrus@citrus-MS-7C94:~/lab/mol-infer/Cyclic_improved/Module_3/files$ python3 infer_cy
clic_graphs_ec_id_vector.py ANN/FP 200 chemical_specification/instance_a.txt result 1
Initializing Time: 0.354
Start Solving Using CPLEX...
Status: Feasible
MILP y*: 203.819
Traceback (most recent call last):
  File "infer_cyclic_graphs_ec_id_vector.py", line 555, in <module>
    main(sys.argv)
  File "infer_cyclic_graphs_ec_id_vector.py", line 472, in main
    fv_result = subprocess.run(
  File "/usr/lib/python3.8/subprocess.py", line 493, in run
    with Popen(*popenargs, **kwargs) as process:
  File "/usr/lib/python3.8/subprocess.py", line 858, in __init__
    self._execute_child(args, executable, preexec_fn, close_fds,
  File "/usr/lib/python3.8/subprocess.py", line 1704, in _execute_child
    raise child_exception_type(errno_num, err_msg, err_filename)
FileNotFoundError: [Errno 2] No such file or directory: './fv'
```

2L-model

Module 3 - Fail

Example is infeasible.

```
citrus@citrus-MS-7C94:~/lab/mol-infer/2L-model/Module_3/files$ python3 infer_gra
ph_2L_fc.py ANN/KOW 3.2 topological_description/instance_a.txt fringe_set/ins_a_
fringe.txt result 1
Initializing Time: 0.463
Number of variables: 7663
 - Integer : 7395
 - Binary  : 6050
Number of constraints: 9162
Status: Infeasible
Solving Time: 0.192
```
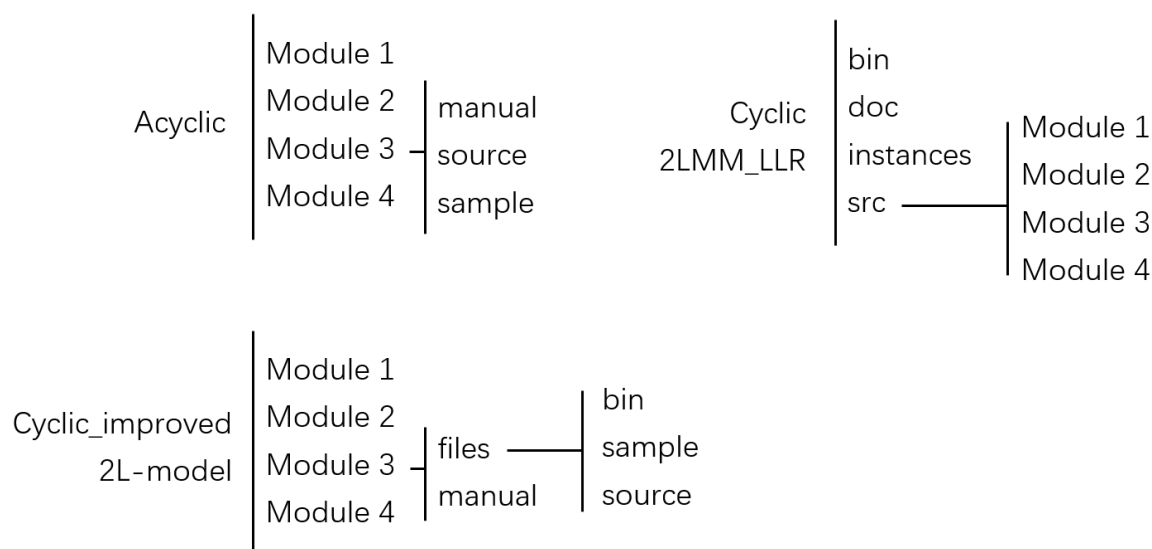
2LMM-LLR

Pass

Documentation / file issues

Overall

Acyclic claims documentation should be written in Markdown. But existing documentation (except the Acyclic Module 1) are using Latex. Should we transfer to Markdown?

Each part have a different file structure.

```
Acyclic     Module 1
            Module 2    manual
            Module 3 —  source
            Module 4    sample

Cyclic      bin
2LMM_LLR    doc
            instances          Module 1
            src —              Module 2
                               Module 3
                               Module 4

Cyclic_improved  Module 1
2L-model         Module 2            bin
                 Module 3 —  files — sample
                 Module 4    manual  source
```

Some underscores ("_") would disappear when copying and pasting commands into the terminal.

Acyclic

Inconsistent manual filename. (`Readme.md` , `Manual_Module_2_en.pdf` , `Manual_MILP_BH_en.pdf` , `Module4_manual_en.pdf`)

Module 2 - `Readme_ja.md` is empty. | Hyperlinks in `Readme.md` are broken.

Module 3 - The second half of `Manual_MILP_BH_en.pdf` is written in Japanese. | Hyperlink in `REDME.md` is broken. | No Japanese documentation.

Module 4 - Folder and file names do not match the manual (It seems lots of folders and files are modified and the manuals have not been updated).

Cyclic

Documentation for all 4 modules are in a single file (`Manual_Cyclic_en.pdf`). Should we separate it into different files?

`.DS_Store` files should be removed. (Use gitignore).

In manual page 12: Should add a `../` to the front of `instances/BP/BP_desc.csv` in example command.

Cyclic_improved

Module 3 - In `infer_cylic_graphs_ec_id.py`, solver type in arguments is ignored (line 26, 27) and hard coded (line 59). (Solver type is provided in command arguments.)

Module 4 - Incorrect filename in English manual (while it's correct in Japanese manual). Claimed `generate_isomers.cpp`, but it should be `main.cpp` (pages 6 & 7).

2L-model

Module 1 - No English documentation.

Module 2 - No English documentation.

Module 3 - No Japanese documentation.

Module 4 - `Manual_Module_4_2L-model_en.pdf` has no menu (it's a blank page). | Unnecessary `\` in English manual (page 5, section 3.2.1, Compiling the program, `g++ -o generate_isomers generate\_isomers.cpp -O3 -std=c++11`).

2LMM-LLR

Module 1 - Missing Makefile.