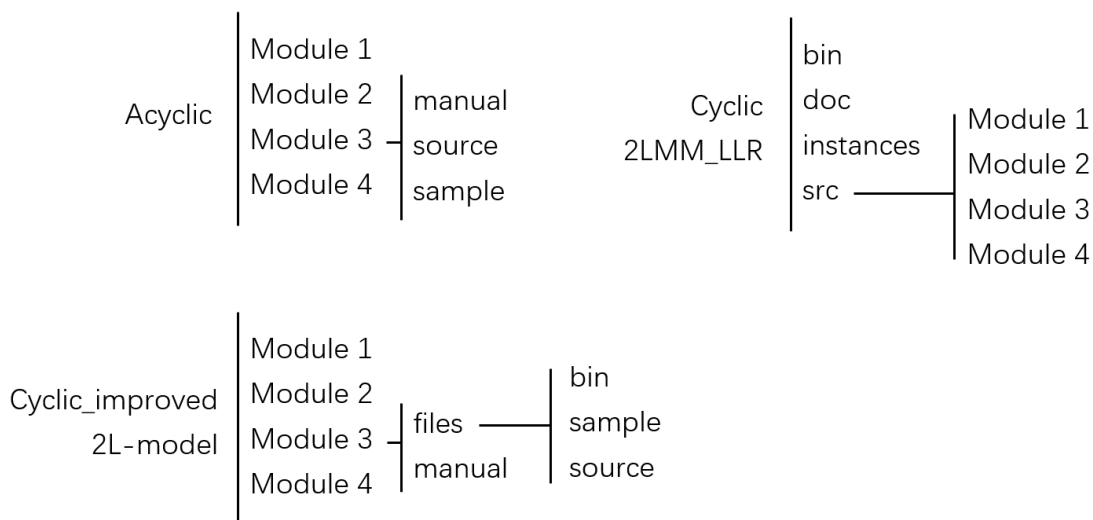


Overall Issues

1. **Acyclic** claims documentation should be written in Markdown. But existing documentation (except the Acyclic Module 1) are using Latex. Should we transfer to Markdown?
2. Each part have a different file structure.



3. Some underscores ("_") would disappear when copying and pasting commands into the terminal.
4. CBC solver cannot find feasible solution for MILPs. Currently not tested with CPLEX (I don't have a software license). Marked as **Not tested**.

Acyclic

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

Module 1 Pass

None

Module 2 Fail

`Readme_ja.md` is empty.

Hyperlinks in `Readme.md` are broken.

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

Module 3 Fail

The second half of `Manual_MILP_BH_en.pdf` is written in Japanese.

Hyperlink in `REDME.md` is broken.

No Japanese documentation.

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

Module 4 Pass

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).

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 ./instances/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 ./instances/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

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).

Module 1 Pass

None

Module 2 Pass

In manual page 12:

```
python predict_values.py output_weights.txt output_biases.txt \
instances/BP/BP_desc.csv predicted.txt
```

should be

```
python predict_values.py output_weights.txt output_biases.txt \
../instances/BP/BP_desc.csv predicted.txt
```

(Adding a `../` to the front of `instances/BP/BP_desc.csv`)

Module 3 Not tested

Solver type is hard coded in `infer_cyclic_graphs_ec_id.py`, line 61.

Module 4 Fail

No concrete example for `generate_isomers` (no idea how to fill in command arguments).

Got Segmentation fault when executing `generate_isomers` (probably due to incorrect arguments).

```
citrus@citrus-MS-7C94:~/lab/mol-infer/Cyclic/bin/linux$ ./generate_isomers ../../instances/chemical_specification/instance_a.txt 10 10000000 5 2 output.sdf ../../instances/KOW/KOW_MILP_partition.txt
Segmentation fault (core dumped)
citrus@citrus-MS-7C94:~/lab/mol-infer/Cyclic/bin/linux$ ./generate_isomers ../../instances/chemical_specification/instance_b1.txt 10 10000000 5 2 output.sdf ../../instances/BP/BP_MILP_partition.txt
Segmentation fault (core dumped)
citrus@citrus-MS-7C94:~/lab/mol-infer/Cyclic/bin/linux$ ./generate_isomers ../../instances/chemical_specification/instance_a.txt 10 10000000 5 2 output.sdf ../../instances/BP/BP_MILP_partition.txt
Segmentation fault (core dumped)
```

Cyclic_improved

Module 1 Pass

None

Module 2 Pass

None

Module 3 Not tested

In `infer_cyclic_graphs_ec_id.py`, solver type in arguments is ignored (line 26, 27) and hardcoded (line 59). (Solver type is provided in command arguments.)

Module 4 Pass

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 Pass

No English documentation.

Module 2 Pass

No English documentation.

Module 3 Not tested

No Japanese documentation.

Module 4 Pass

`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

All references In the manual are corrupted. (displayed as "?" or "??").

Lots of `src` are misspelled as a `scr`: page 3, 25, 26.

Module 1 Pass

Missing Makefile.

Typo:

1. `src/Module1/fringe/RootedGraph.hpp`. Should be `RootedGraph.hpp`
2. In manual page 3, `./FV_2LMM_V018 ../scr/Module1/sample_instance/sample1.sdf`
`output.csv`. `scr` should be `src`.

Module 2 Pass

None

Module 3 Not tested

In manual page 16, last line: `python infer_2LMM_L.py ../src/Module 3/sample instance/Hc`
`1900 1920`, `infer_2LMM_L.py` should be `infer_2LMM_LL.R.py`

Module 4 Pass

None