

# GSEE Benchmark Standard Report

Report based on data from 2025-01-28T21:50:06.833854+00:00

<https://github.com/isi-usc-edu/qb-gsee-benchmark>

Input data: Hamiltonian\_features.csv, last modified Tue Jan 28 11:45:36 2025

Input data: GSEE-HC\_utility\_estimates\_all\_instances\_task\_uuids\_v2.csv, last modified Thu Jan 9 12:11:19 2025

Latest creation time for a problem\_instance.json file: Mon Jan 27 11:42:37 2025

Latest creation time for a solution.json file: Tue Jan 28 11:45:36 2025

## Problem Instance Summary Statistics

number of problem\_instances: 84.

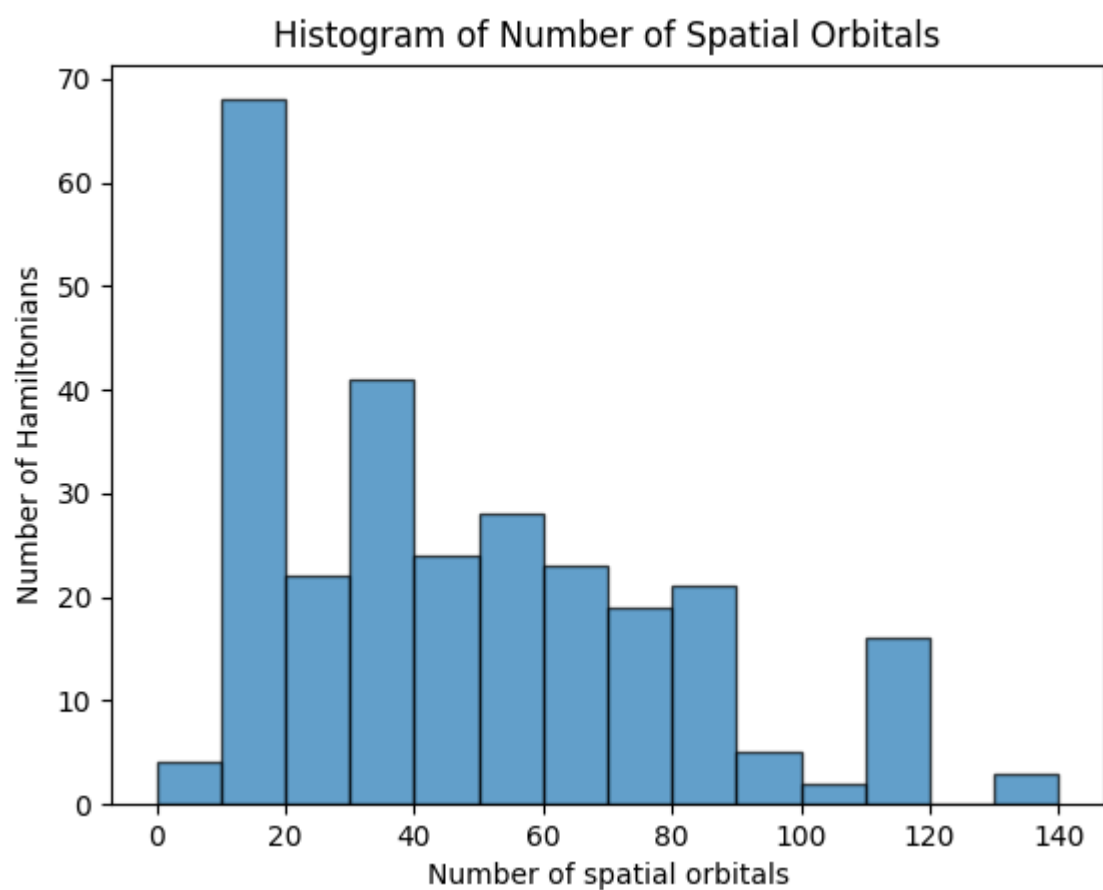
problem\_instance.json with the most tasks: 30 (hubbard\_square/614c4444-a31a-4348-b24d-01040208651c)

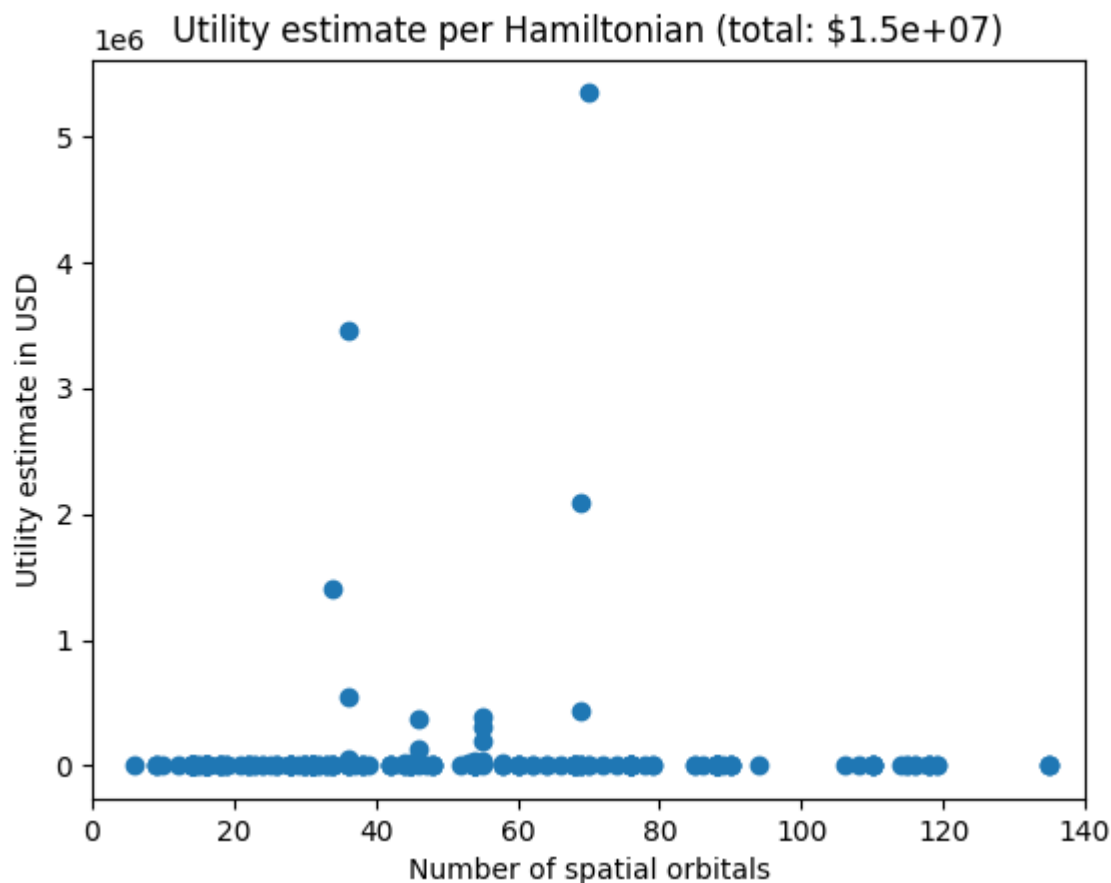
number of Hamiltonians (i.e., tasks) we have features calculated for: 276

minimum number of orbitals: 6

median number of orbitals: 42.0

maximum number of orbitals: 135





## Solver Summary Statistics

number of unique participating solvers: 16

Solver: SHCI\_opt/2dde727e-a881-44fa-aabf-bba6248e4baf, ML Solvability Ratio: 1.0, F1 Score: [0.83333333 0.99342105]

Solver: SHCI\_pt\_1e-4/4ed500f1-0650-41e3-af00-e4d0359394b4, ML Solvability Ratio: 0.9859, F1 Score: [0.71428571 0.97222222]

Solver: SHCI\_var\_1e-4/7e730dfb-57ee-480b-a8a1-4b73f5f07c54, ML Solvability Ratio: 0.8794, F1 Score: [0.99212598 0.99470899]

Solver: SHCI\_pt\_2e-4/ad964781-302e-4728-a26d-39918e0a6cdb, ML Solvability Ratio: 1.0, F1 Score: [0.64516129 0.96140351]

Solver: SHCI\_pt\_2e-5/c71b90bd-3250-4c0c-b4e7-fc9878f141f6, ML Solvability Ratio: 1.0, F1 Score: [0.375 0.96666667]

Solver: SHCI\_pt\_5e-5/d626506c-7aae-4ad6-802a-b29af5f2bb93, ML Solvability Ratio: 1.0, F1 Score: [0.9375 0.99295775]

Solver: SHCI\_var\_2e-4/0db183e3-a86d-491b-9125-599556e37c7a, ML Solvability Ratio: 0.0833, F1 Score: [0.95364238 0.95757576]

Solver: SHCI\_var\_2e-5/86bfe50c-9342-4d54-bb68-abc8abd95688, ML  
Solvability Ratio: 0.3942, F1 Score: [0.8627451 0.97358491]

Solver: SHCI\_var\_5e-5/01949b95-c427-4693-9134-01f47f688c09, ML  
Solvability Ratio: 0.3549, F1 Score: [0.83950617 0.94468085]

Solver: DF\_QPE/5dad4064-cd11-412f-85cb-d722afe3b3de, Model could not  
be calculated.

Solver: CISD/418f060e-496b-4024-8d2d-9b1f8791e76d, ML Solvability  
Ratio: 0.003, F1 Score: [0.97826087 0.85 ]

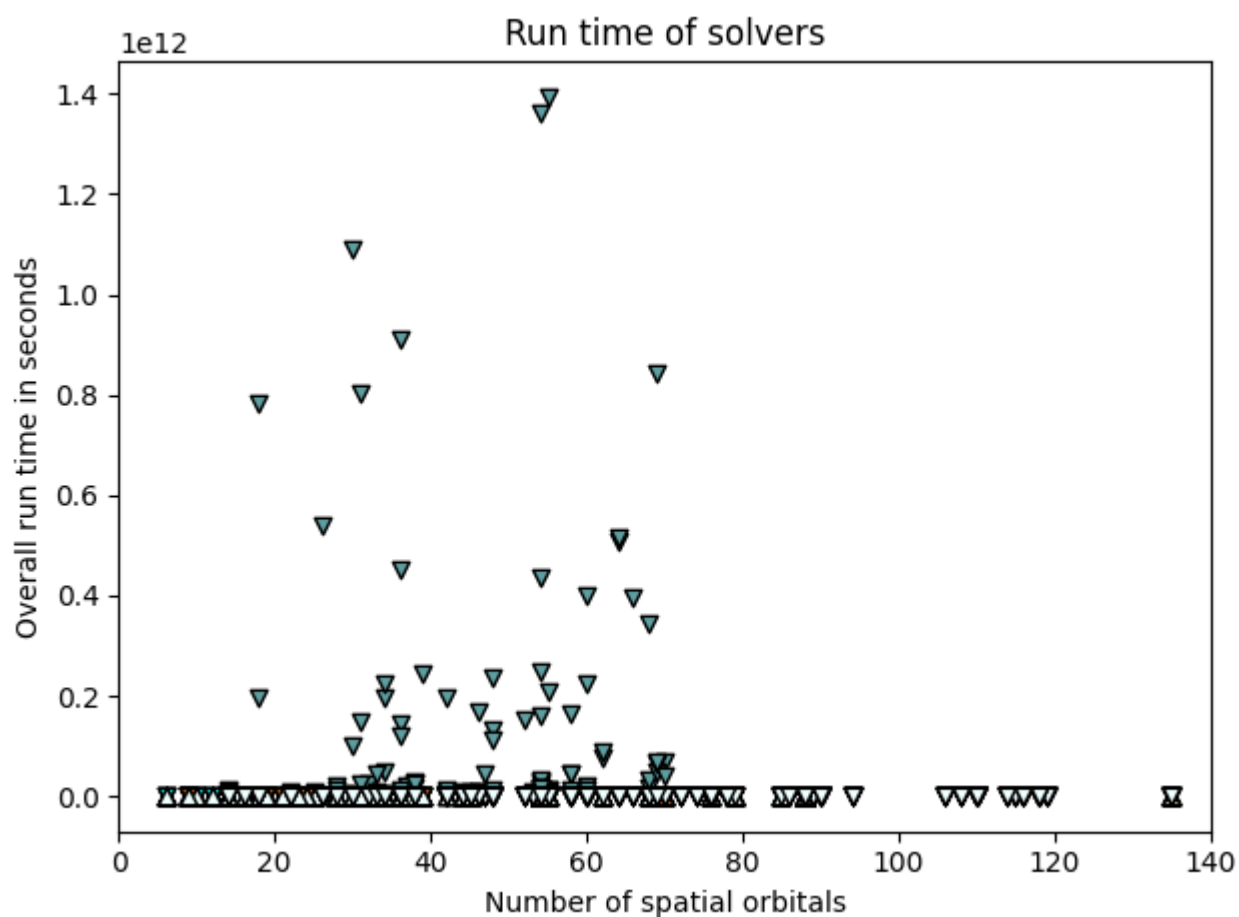
Solver: CCSD(T)/c09217e6-d0f7-4b0f-81c4-79210b7ac878, ML Solvability  
Ratio: 0.8102, F1 Score: [0.86956522 0.86451613]

Solver: HF/5f5e617a-19c2-4d82-bebc-b2d6b3dcb012, ML Solvability Ratio:  
0.0, F1 Score: [0.98675497 0.71428571]

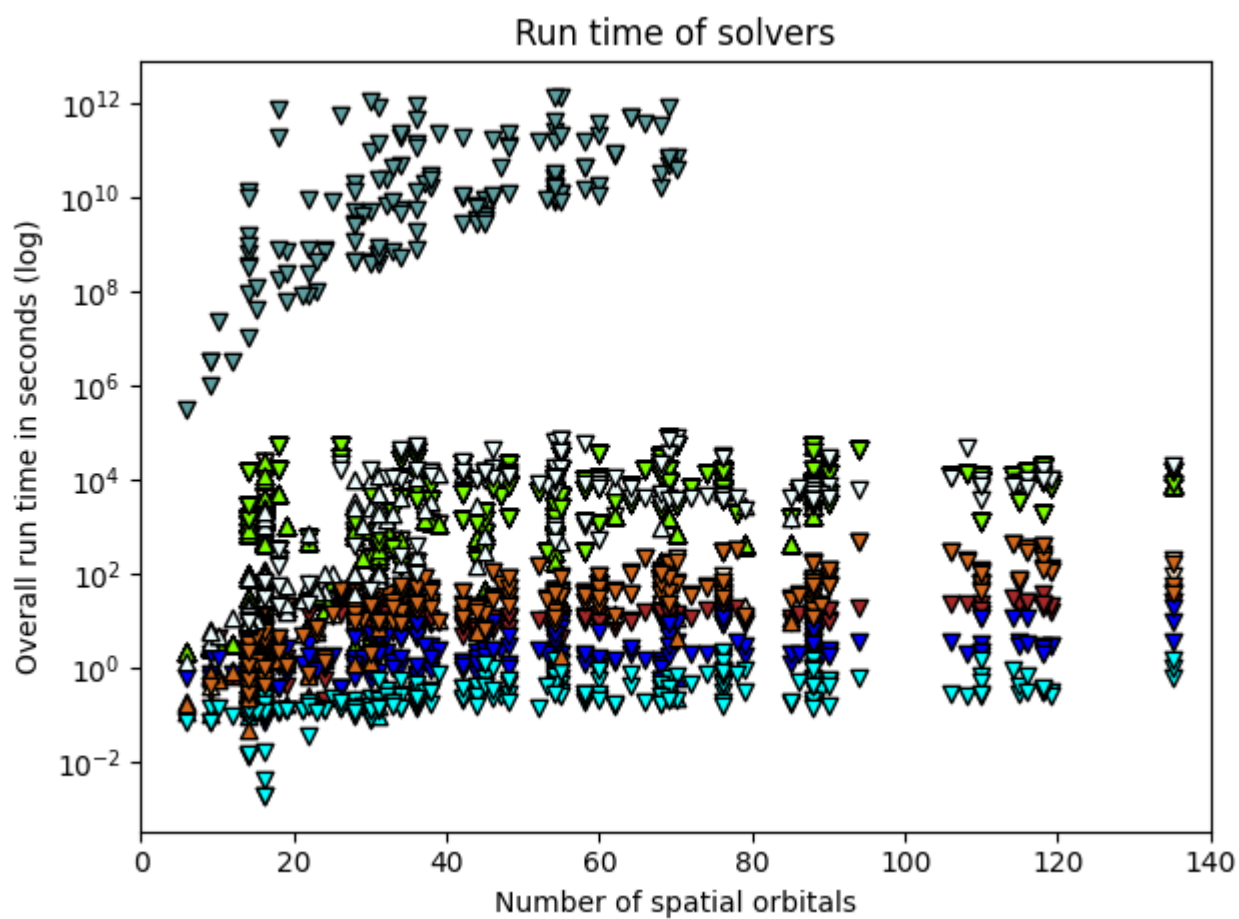
Solver: MP2/b420358b-5def-41e6-8c5d-b9d93b6aec2, ML Solvability Ratio:  
0.0, F1 Score: [0.98675497 0.71428571]

Solver: CCSD/0a29e54f-bef9-4d19-bafa-d94b1c4b37aa, ML Solvability Ratio:  
0.0197, F1 Score: [0.98867925 0.94117647]

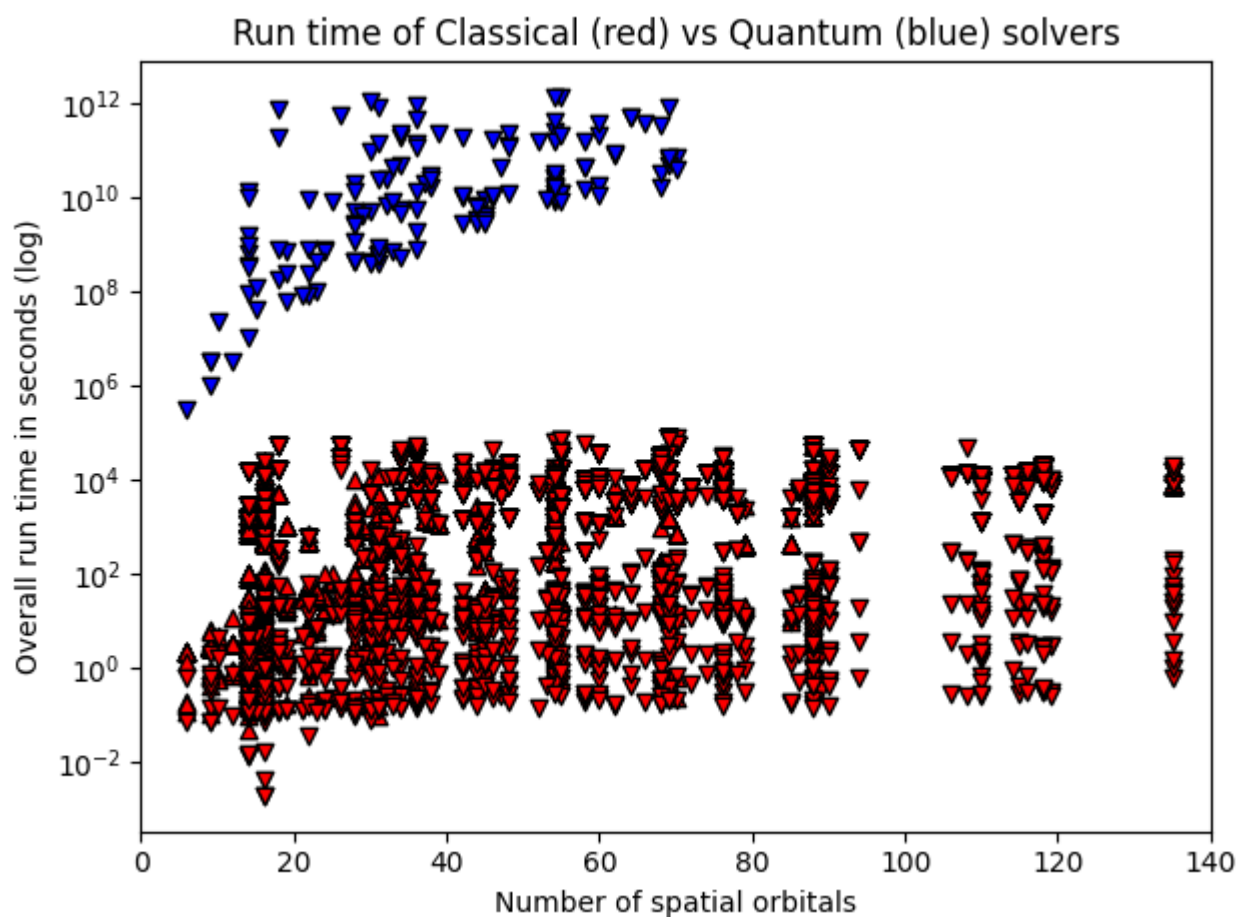
Solver: DMRG\_Niagara\_cluster\_lowest\_energy/16537433-9f4c-4eae-  
a65d-787dc3b35b59, ML Solvability Ratio: 0.6106, F1 Score: [0.96629213  
0.98678414]



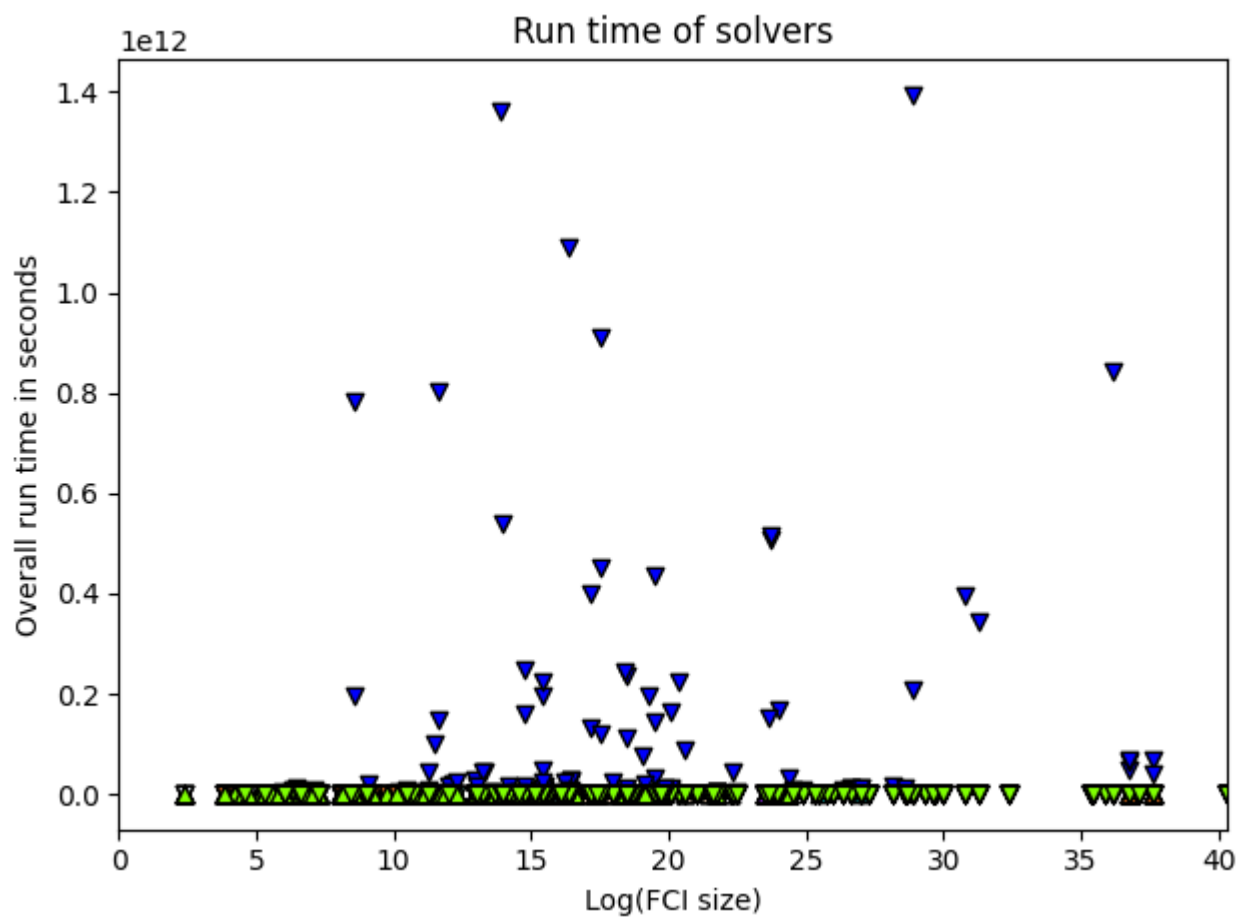
NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.



NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

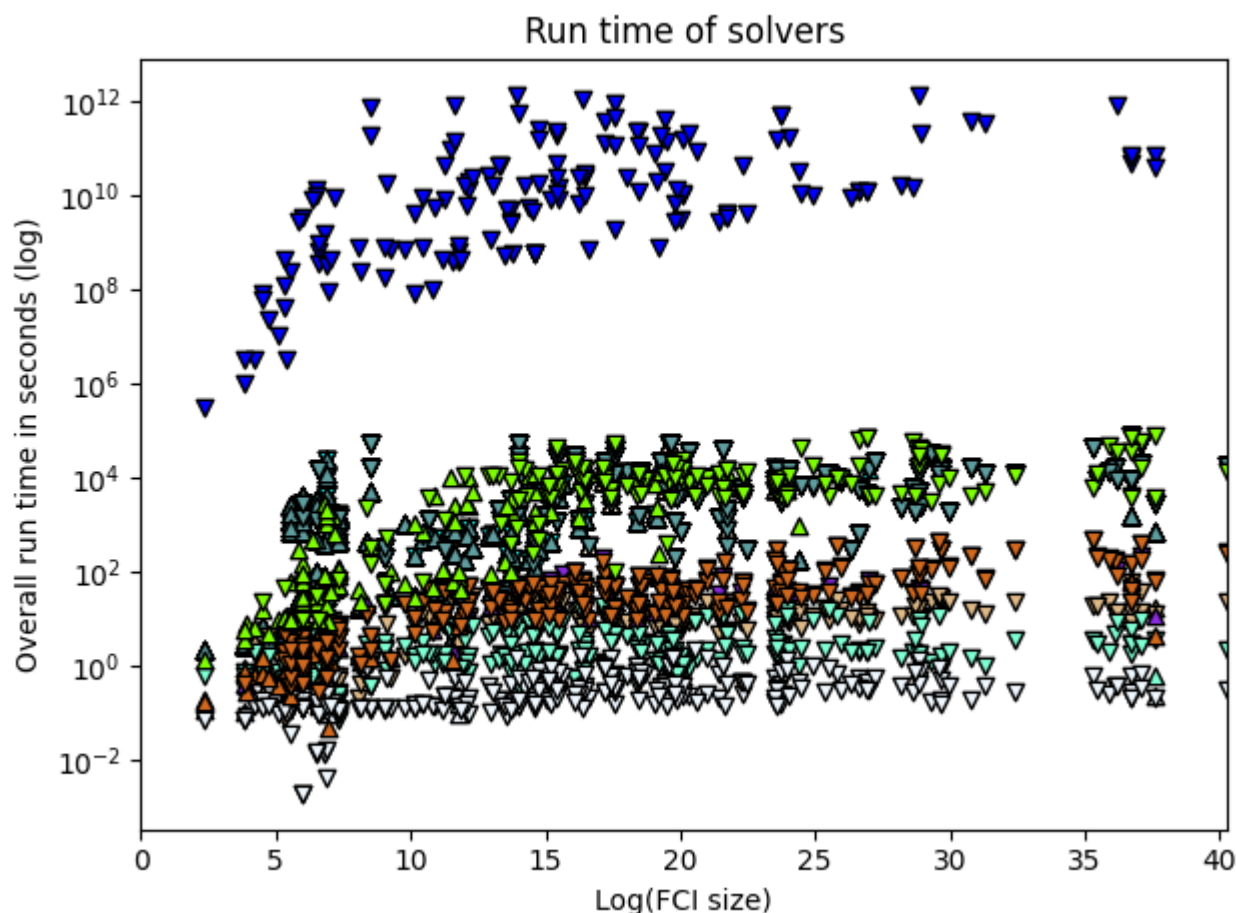


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.



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## **Solver SHCI\_opt, 2dde727e-a881-44fa-aabf-bba6248e4baf**

solver\_uuid:2dde727e-a881-44fa-aabf-bba6248e4baf

solver\_short\_name:SHCI\_opt

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with optimized orbitals followed by SHCI+PT

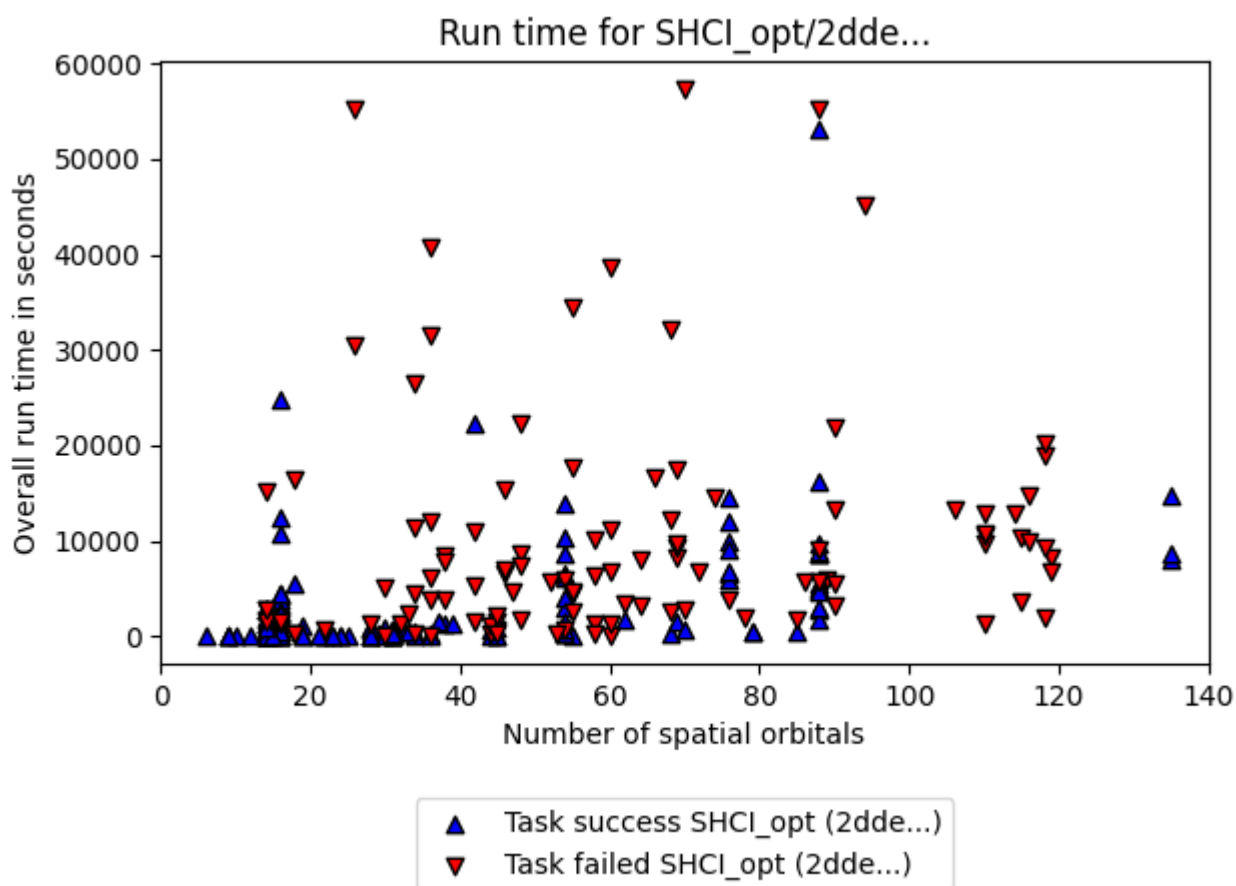
software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 0503c522-5530-488b-b5d3-3a26b4544d21

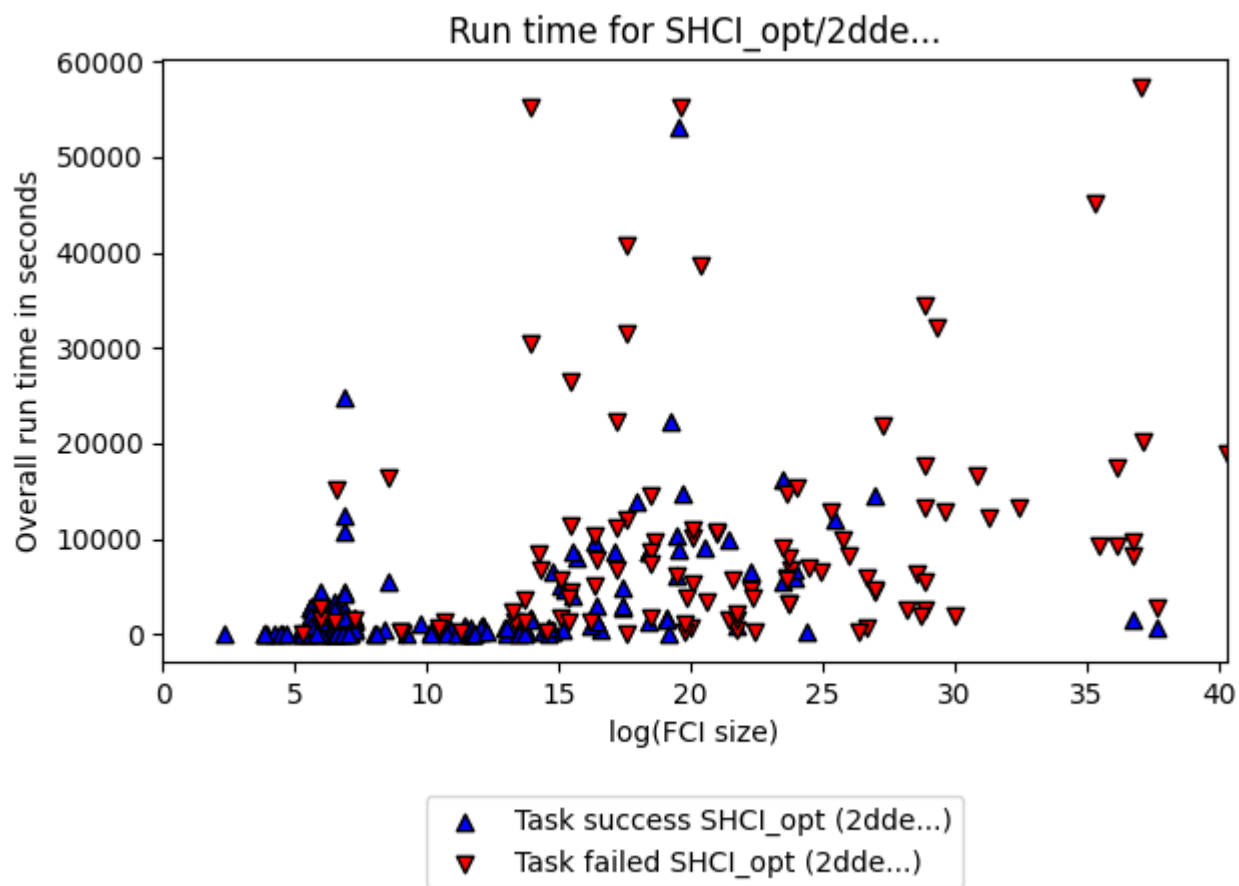
creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 80  
number\_of\_problem\_instances\_solved: 33  
number\_of\_tasks: 276  
number\_of\_tasks\_attempted: 265  
number\_of\_tasks\_solved: 153  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 265  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 153  
max\_run\_time\_of\_attempted\_tasks: 57334.2  
sum\_of\_run\_time\_of\_attempted\_tasks: 1553340.6179999998  
solvability\_ratio: 1.0  
f1\_score: [0.8333333333333334, 0.993421052631579]  
ml\_metrics\_calculator\_version: 1



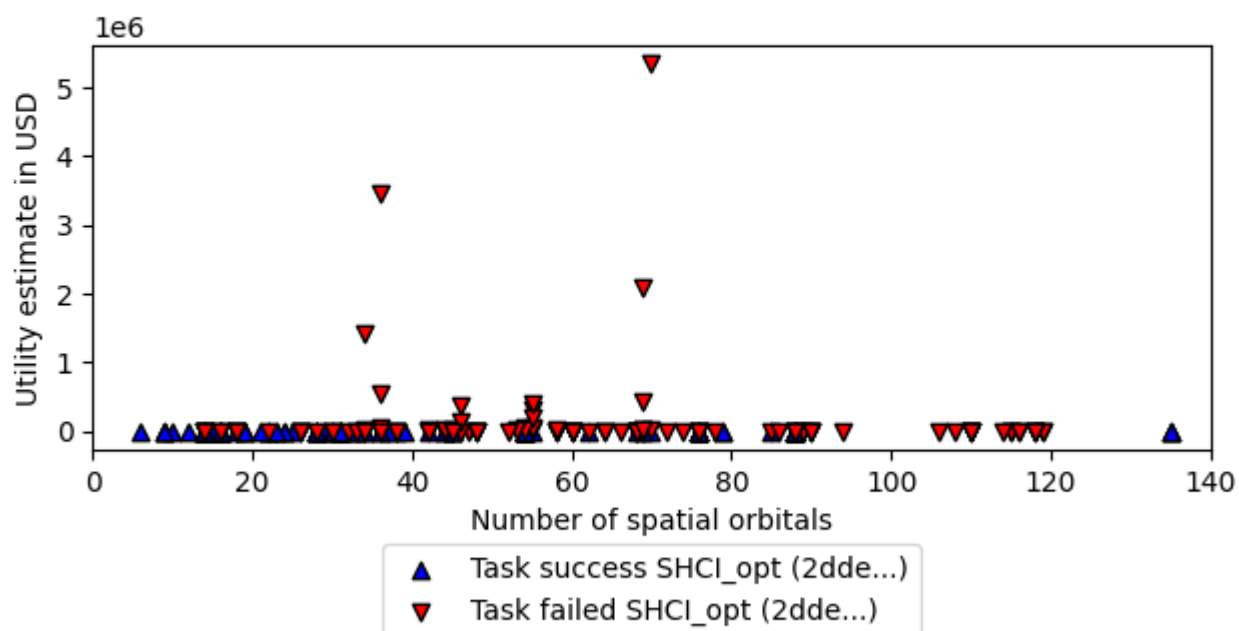
Note: plot only contains attempted tasks.

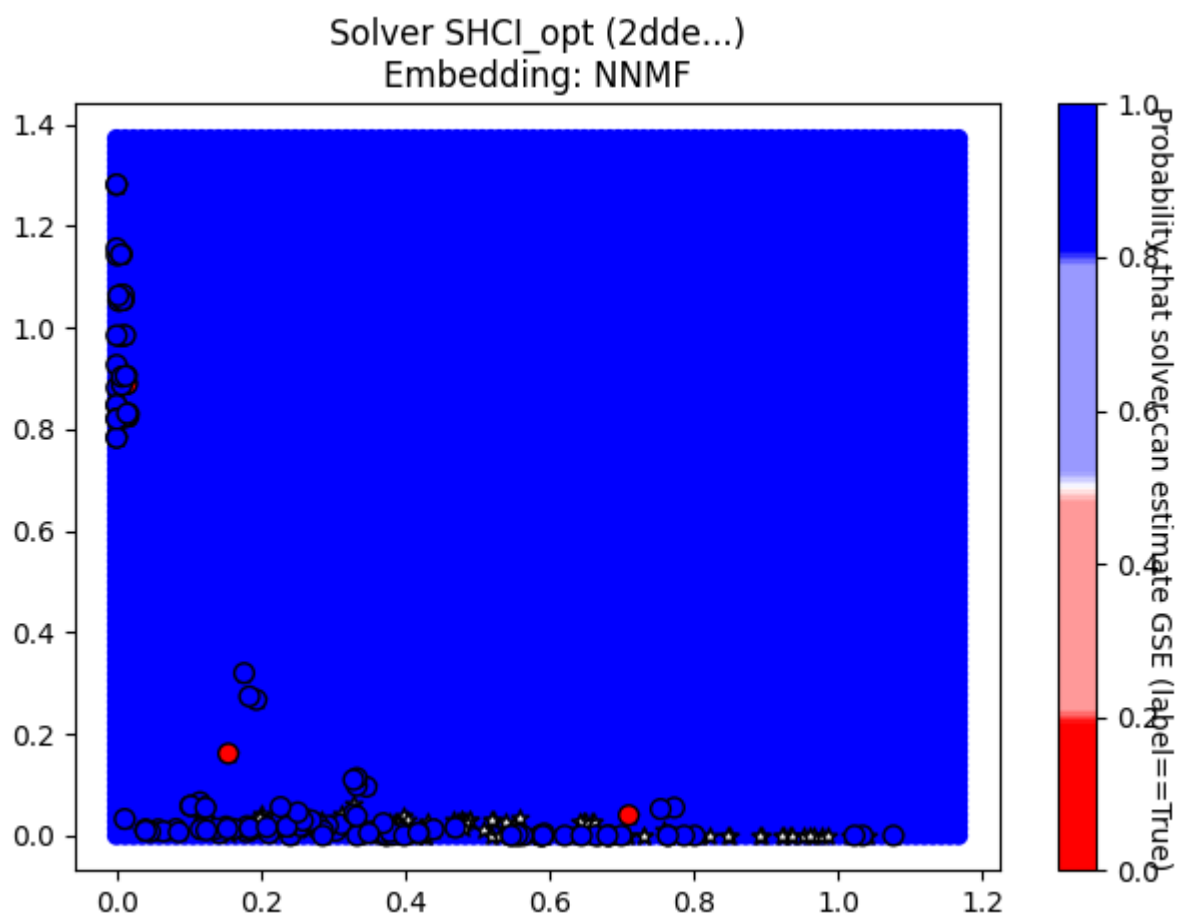


Note: plot only contains attempted tasks.

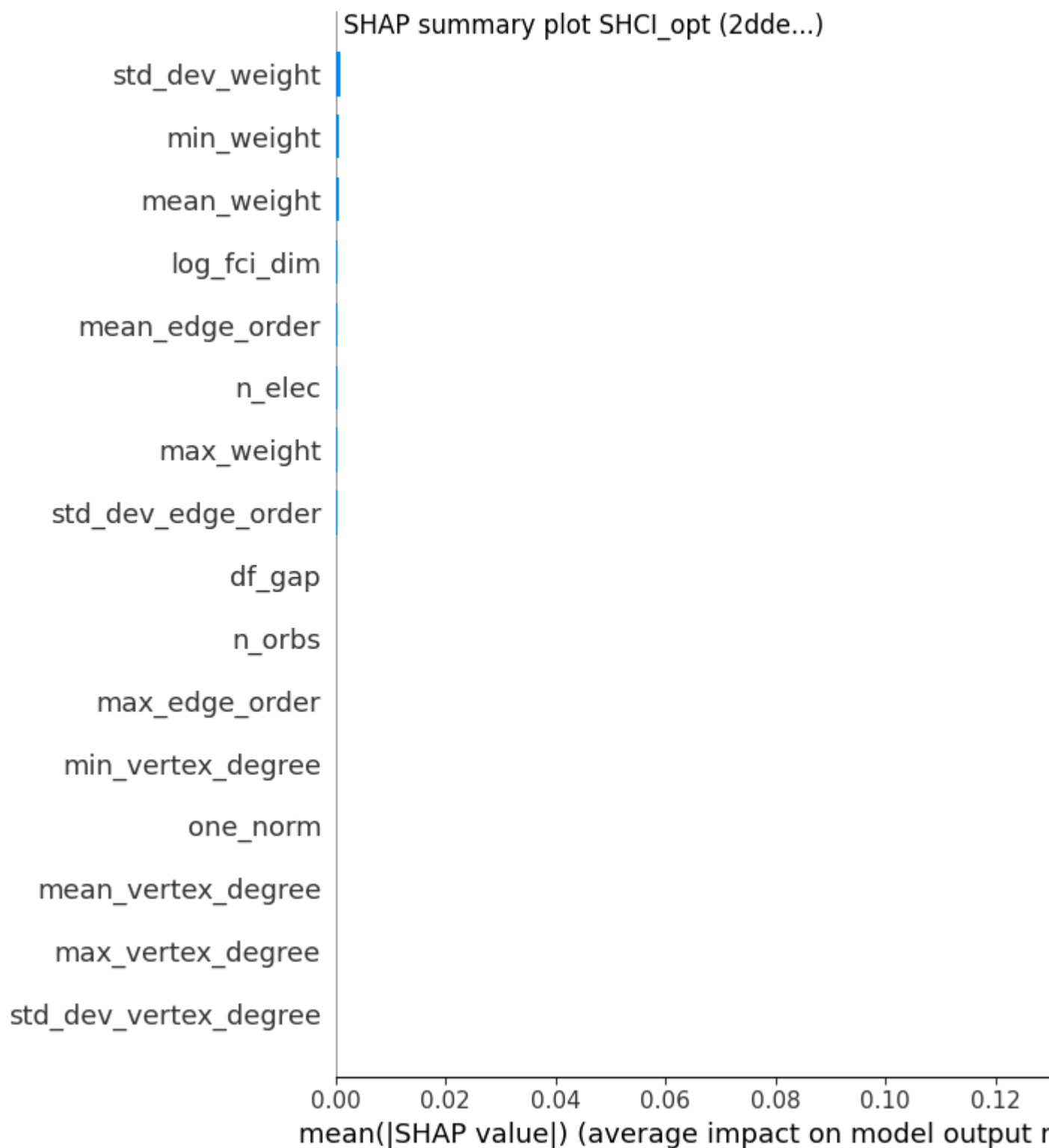
# Utility capture from SHCI\_opt/2dde...

(captured:  $\$8.0\text{e}+02/1.5\text{e}+07$ , approximately  $5.3\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_pt\_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4**

solver\_uuid:4ed500f1-0650-41e3-af00-e4d0359394b4

solver\_short\_name:SHCI\_pt\_1e-4

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 1e-4 + PT

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 705809bf-aa08-4c34-942a-1164cf5861d8

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 22

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 140

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 140

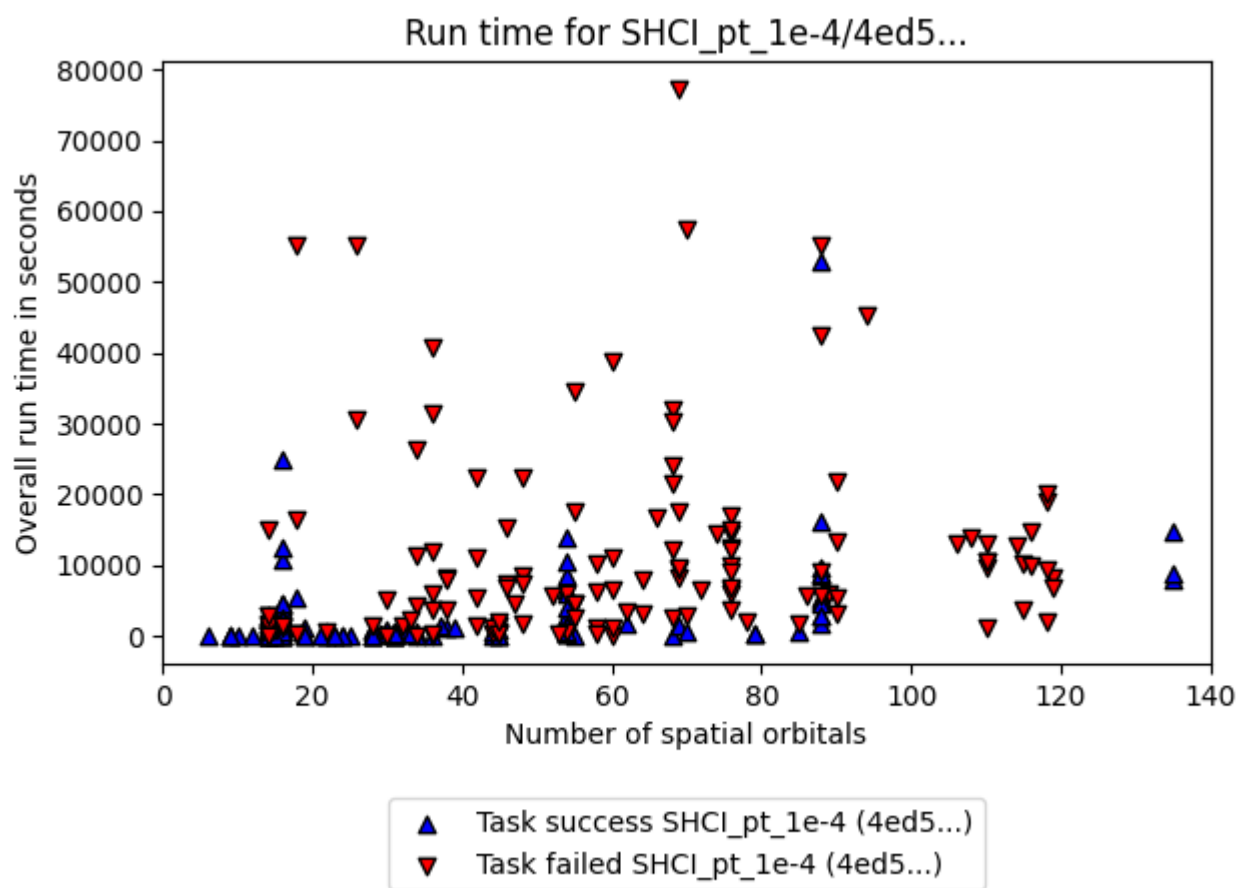
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

solvability\_ratio: 0.9859

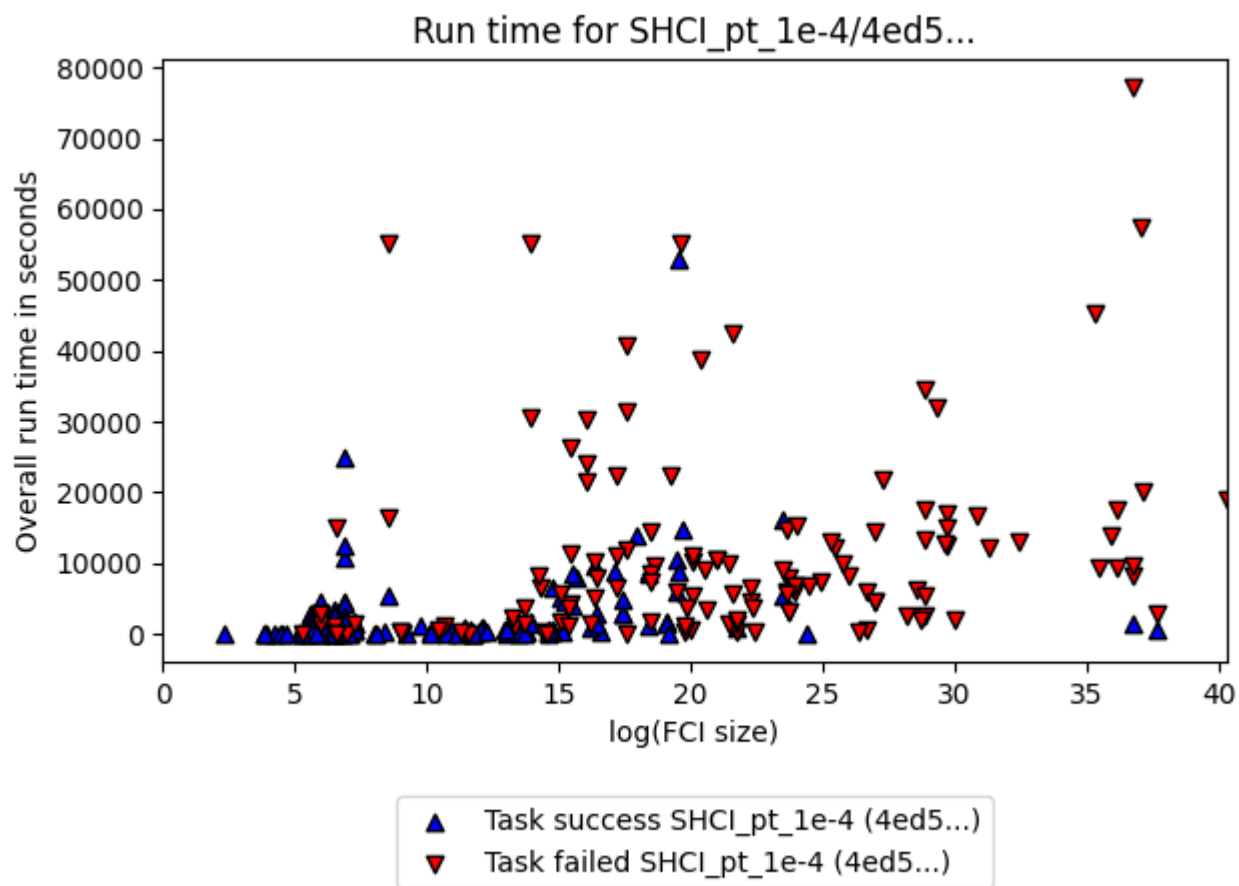
f1\_score: [0.7142857142857143, 0.9722222222222222]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

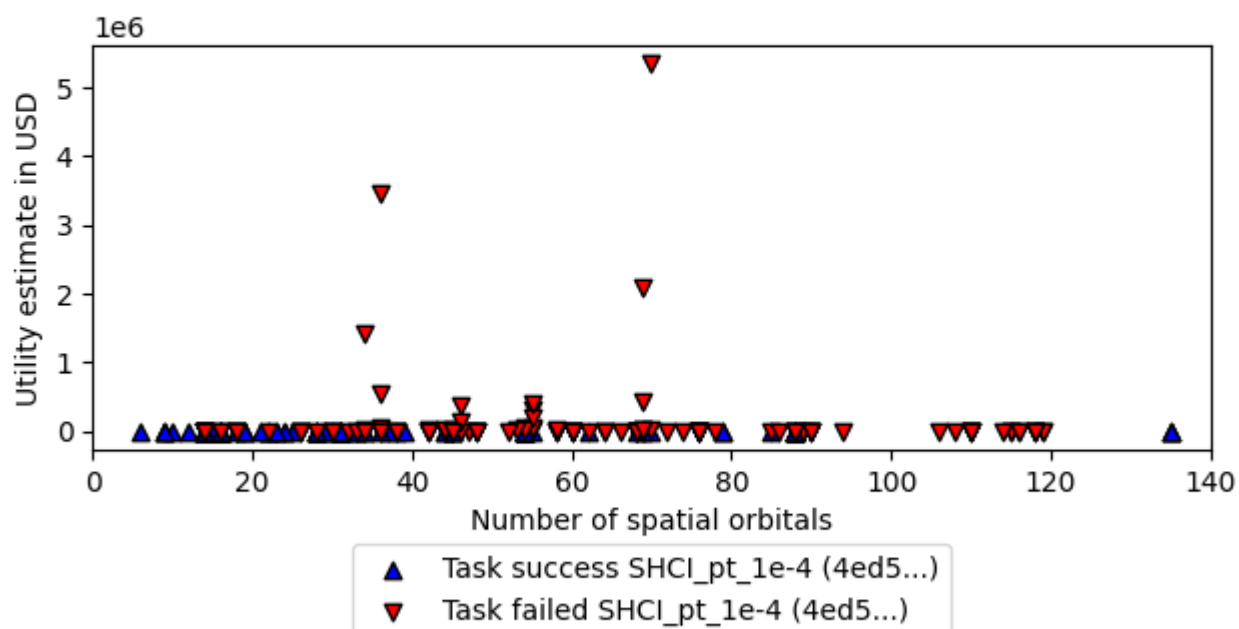


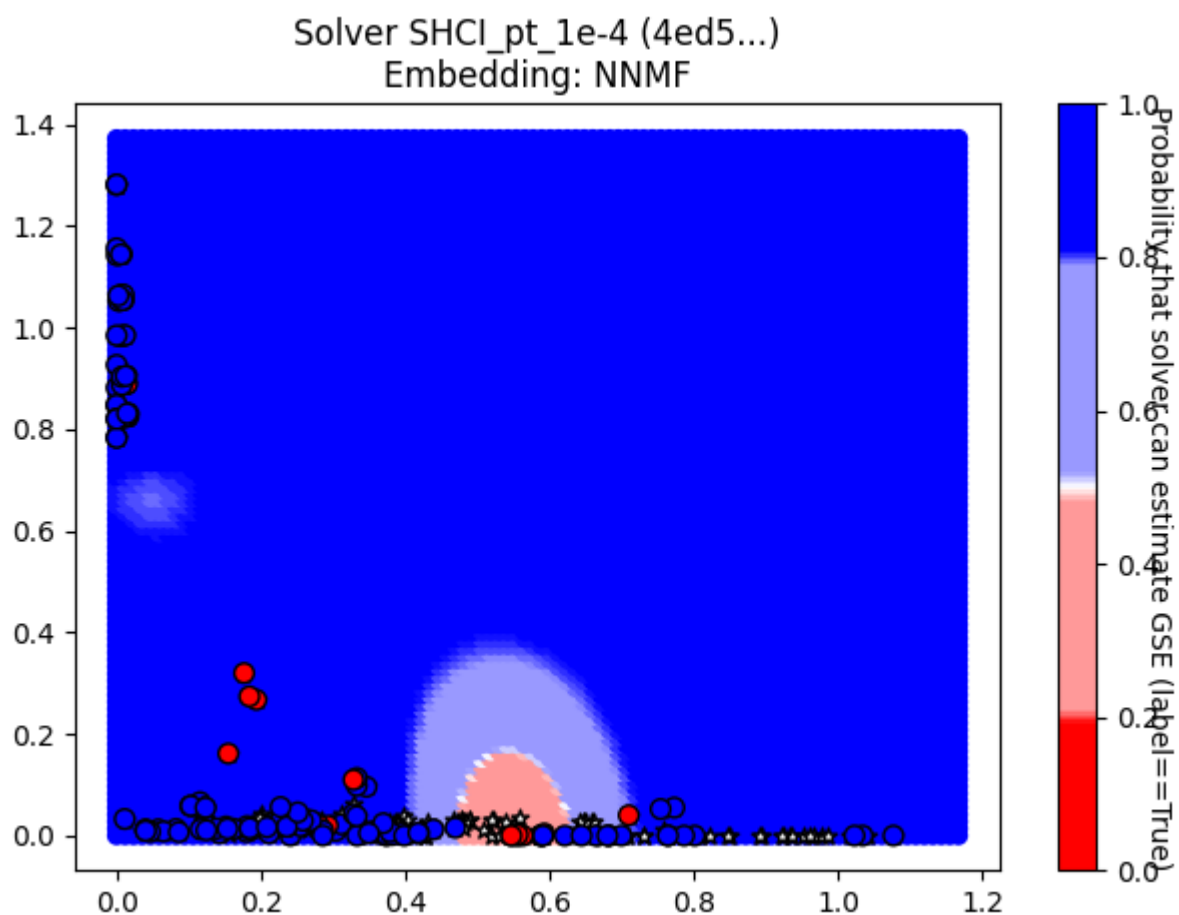


Note: plot only contains attempted tasks.

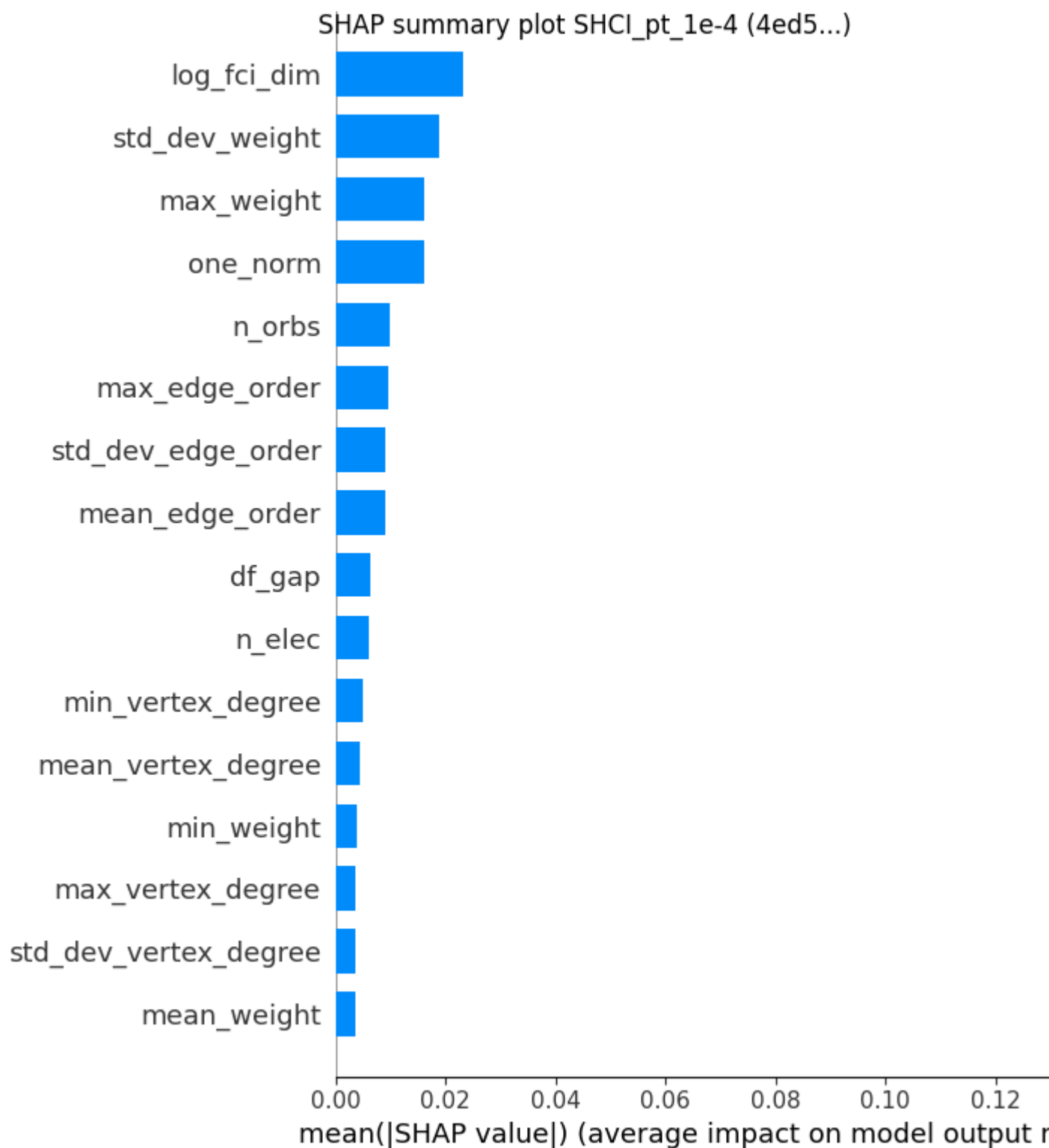
### Utility capture from SHCI\_pt\_1e-4/4ed5...

(captured:  $\$4.9\text{e}+02/1.5\text{e}+07$ , approximately  $3.3\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_var\_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54**

solver\_uuid:7e730dfb-57ee-480b-a8a1-4b73f5f07c54

solver\_short\_name:SHCI\_var\_1e-4

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 1e-4

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: f6651392-bd78-4907-bffc-502553f28bfd

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 13

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 95

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 95

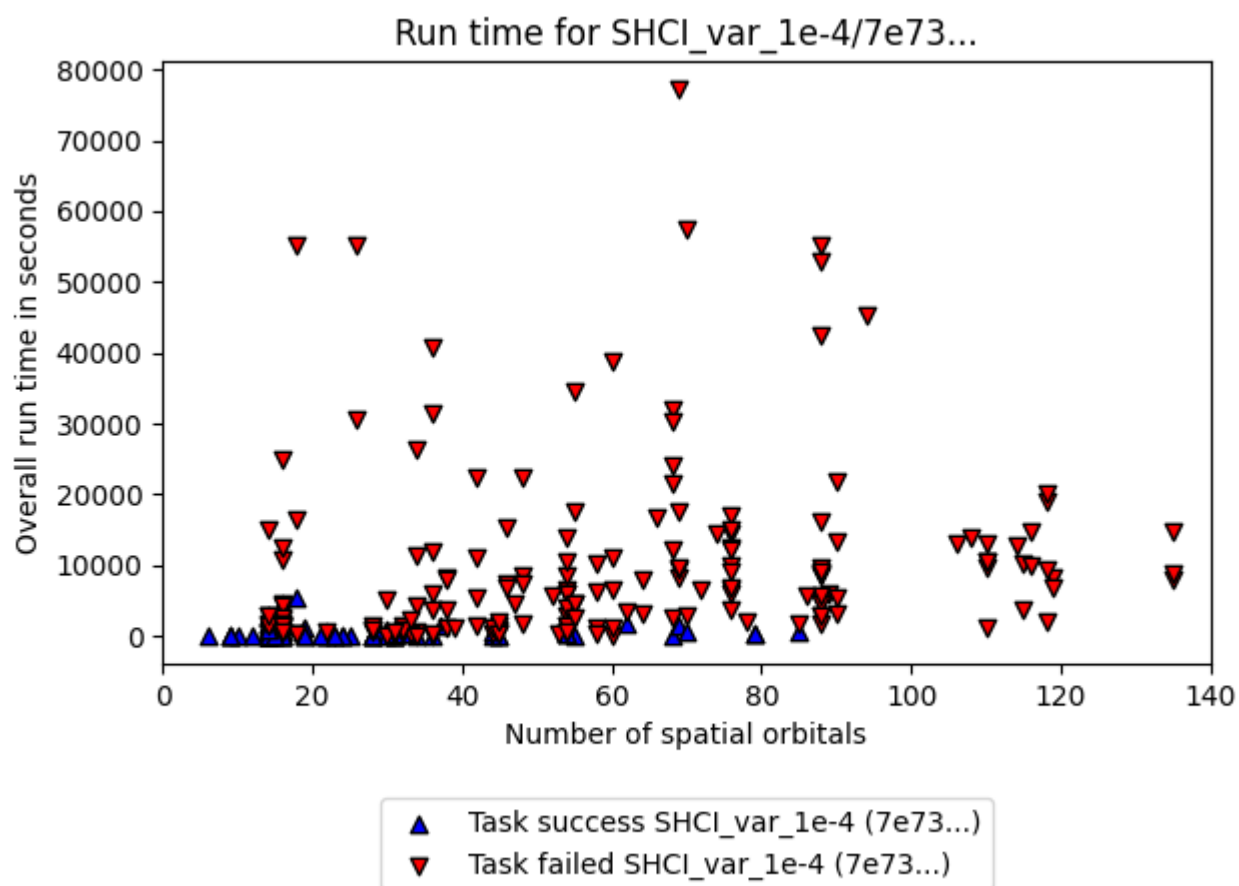
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

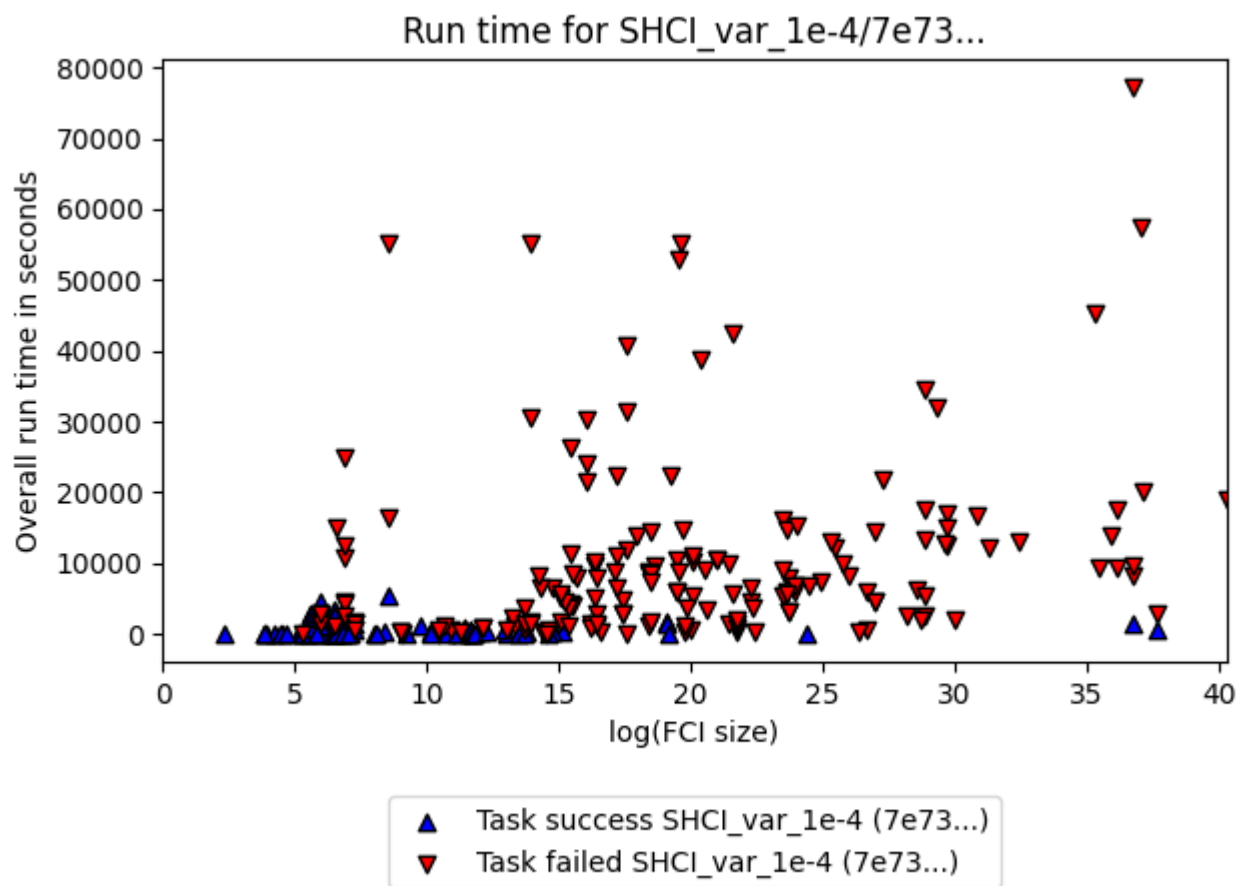
solvability\_ratio: 0.8794

f1\_score: [0.9921259842519685, 0.9947089947089947]

ml\_metrics\_calculator\_version: 1



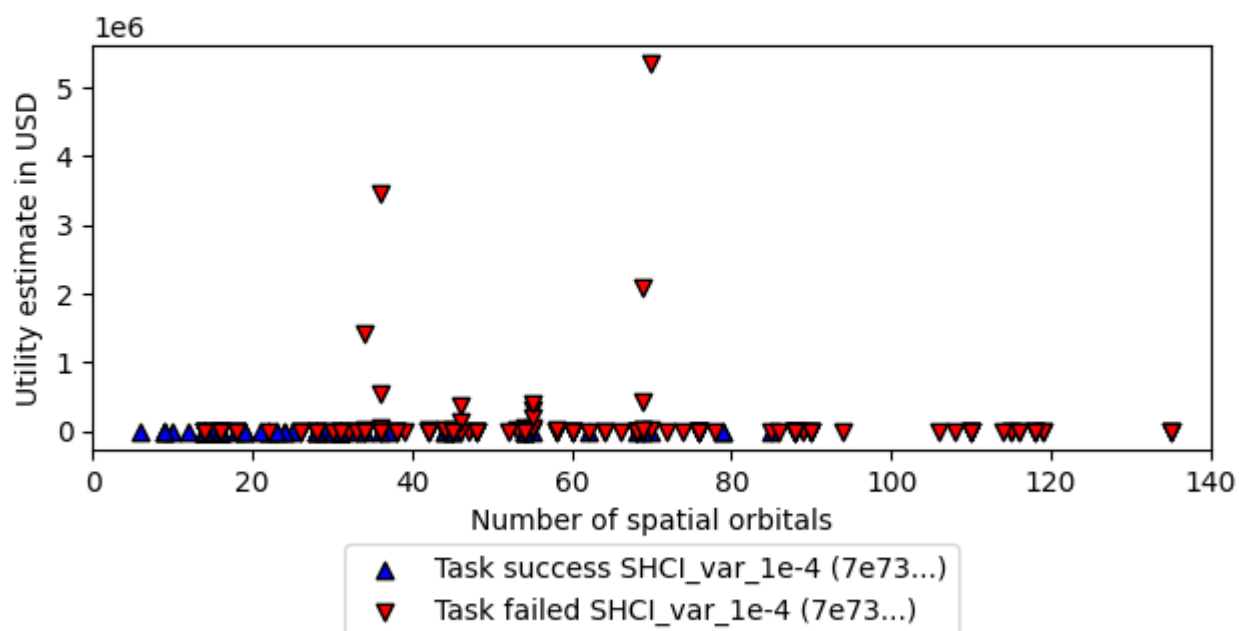
Note: plot only contains attempted tasks.



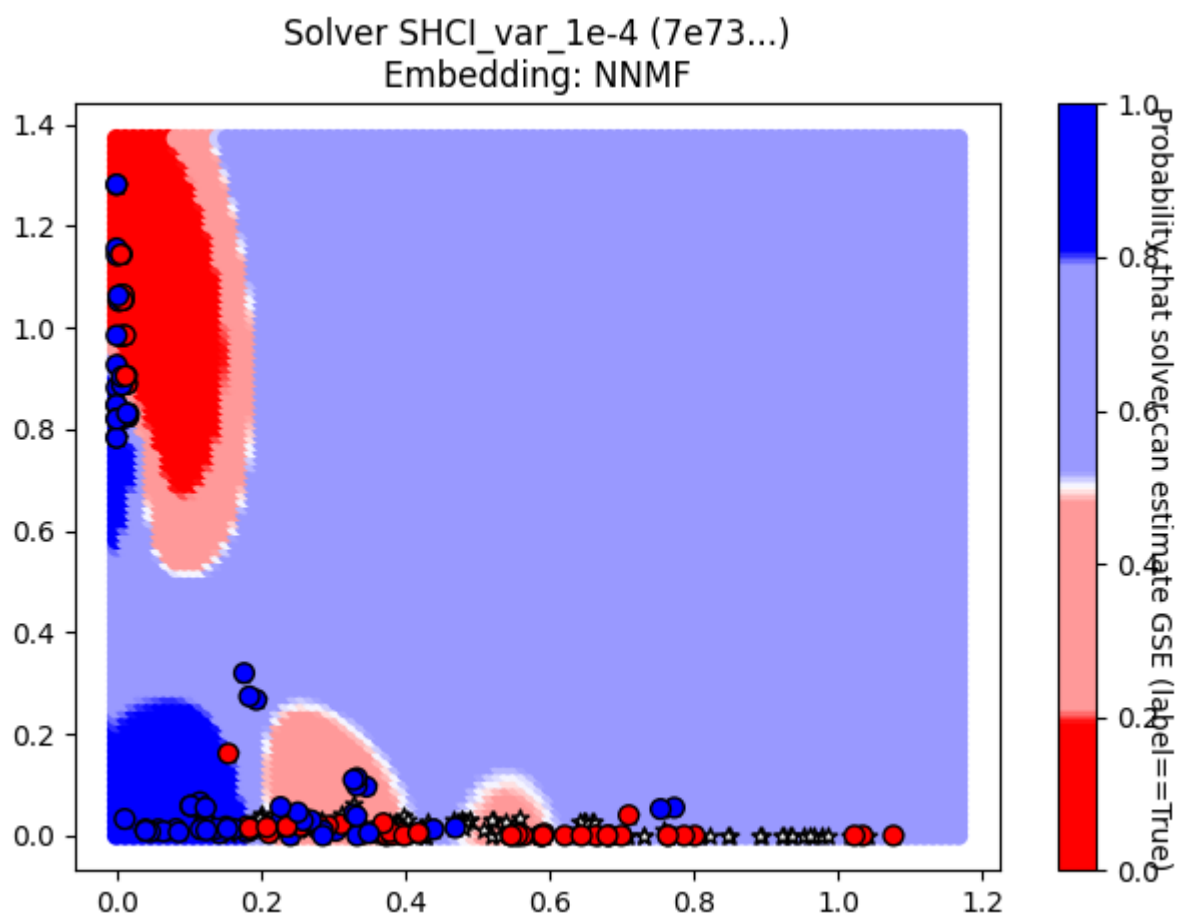
Note: plot only contains attempted tasks.

### Utility capture from SHCI\_var\_1e-4/7e73...

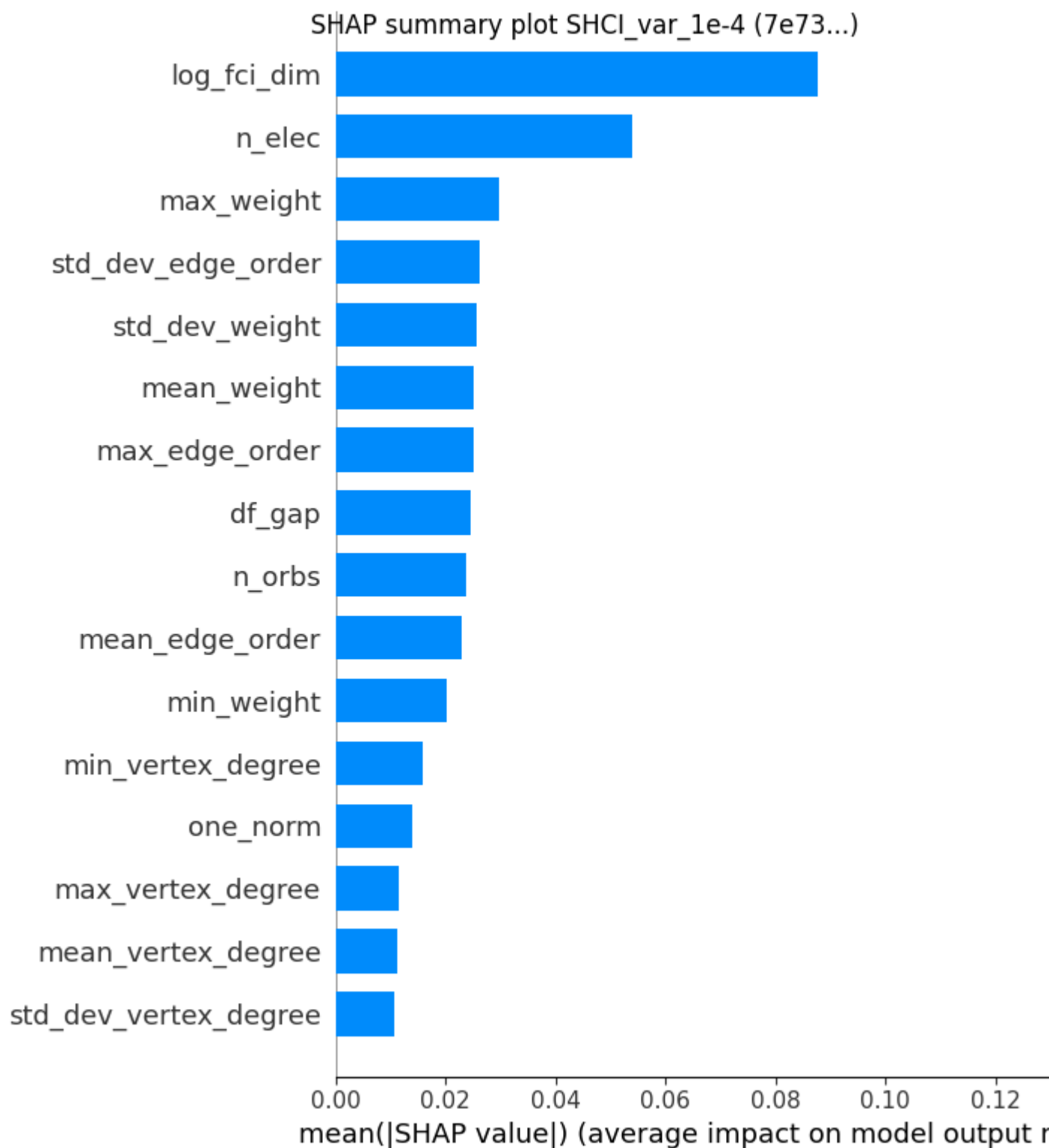
(captured: \$1.0e+02/1.5e+07, approximately 6.8e-04%)







Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_pt\_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb**

solver\_uuid:ad964781-302e-4728-a26d-39918e0a6cdb

solver\_short\_name:SHCI\_pt\_2e-4

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 2e-4 + PT

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: f29b193d-5cdc-4078-9bbb-5e12187184e1

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 22

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 137

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 137

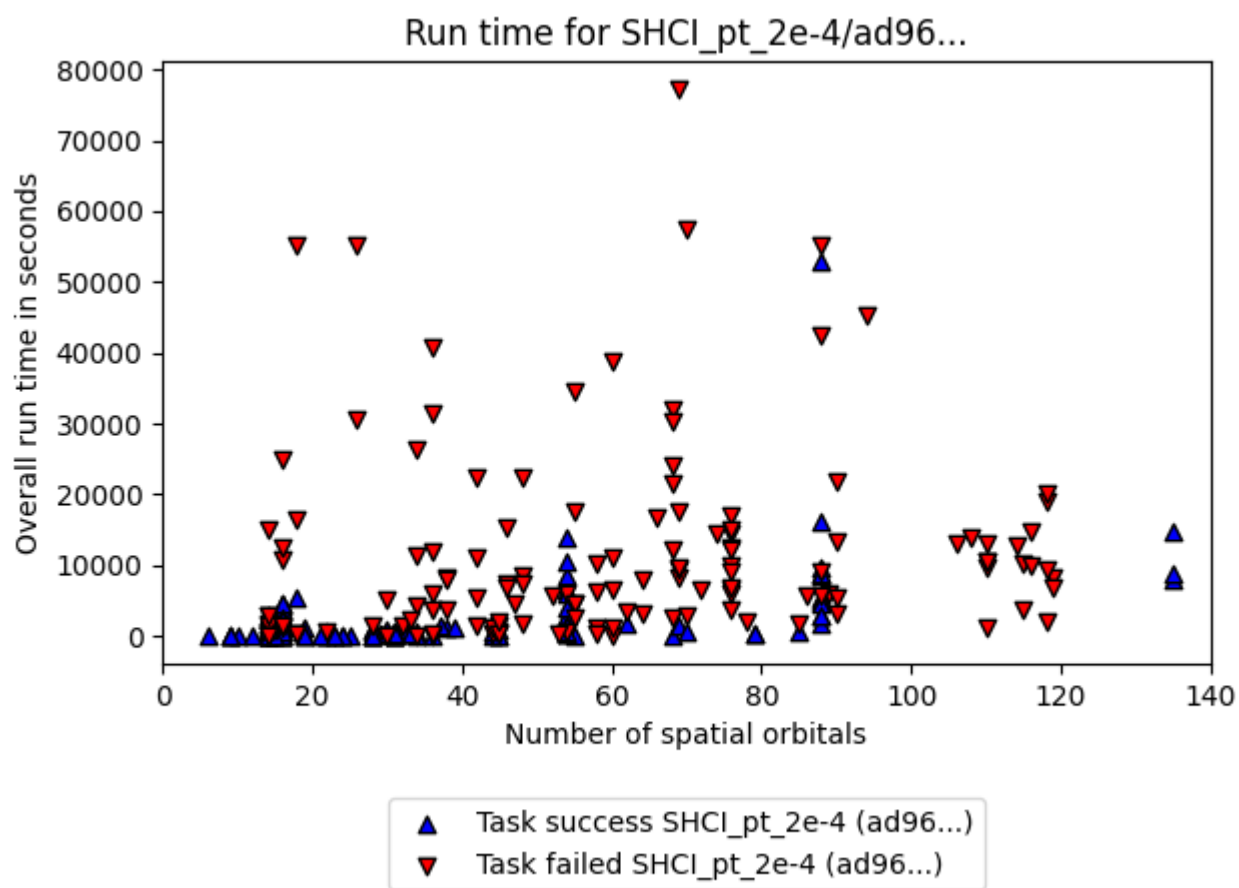
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

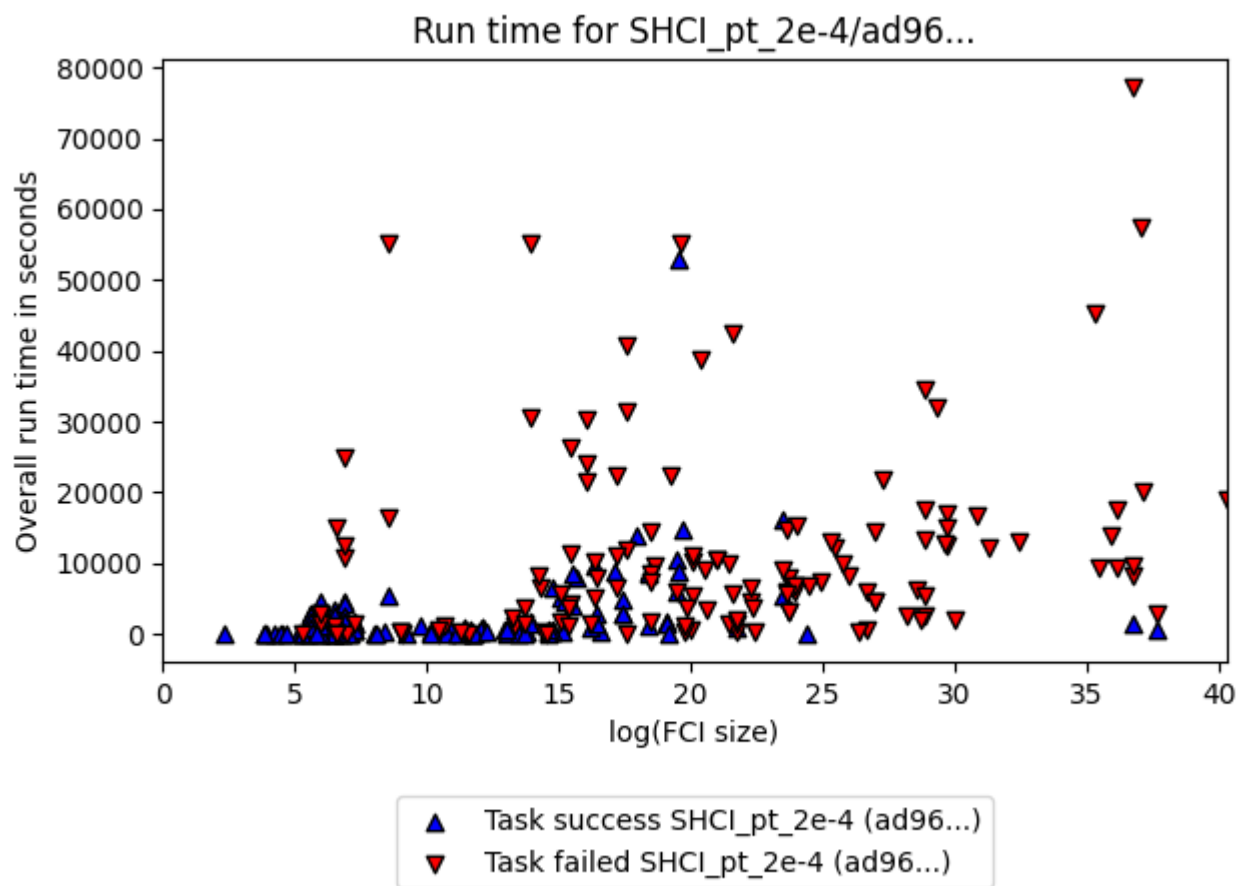
solvability\_ratio: 1.0

f1\_score: [0.6451612903225806, 0.9614035087719298]

ml\_metrics\_calculator\_version: 1



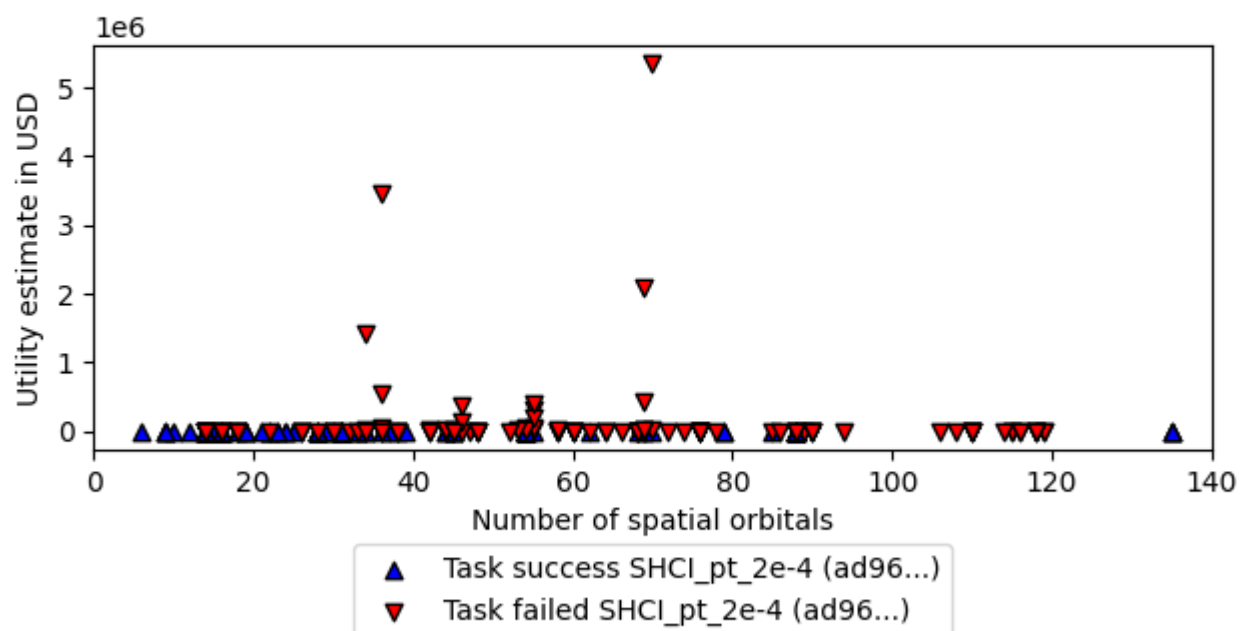
Note: plot only contains attempted tasks.

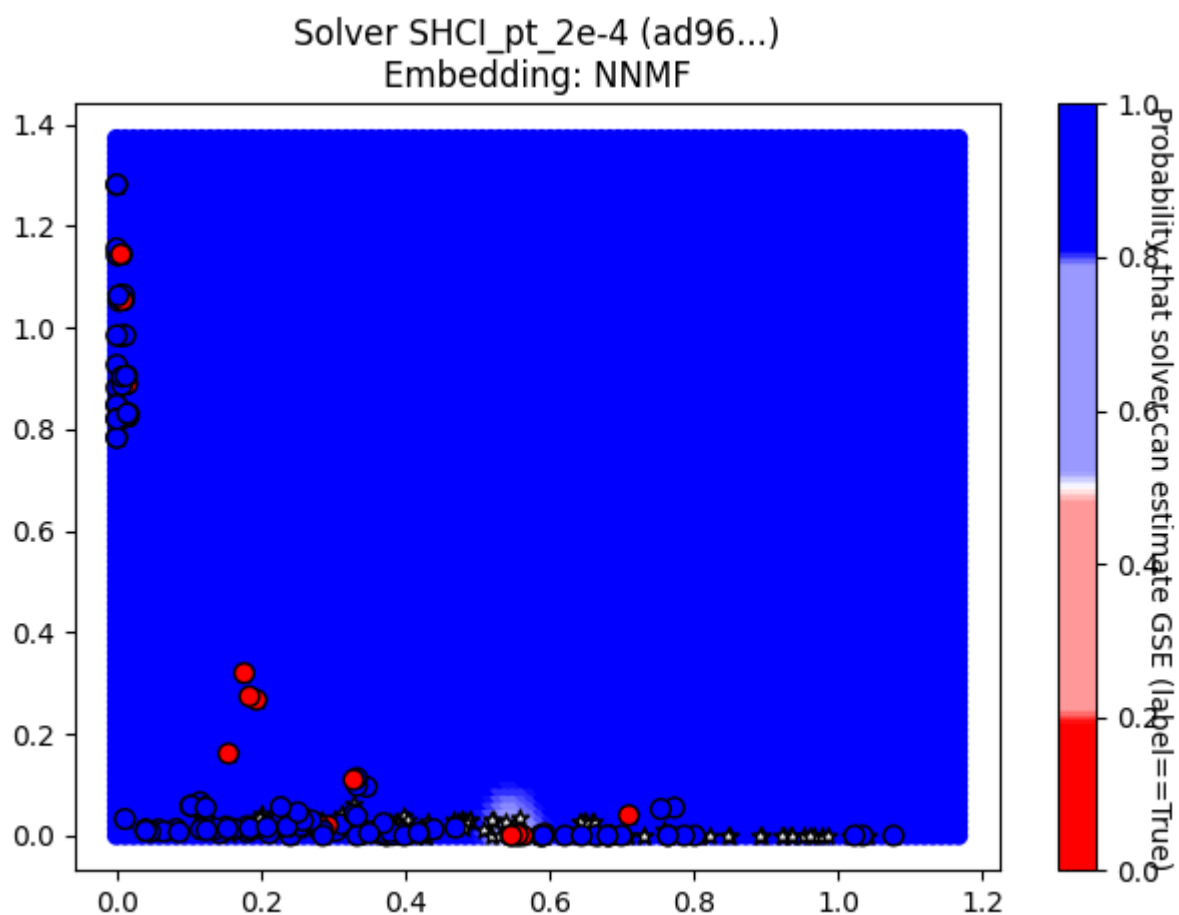


Note: plot only contains attempted tasks.

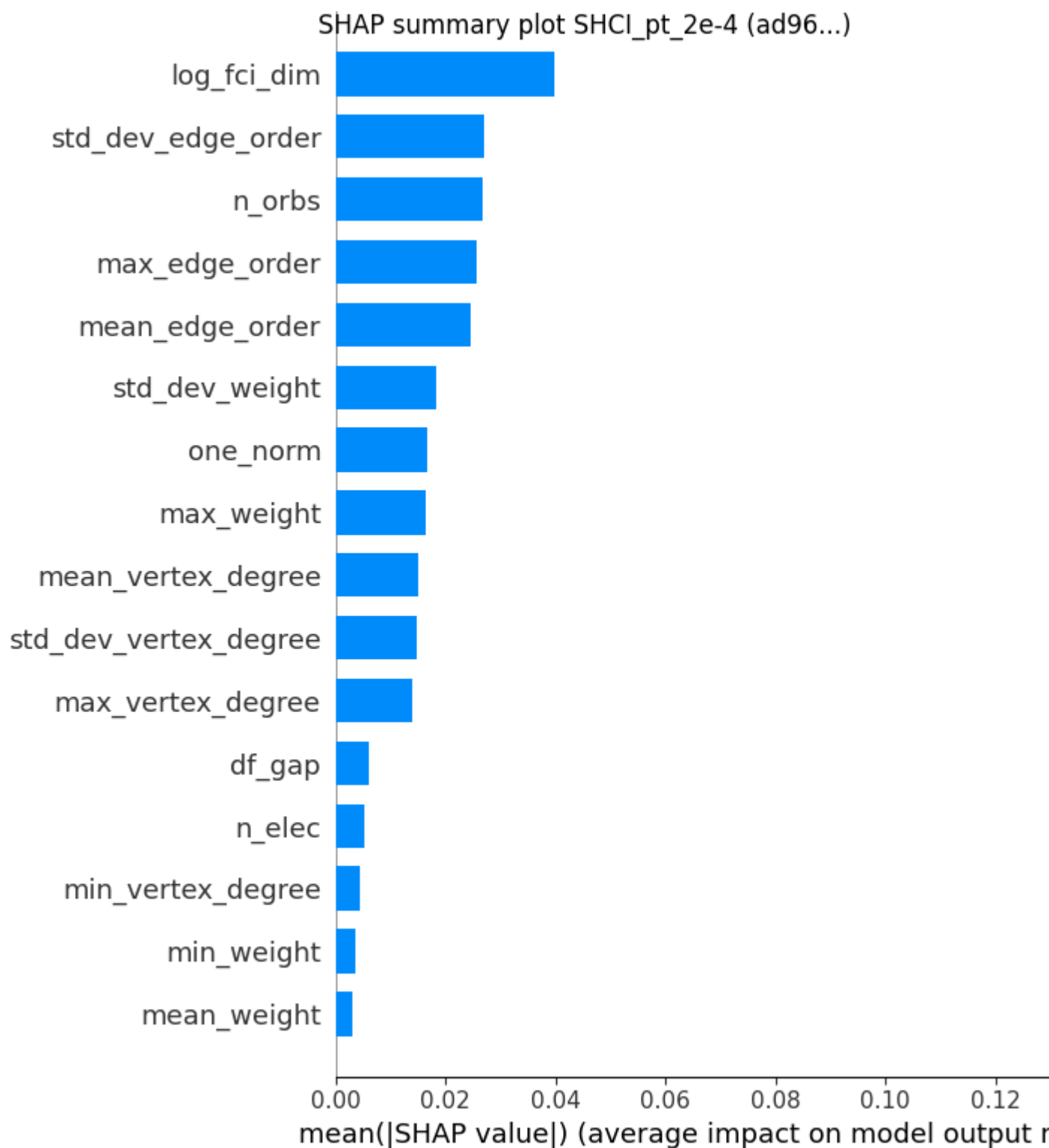
# Utility capture from SHCI\_pt\_2e-4/ad96...

(captured:  $\$4.9\text{e}+02/1.5\text{e}+07$ , approximately  $3.3\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_pt\_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6**

solver\_uuid:c71b90bd-3250-4c0c-b4e7-fc9878f141f6

solver\_short\_name:SHCI\_pt\_2e-5



compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 2e-5 + PT

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 7be4c9eb-e050-4a17-9162-2472de6b20ea

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 26

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 145

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 145

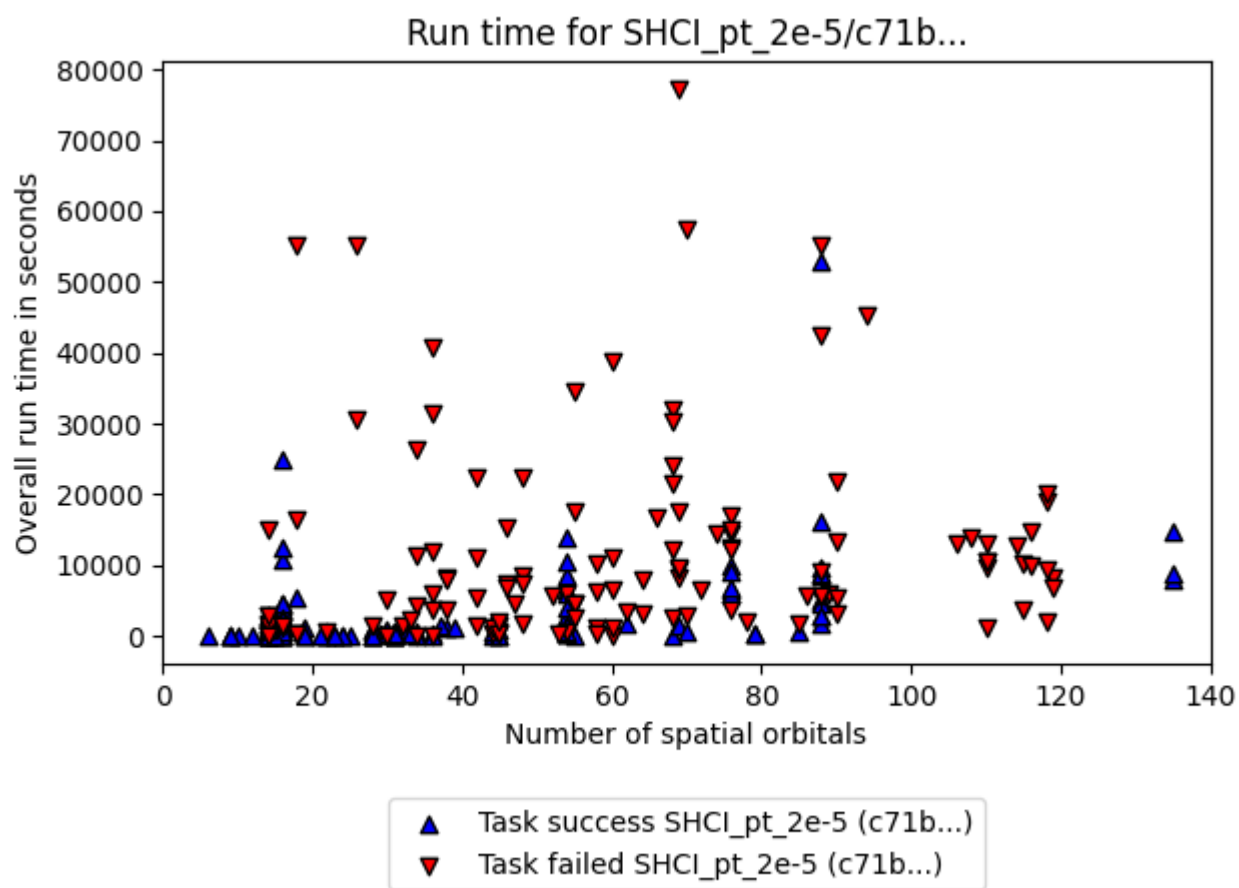
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

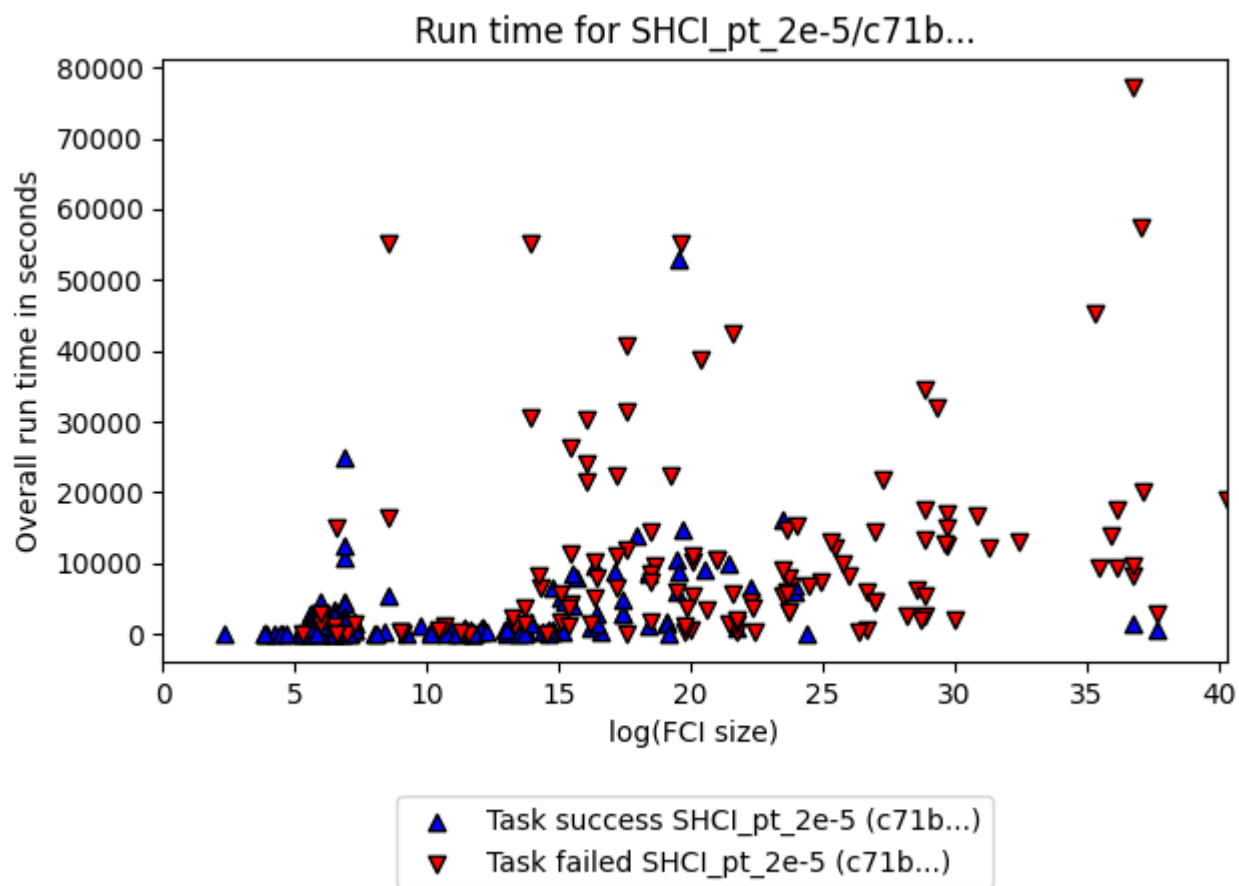
solvability\_ratio: 1.0

f1\_score: [0.375, 0.9666666666666667]

ml\_metrics\_calculator\_version: 1



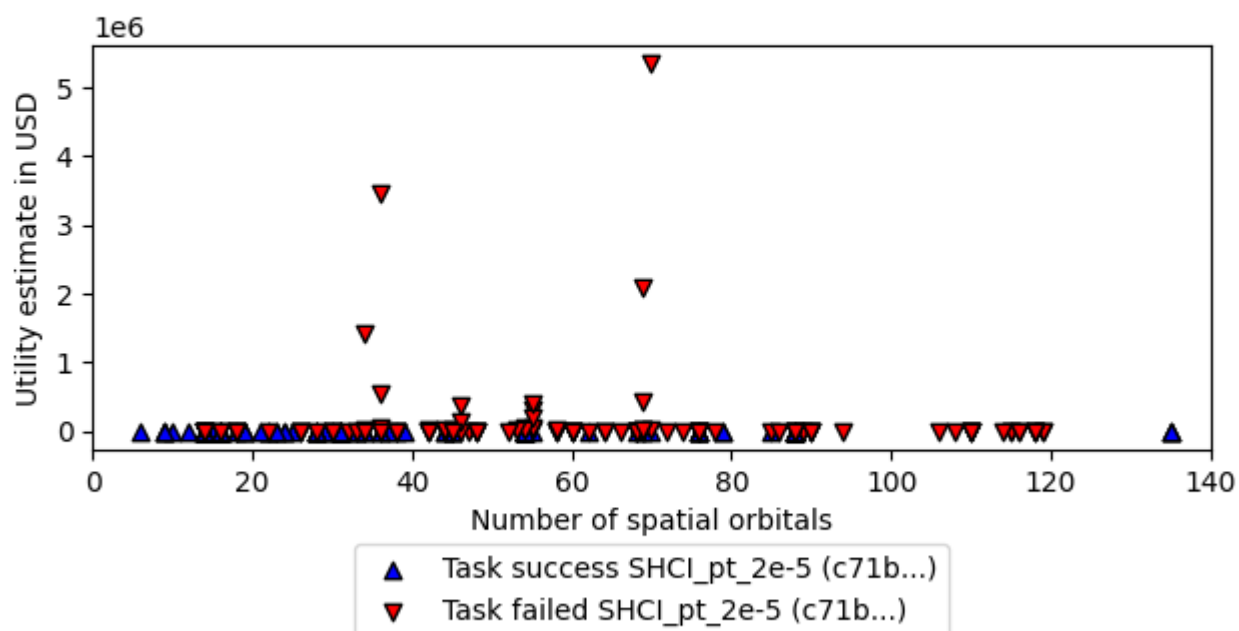
Note: plot only contains attempted tasks.

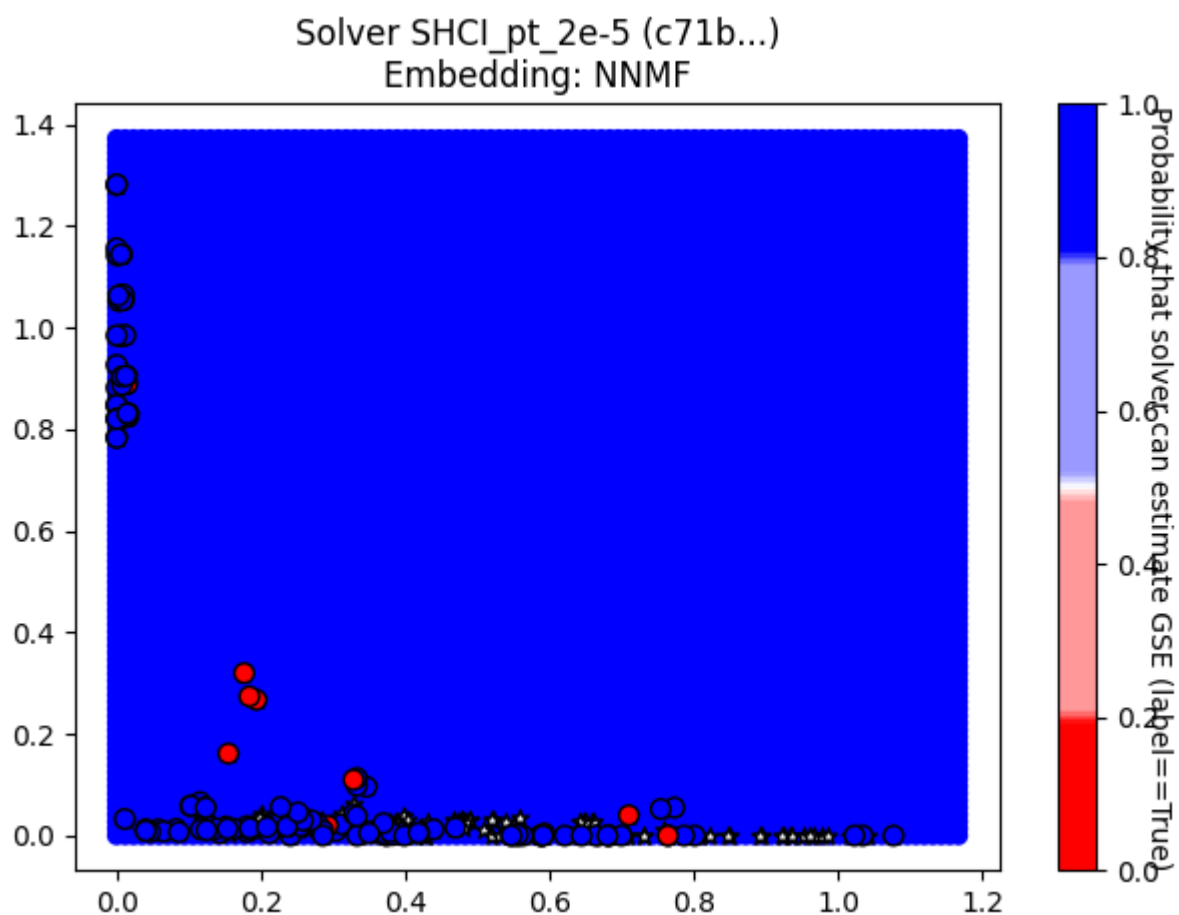


Note: plot only contains attempted tasks.

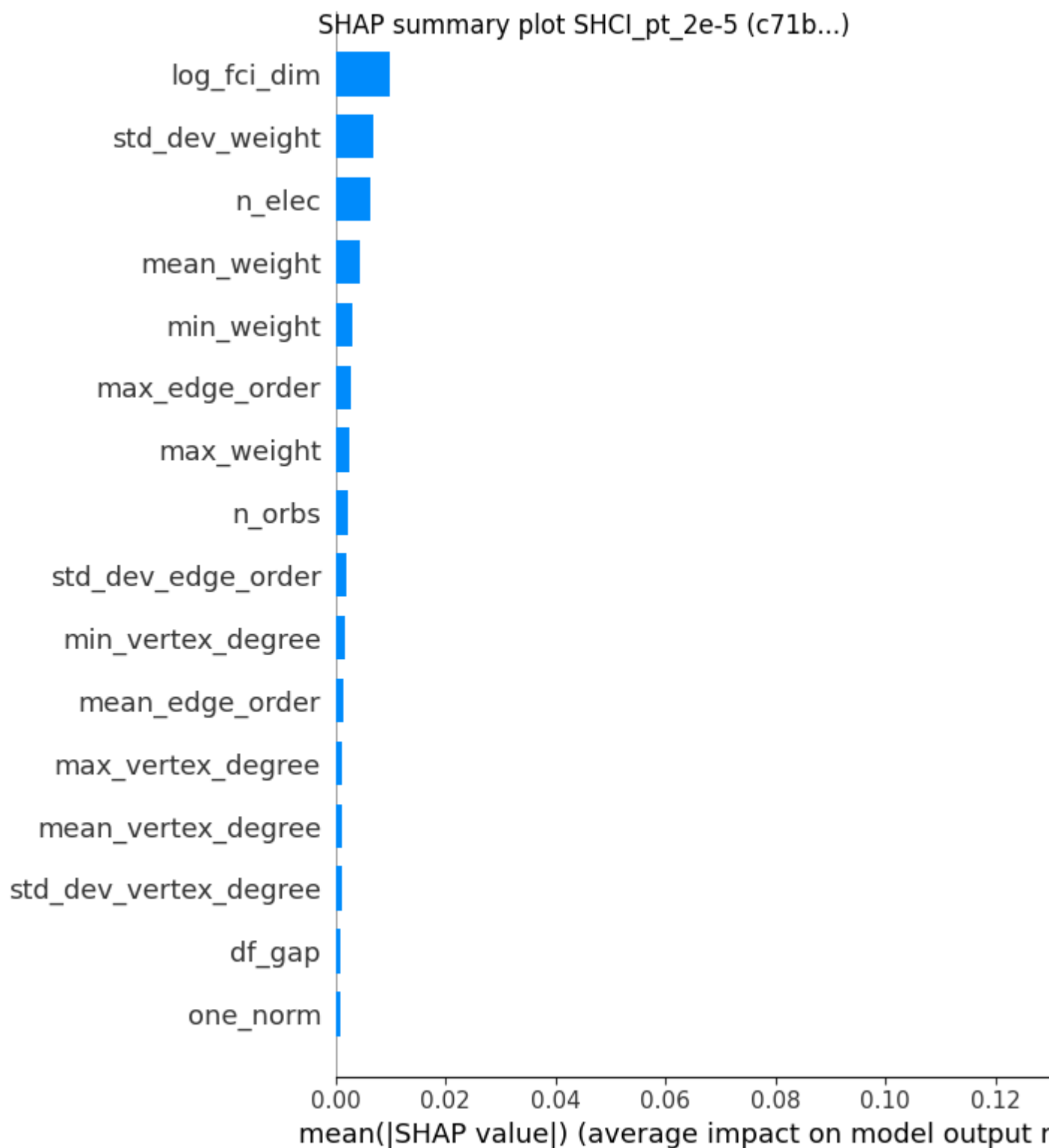
### Utility capture from SHCI\_pt\_2e-5/c71b...

(captured:  $\$8.0\text{e}+02/1.5\text{e}+07$ , approximately  $5.3\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_pt\_5e-5,  
d626506c-7aae-4ad6-802a-b29af5f2bb93**

solver\_uuid:d626506c-7aae-4ad6-802a-b29af5f2bb93

solver\_short\_name:SHCI\_pt\_5e-5

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 5e-5 + PT

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: a5691c59-71c7-4631-82ac-202f187e92b0

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 24

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 143

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 143

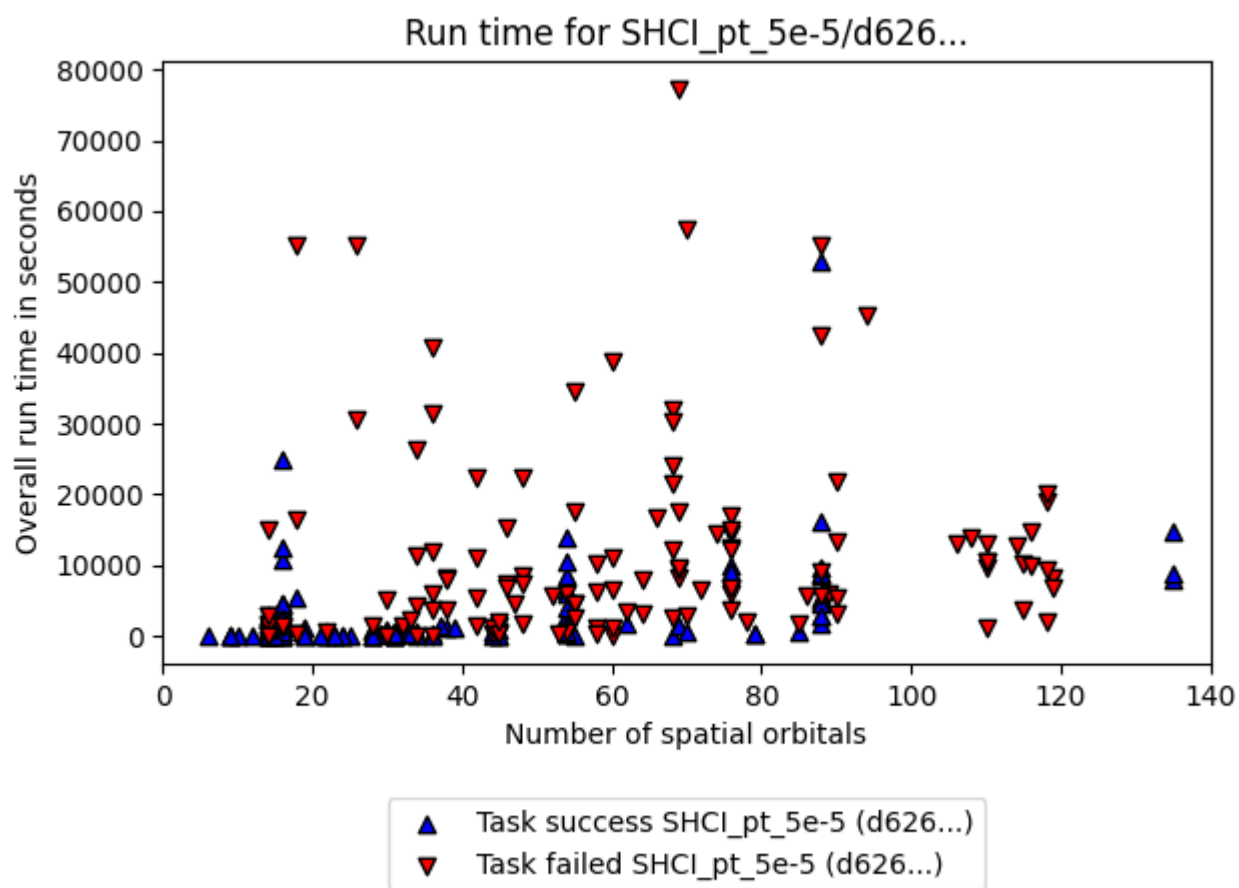
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

solvability\_ratio: 1.0

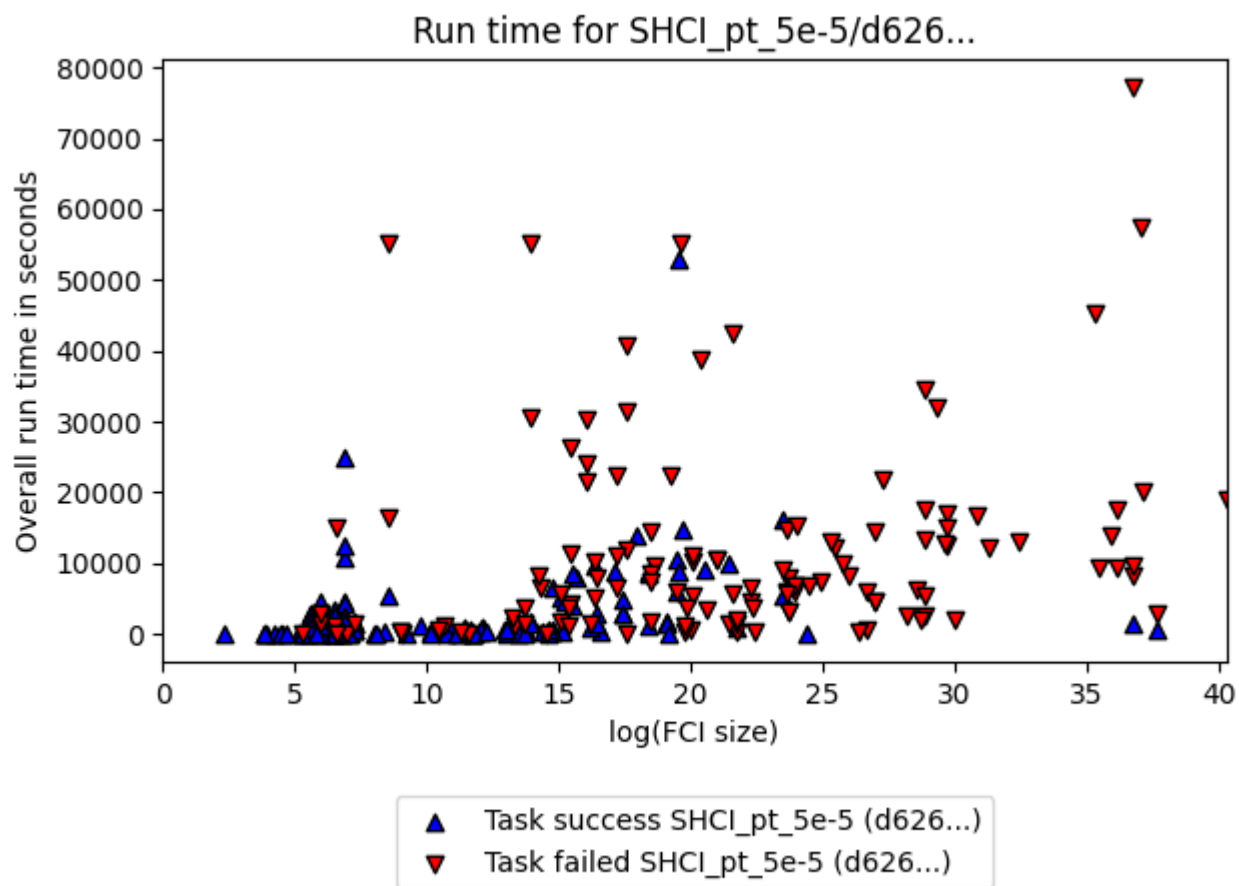
f1\_score: [0.9375, 0.9929577464788732]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

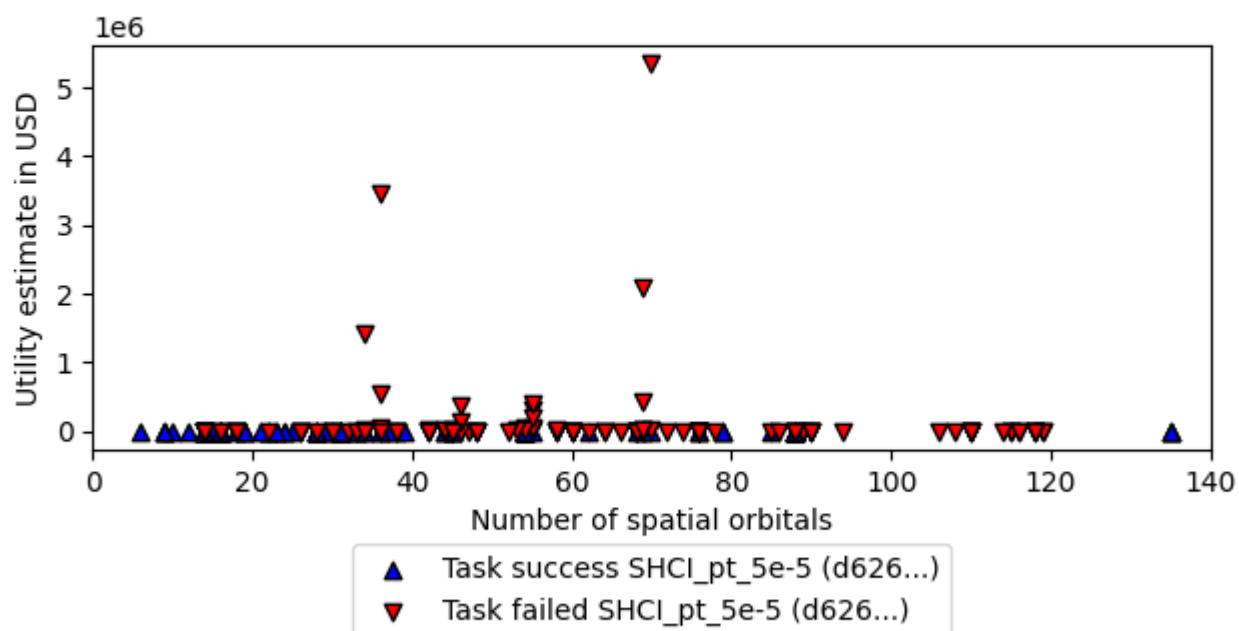


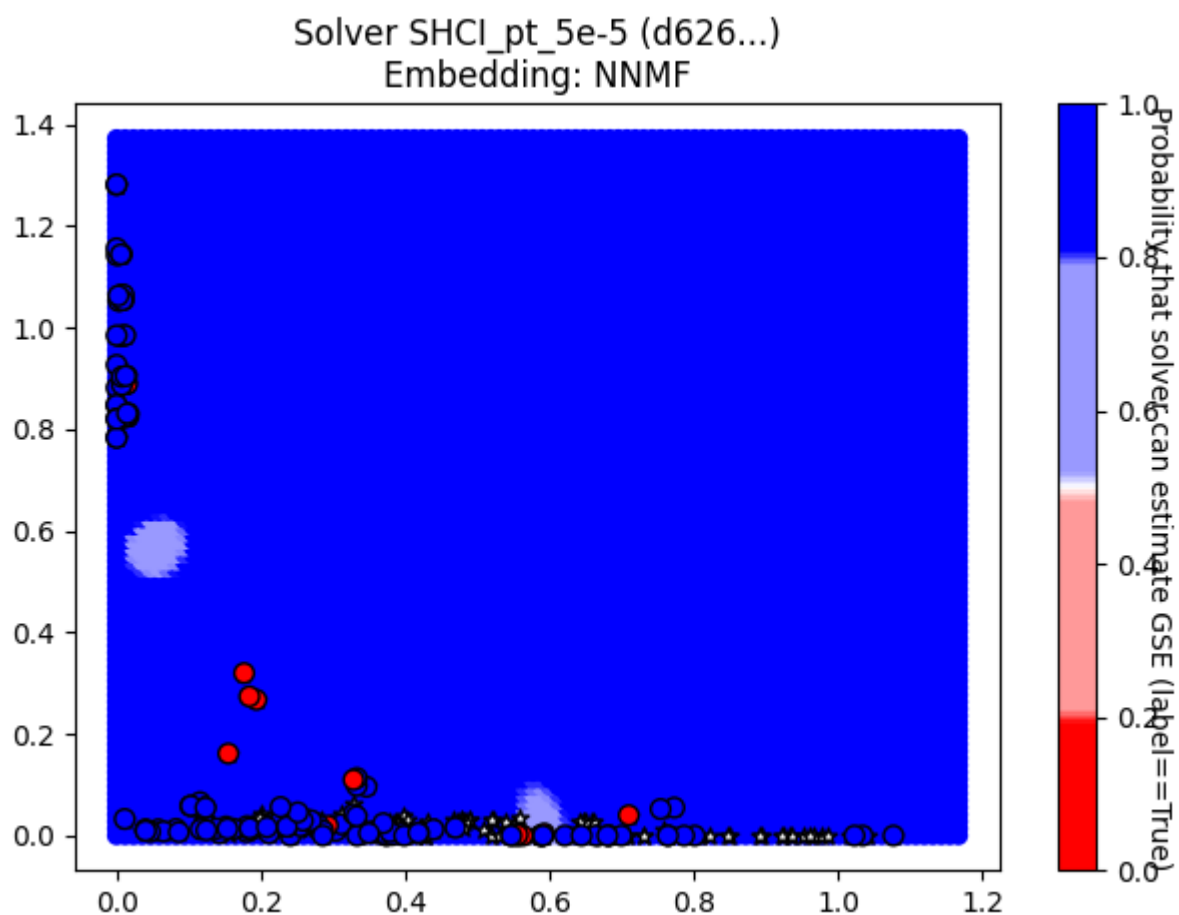


Note: plot only contains attempted tasks.

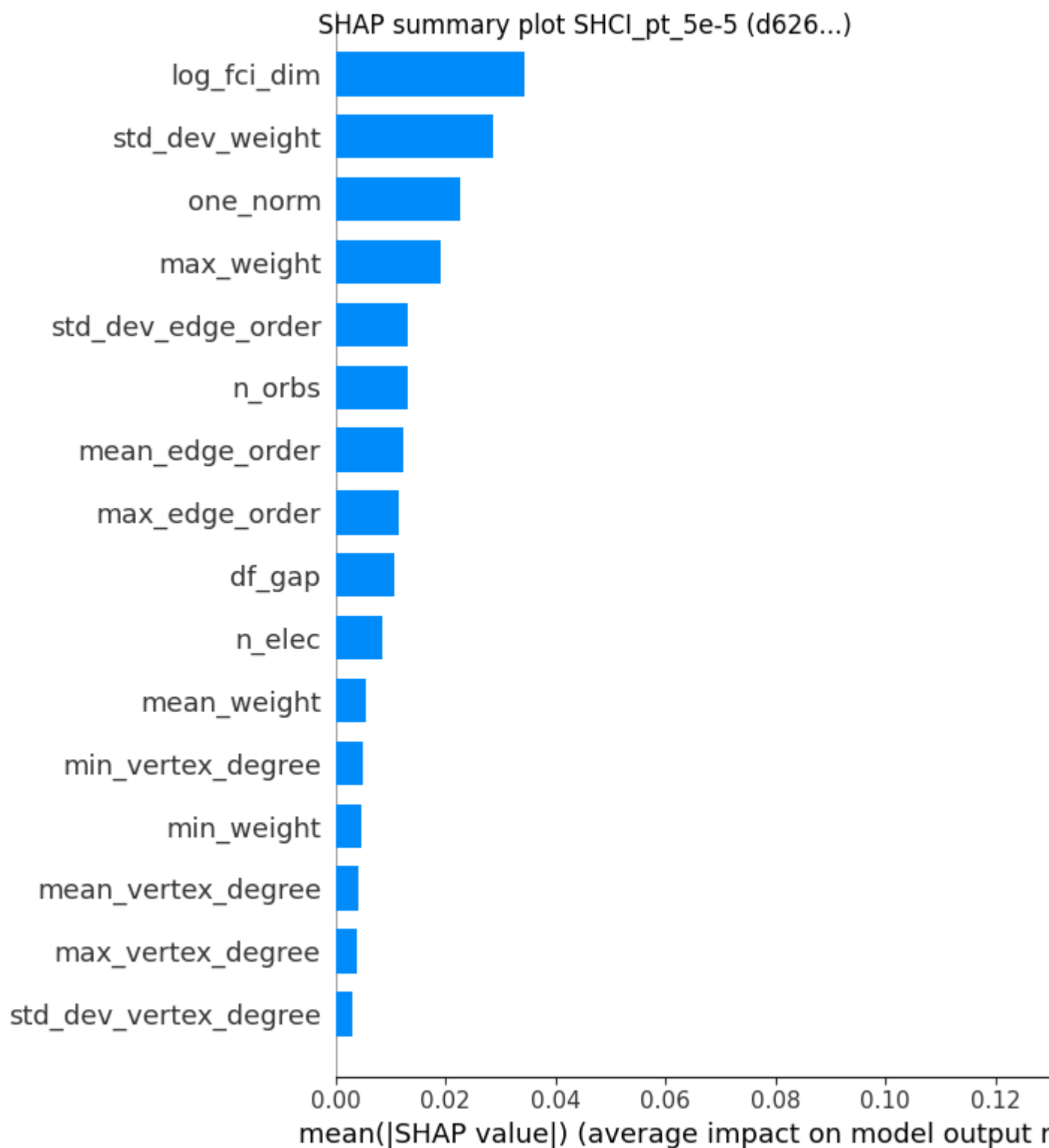
### Utility capture from SHCI\_pt\_5e-5/d626...

(captured:  $\$8.0\text{e}+02/1.5\text{e}+07$ , approximately  $5.3\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_var\_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a**

solver\_uuid:0db183e3-a86d-491b-9125-599556e37c7a

solver\_short\_name:SHCI\_var\_2e-4

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 2e-4

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 9315c8ca-3e06-4795-b27a-cb483f5977ea

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 13

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 84

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 84

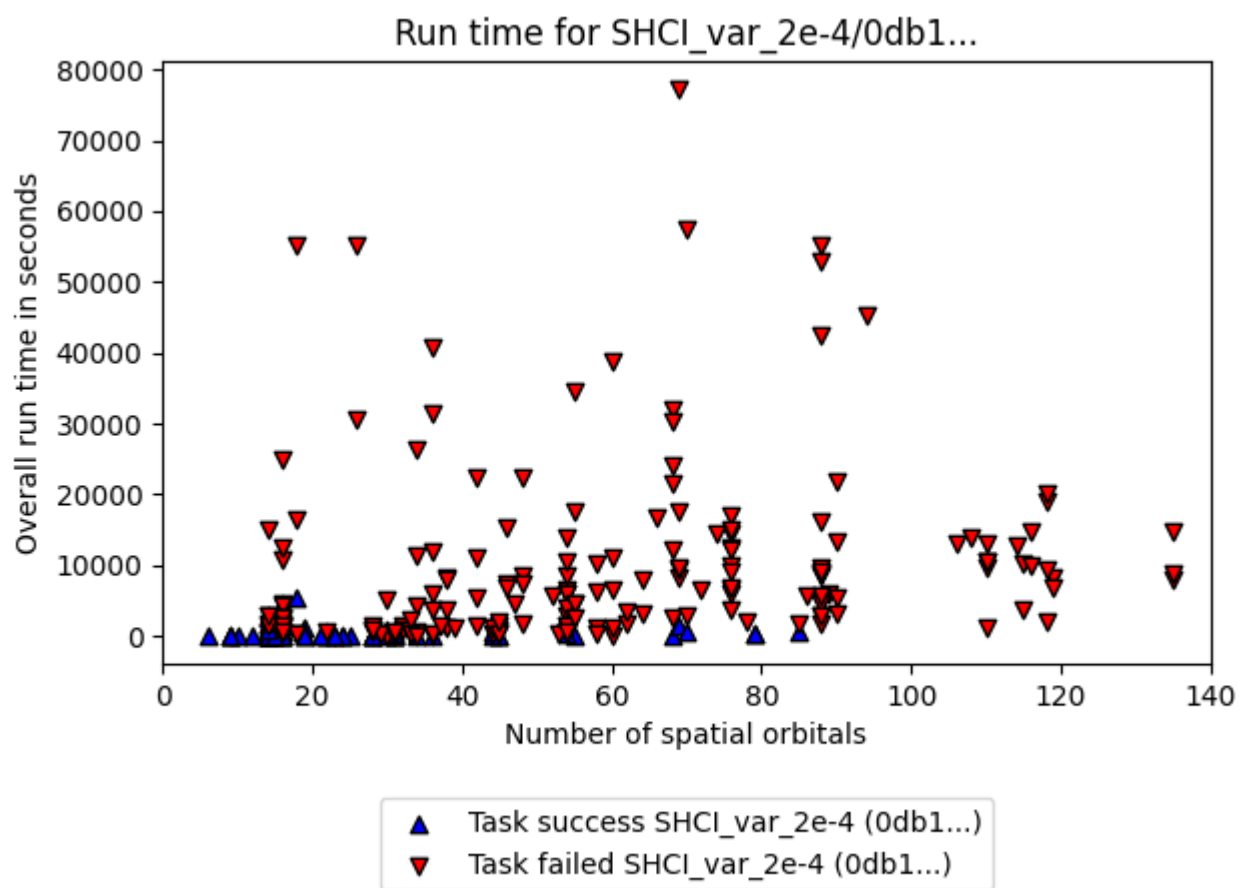
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

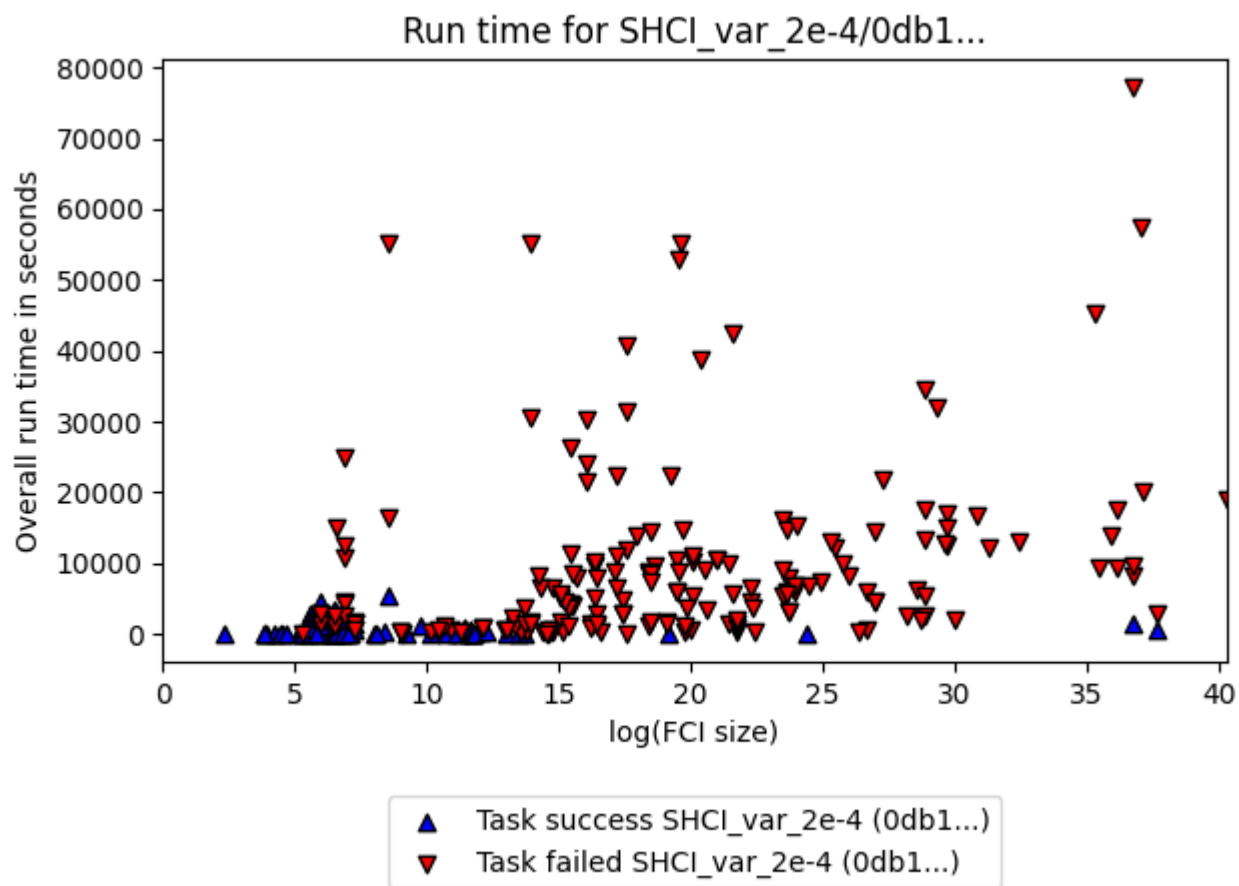
solvability\_ratio: 0.0833

f1\_score: [0.9536423841059603, 0.9575757575757575]

ml\_metrics\_calculator\_version: 1



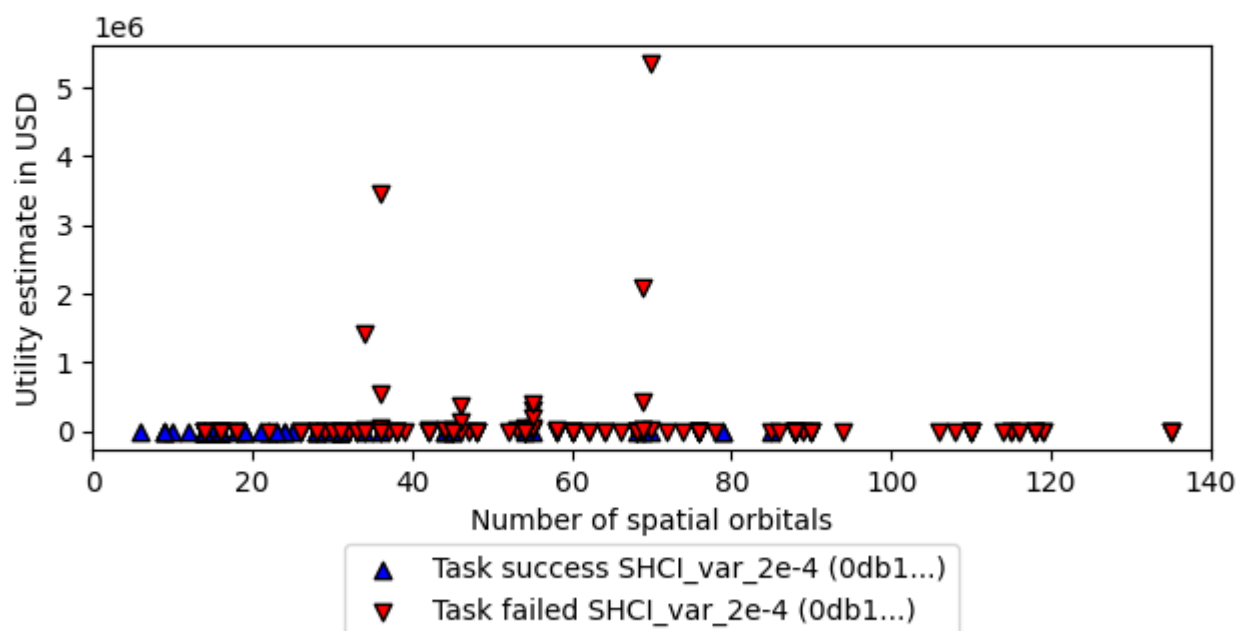
Note: plot only contains attempted tasks.



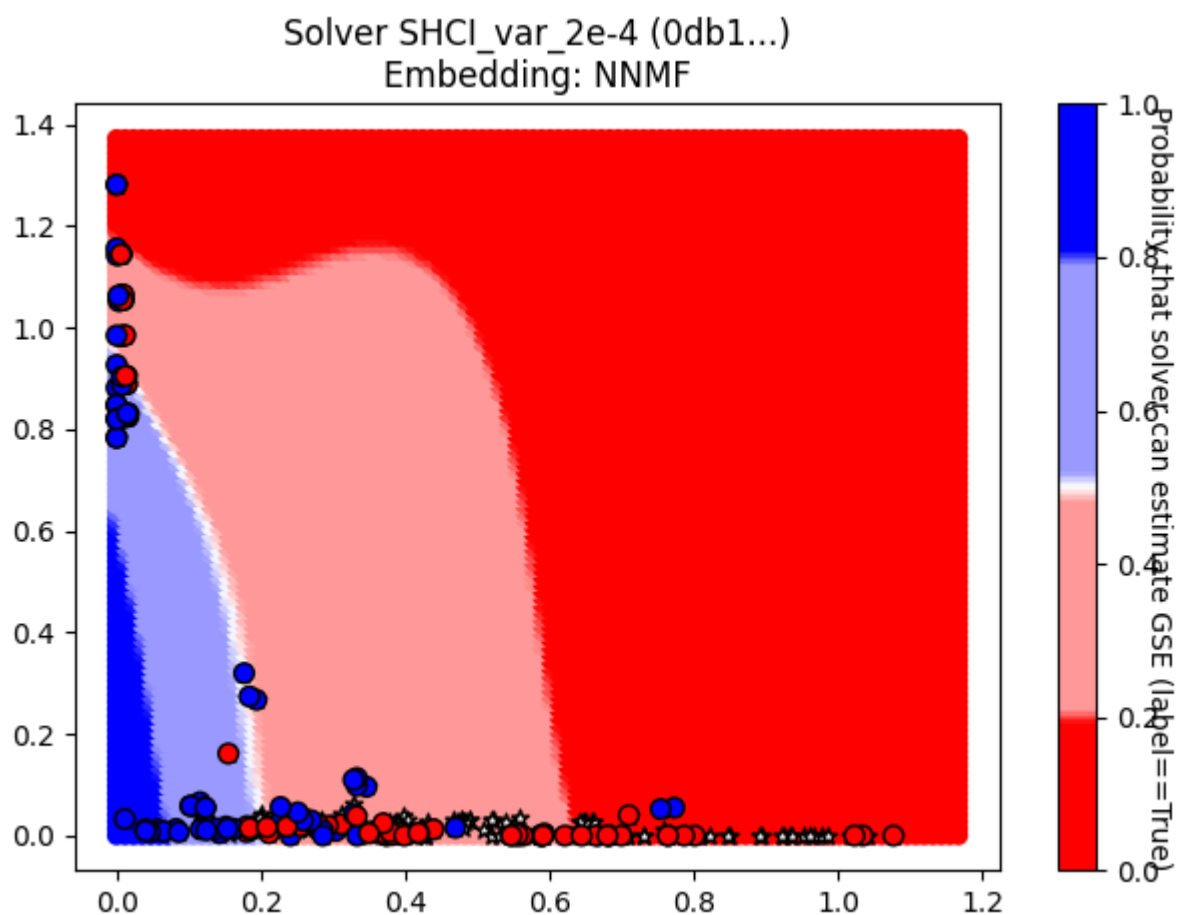
Note: plot only contains attempted tasks.

# Utility capture from SHCI\_var\_2e-4/0db1...

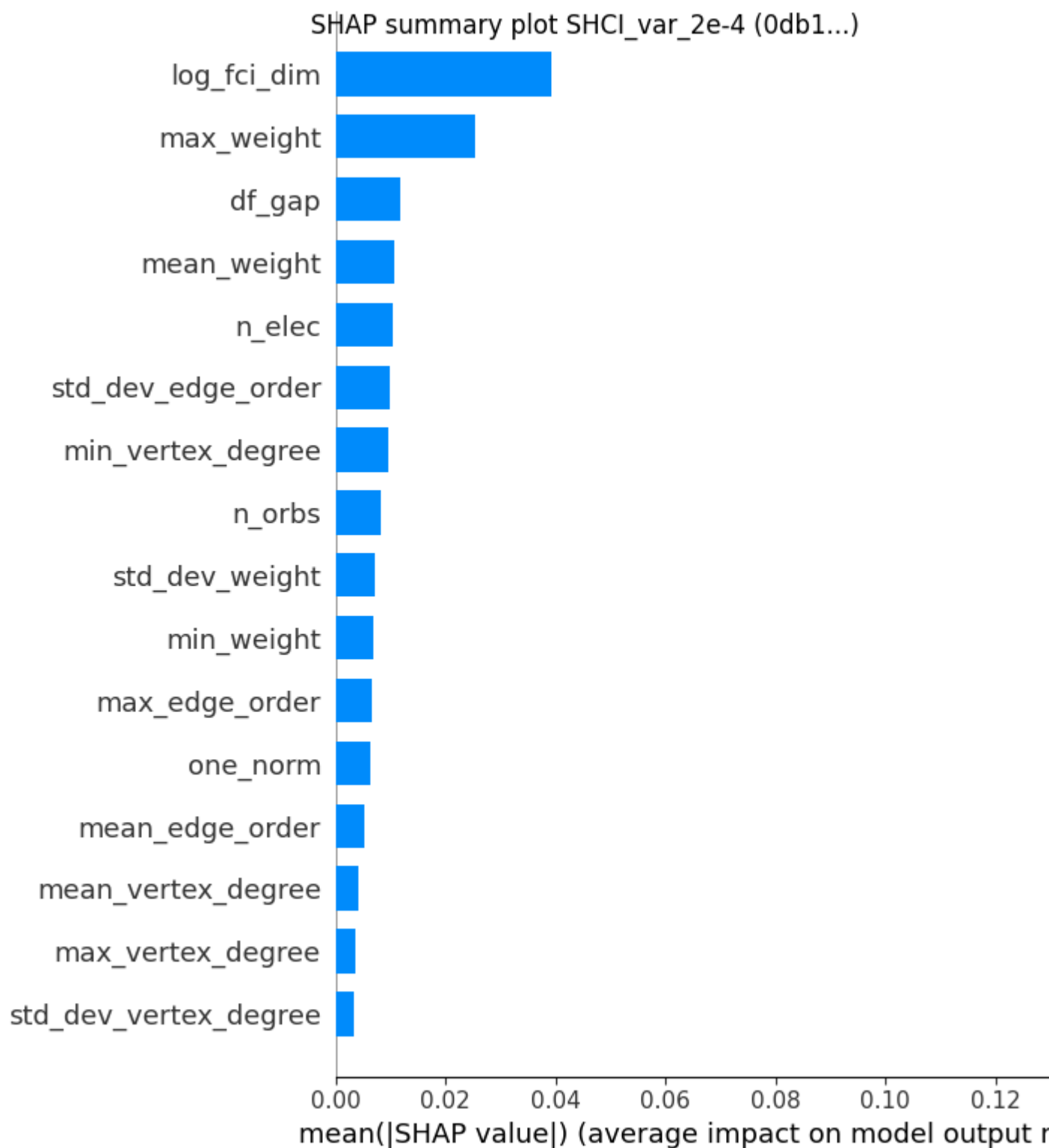
(captured:  $\$8.6\text{e}+01/1.5\text{e}+07$ , approximately  $5.8\text{e}-04\%$ )







Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_var\_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688**

solver\_uuid:86bfe50c-9342-4d54-bb68-abc8abd95688

solver\_short\_name:SHCI\_var\_2e-5

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 2e-5

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 7643a400-ea13-40b9-ad74-561667281b66

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 18

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 133

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 133

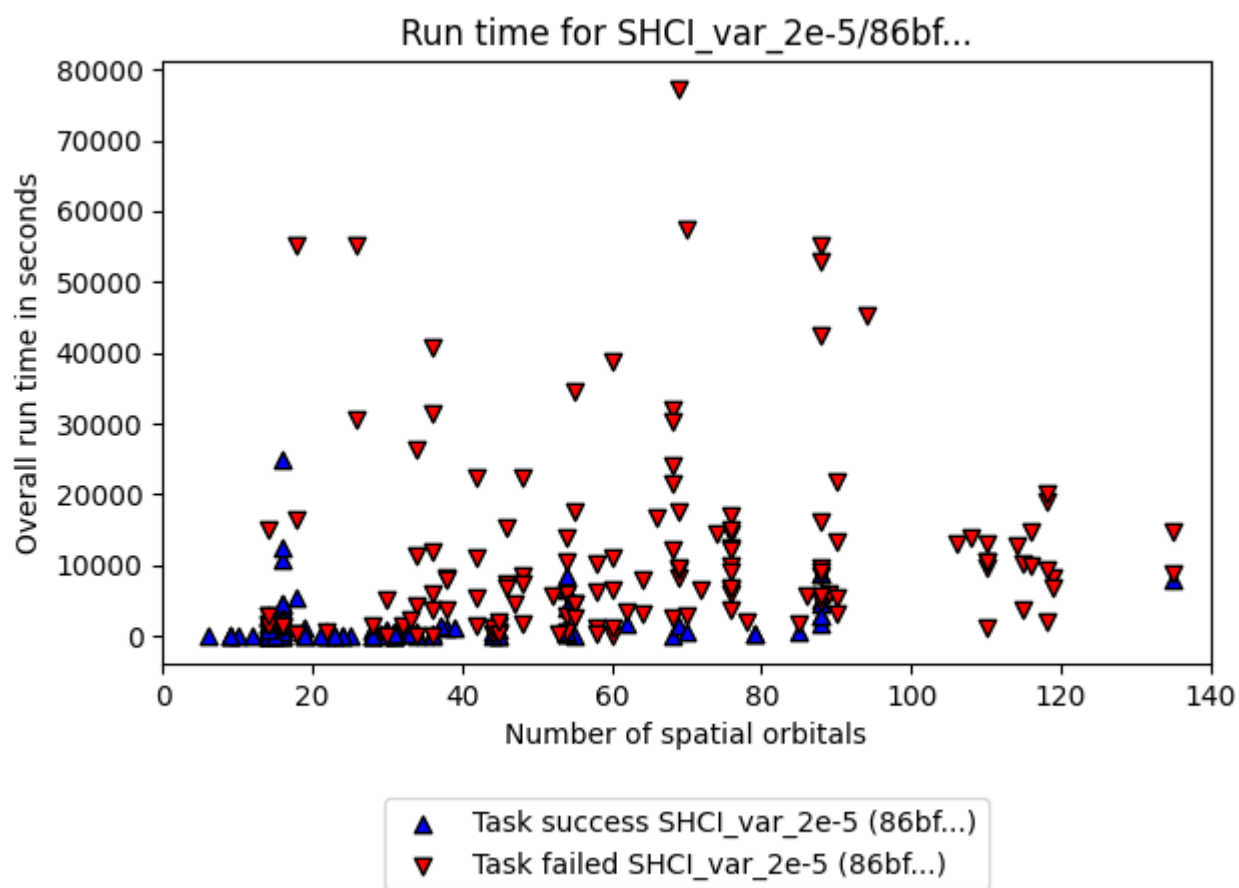
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

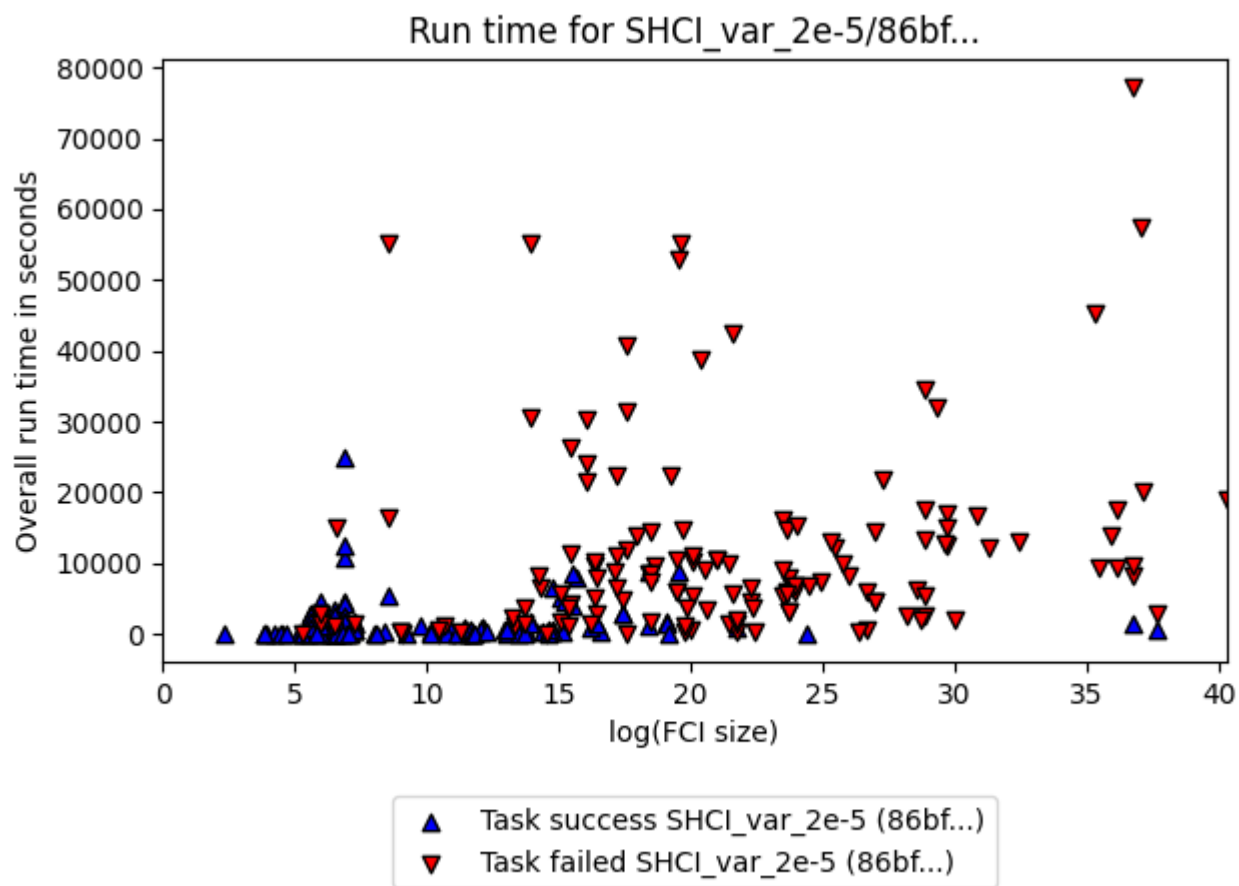
solvability\_ratio: 0.3942

f1\_score: [0.8627450980392157, 0.9735849056603774]

ml\_metrics\_calculator\_version: 1



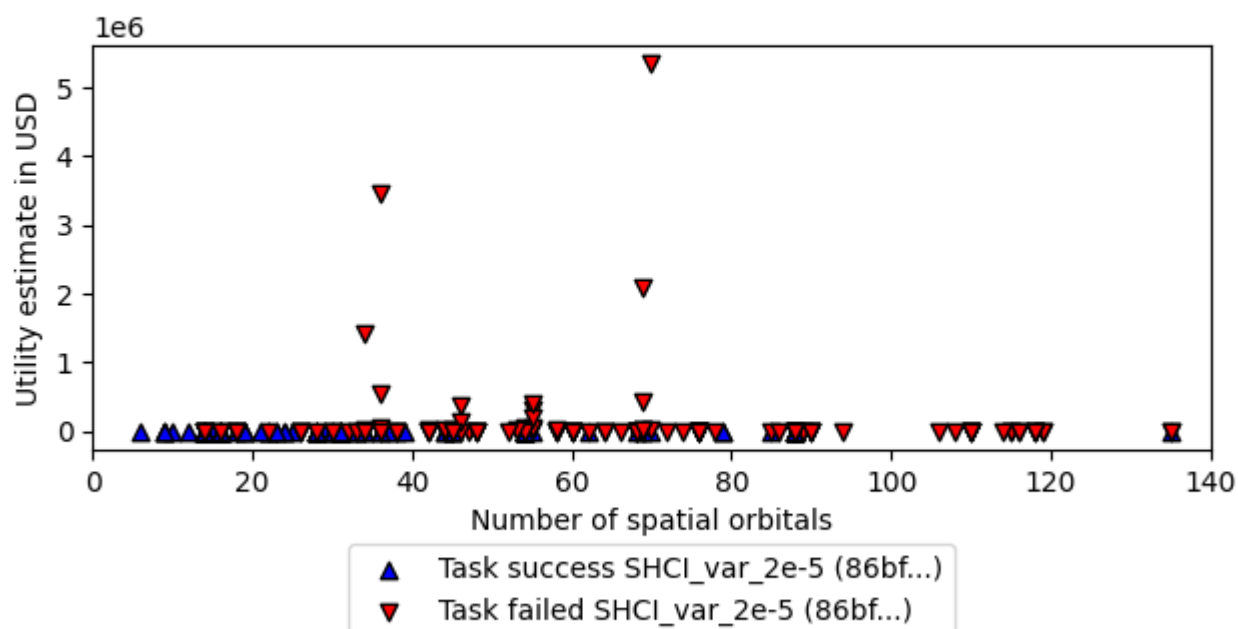
Note: plot only contains attempted tasks.

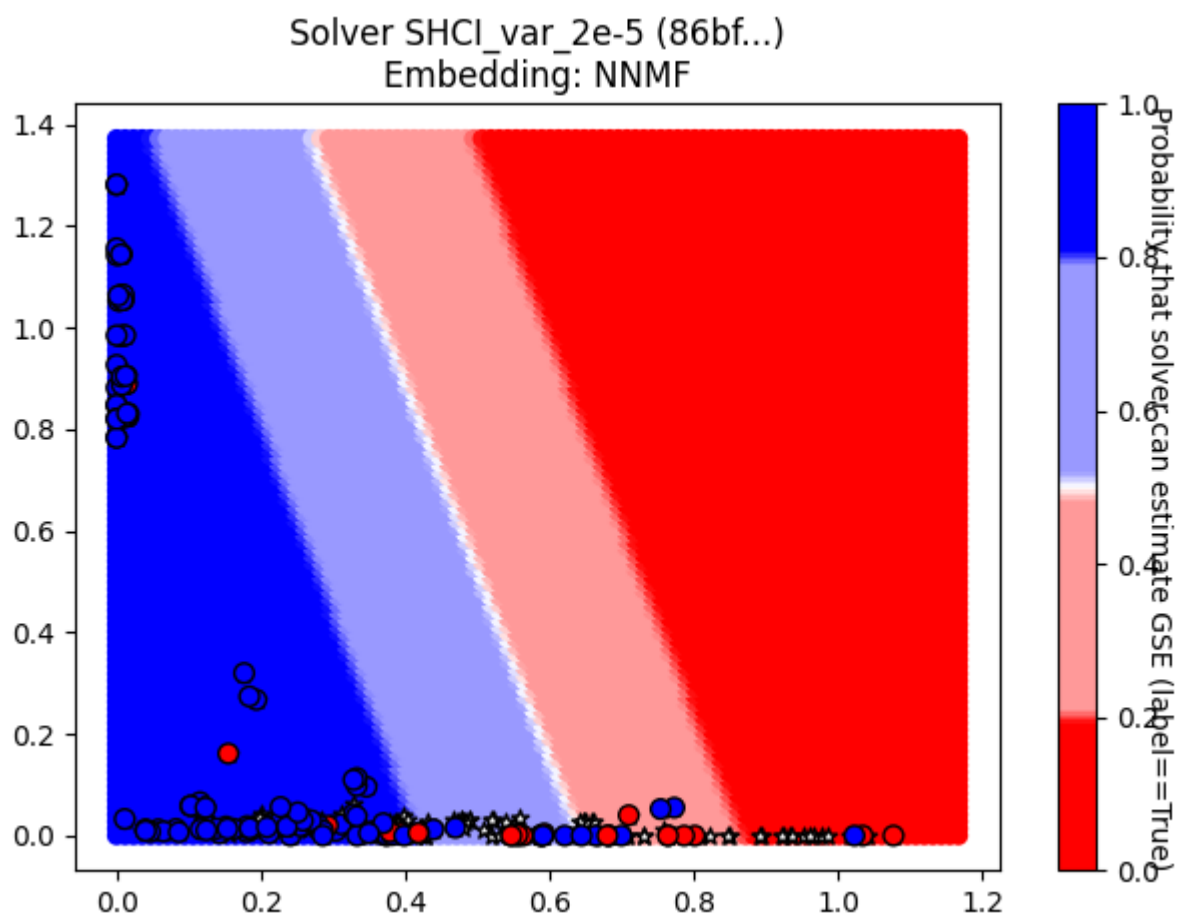


Note: plot only contains attempted tasks.

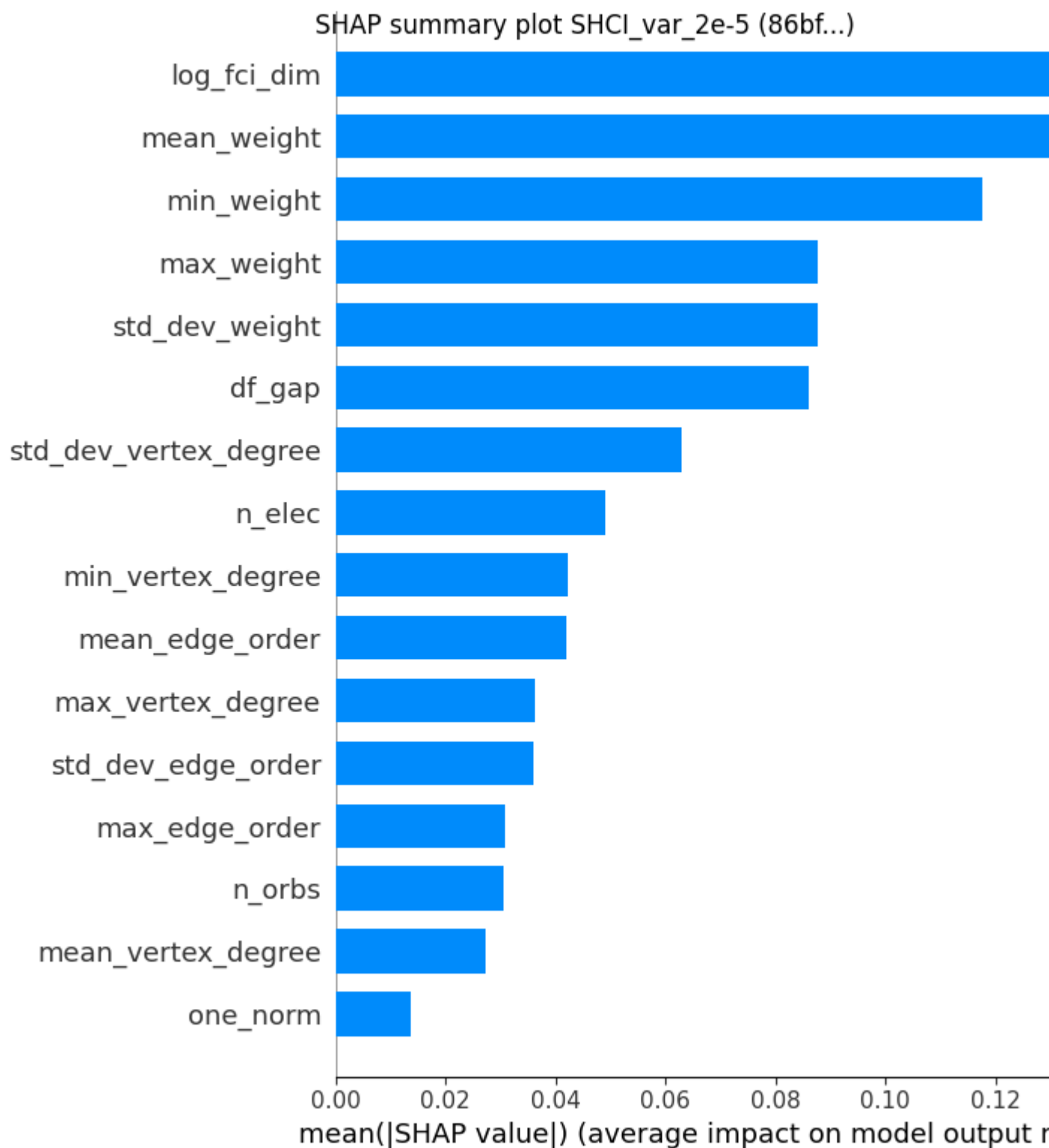
# Utility capture from SHCI\_var\_2e-5/86bf...

(captured:  $\$8.0\text{e}+02/1.5\text{e}+07$ , approximately  $5.3\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver SHCI\_var\_5e-5, 01949b95-c427-4693-9134-01f47f688c09**

solver\_uuid:01949b95-c427-4693-9134-01f47f688c09

solver\_short\_name:SHCI\_var\_5e-5



compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:SHCI with eps\_var 5e-5

software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 2eccdee5-615c-4be6-977b-5e6e18702f4e

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 83

number\_of\_problem\_instances\_solved: 14

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 275

number\_of\_tasks\_solved: 120

number\_of\_tasks\_solved\_within\_run\_time\_limit: 275

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 120

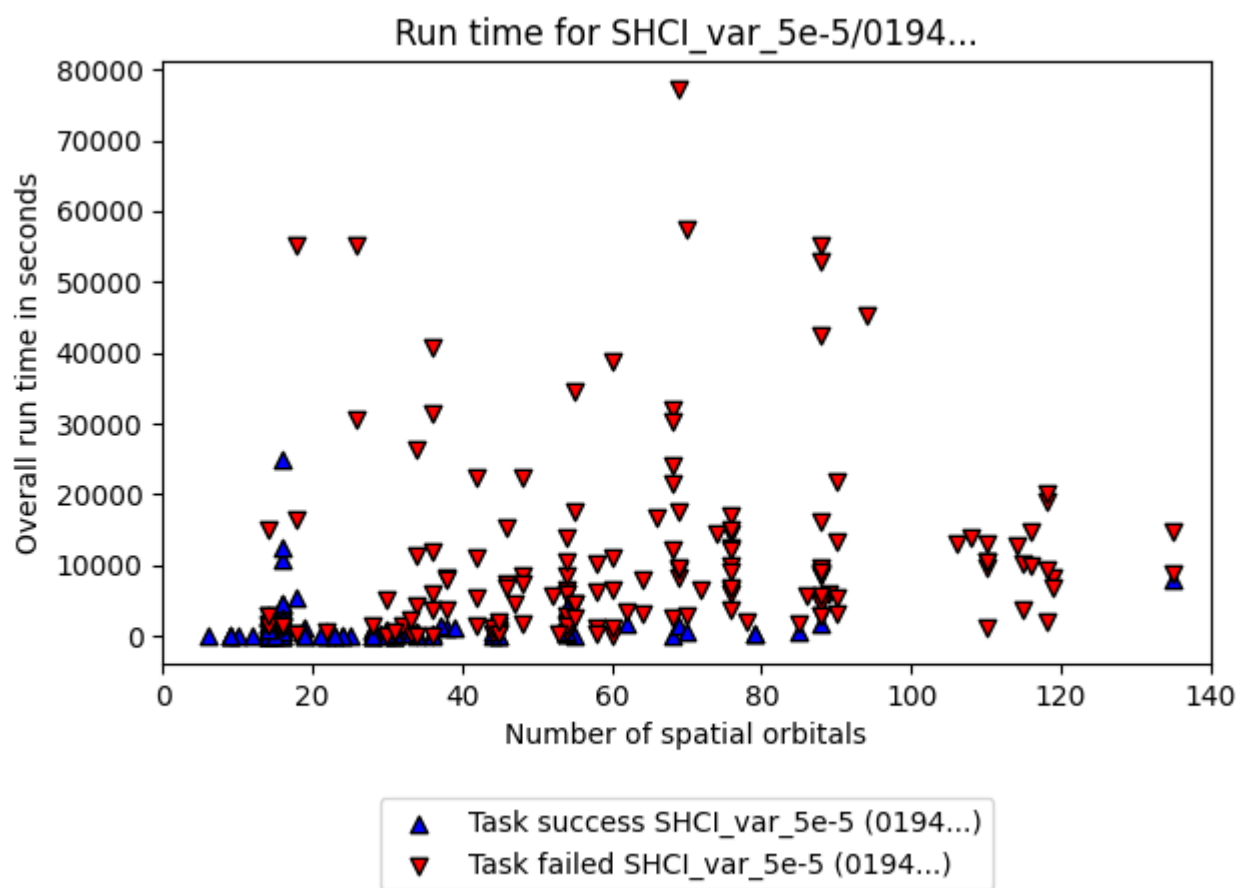
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

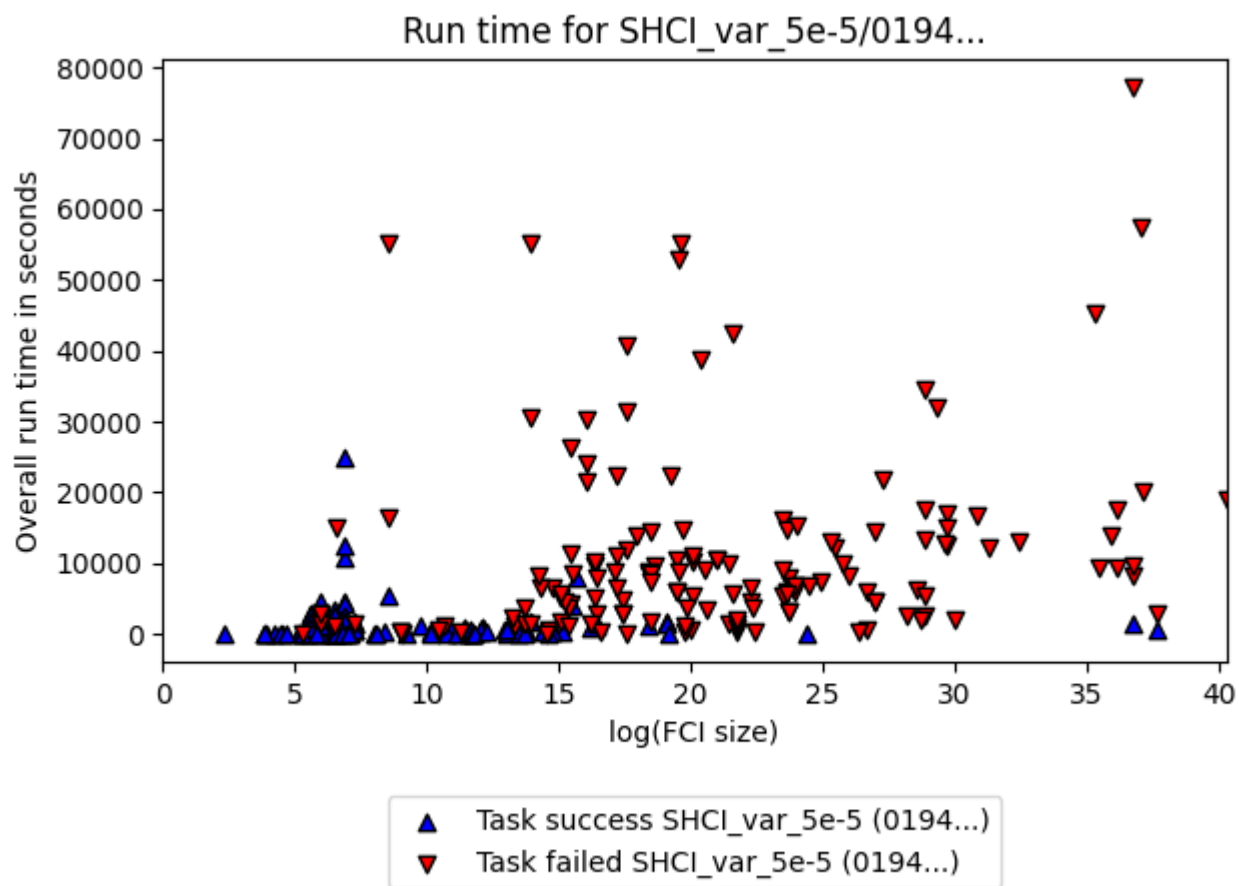
solvability\_ratio: 0.3549

f1\_score: [0.8395061728395061, 0.9446808510638298]

ml\_metrics\_calculator\_version: 1



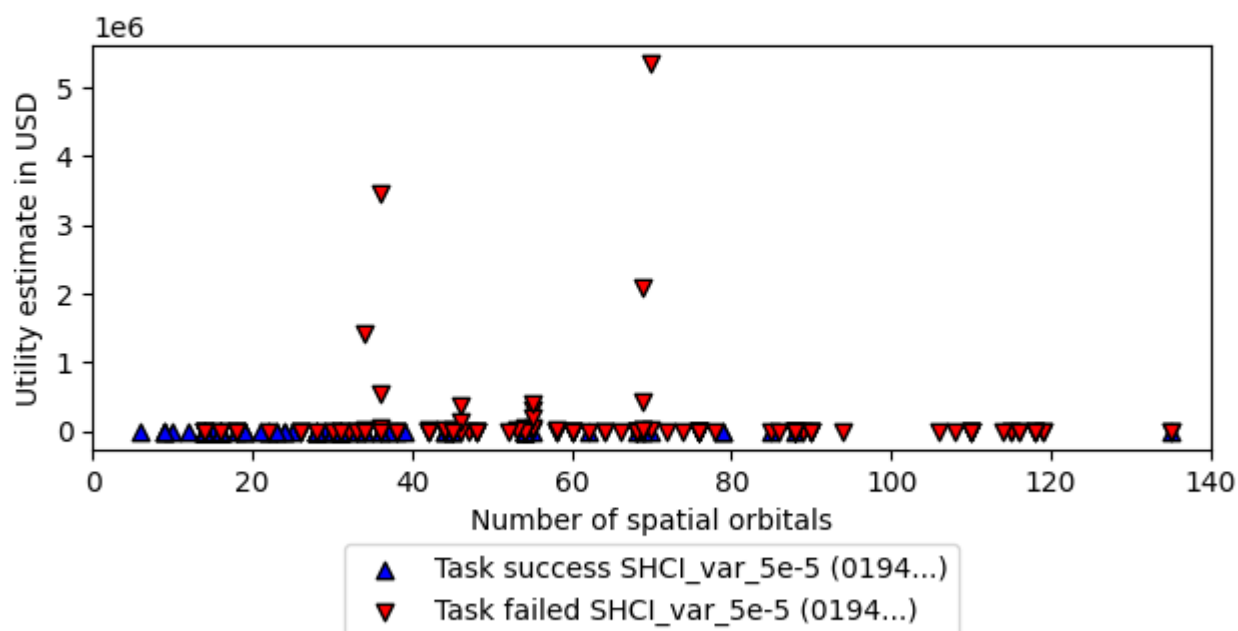
Note: plot only contains attempted tasks.

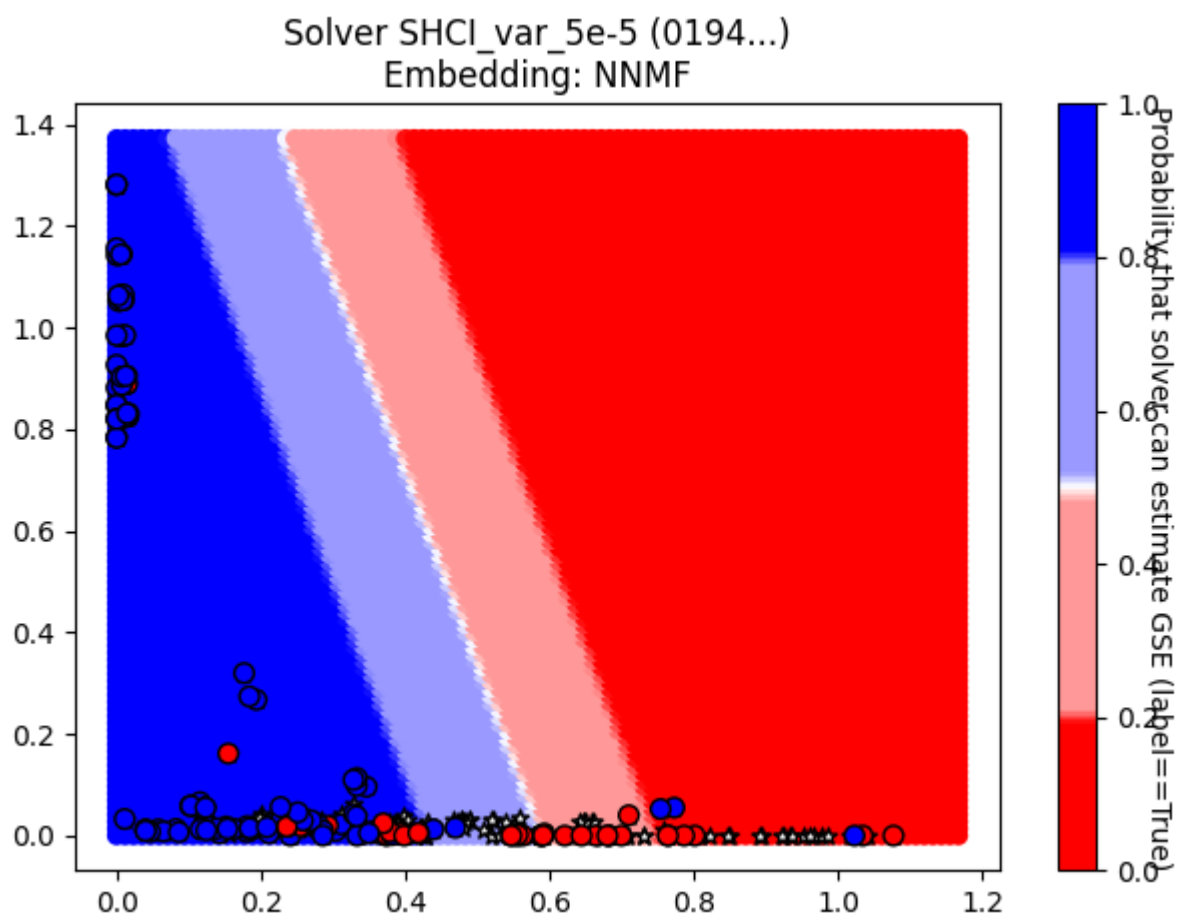


Note: plot only contains attempted tasks.

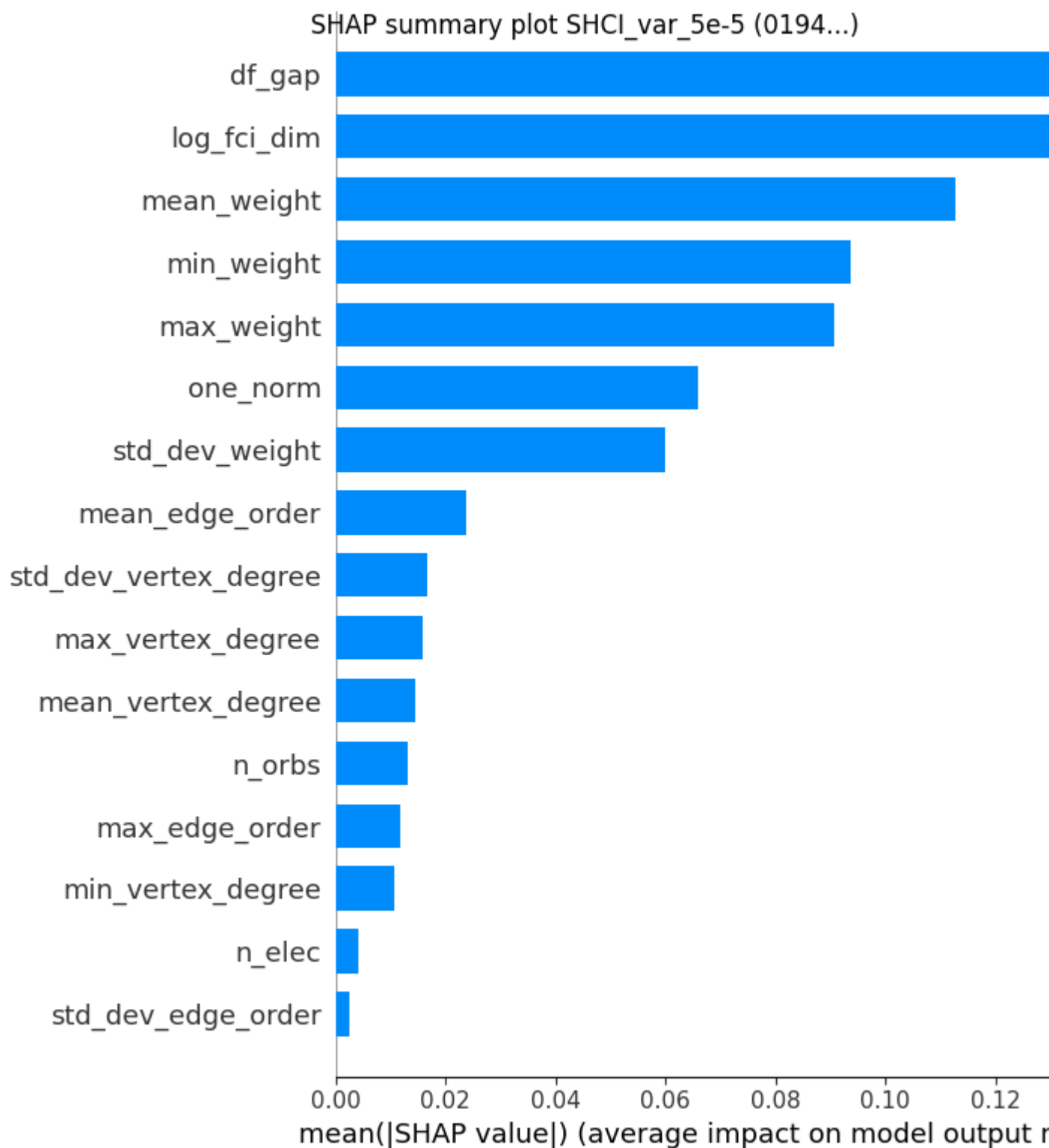
# Utility capture from SHCI\_var\_5e-5/0194...

(captured:  $\$4.5\text{e}+02/1.5\text{e}+07$ , approximately  $3.0\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver DF\_QPE, 5dad4064-cd11-412f-85cb-d722afe3b3de**

solver\_uuid:5dad4064-cd11-412f-85cb-d722afe3b3de

solver\_short\_name:DF\_QPE

compute\_hardware\_type:quantum\_computer

algorithm\_details: {'algorithm\_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm\_parameters': {'overlap\_csv': 'overlaps.csv', 'sf\_threshold': 1e-12, 'df\_threshold': 0.001, 'max\_orbitals': 70}}

software\_details: [{'software\_name': 'pyLIQTR', 'software\_version': '1.3.4'}, {'software\_name': 'qb-gsee-benchmark', 'software\_version': '0.1.0a2.dev193+g879c00d'}, {'software\_name': 'Python', 'software\_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]'}, {'software\_name': 'qualtran', 'software\_version': '0.4.0'}]

quantum\_hardware\_details: {'quantum\_hardware\_description': 'Optimistic superconducting hardware model based on that described in <https://arxiv.org/abs/2011.03494>.', 'quantum\_hardware\_parameters': {'num\_factories': 4, 'physical\_error\_rate': 0.0001, 'cycle\_time\_microseconds': 1}}

logical\_resource\_estimate\_solution\_uuid:fc17e113-d2e0-49ab-955a-6fc08c6eb2f9

logical\_resource\_estimate\_solver\_uuid:f2d73e1f-3058-43c4-a634-b6c267c84ff1

performance\_metrics\_uuid: dfb6f14e-3619-4557-9e95-d22067ccef5c

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 22

number\_of\_problem\_instances\_solved: 0

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 154

number\_of\_tasks\_solved: 0

number\_of\_tasks\_solved\_within\_run\_time\_limit: 0

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 154

max\_run\_time\_of\_attempted\_tasks: 1394068547267.4111

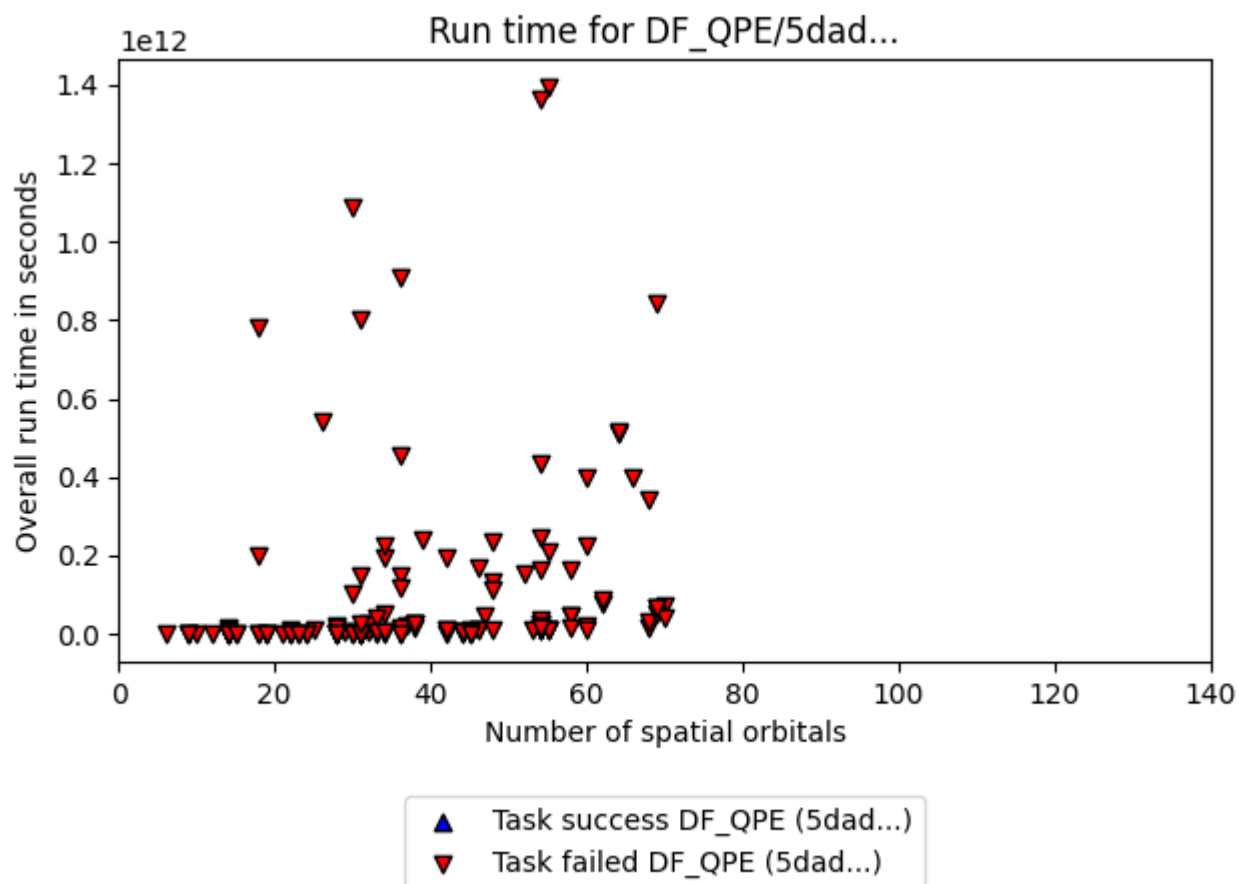
sum\_of\_run\_time\_of\_attempted\_tasks: 15652541022388.93

solvability\_ratio: None

f1\_score: None

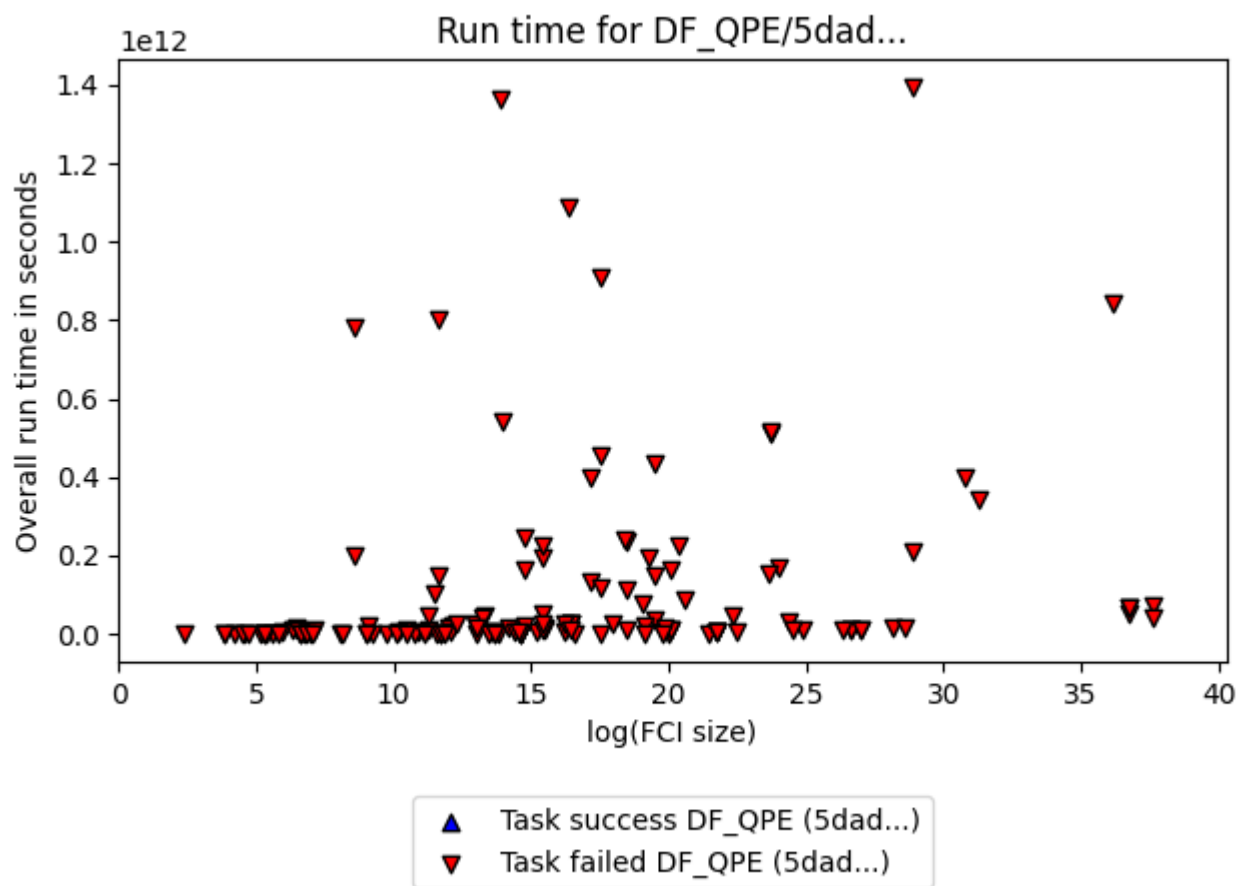
ml\_metrics\_calculator\_version: 1

comment: All labels were either all True or all False and we cannot create an ML model with only one class.



Note: plot only contains attempted tasks.

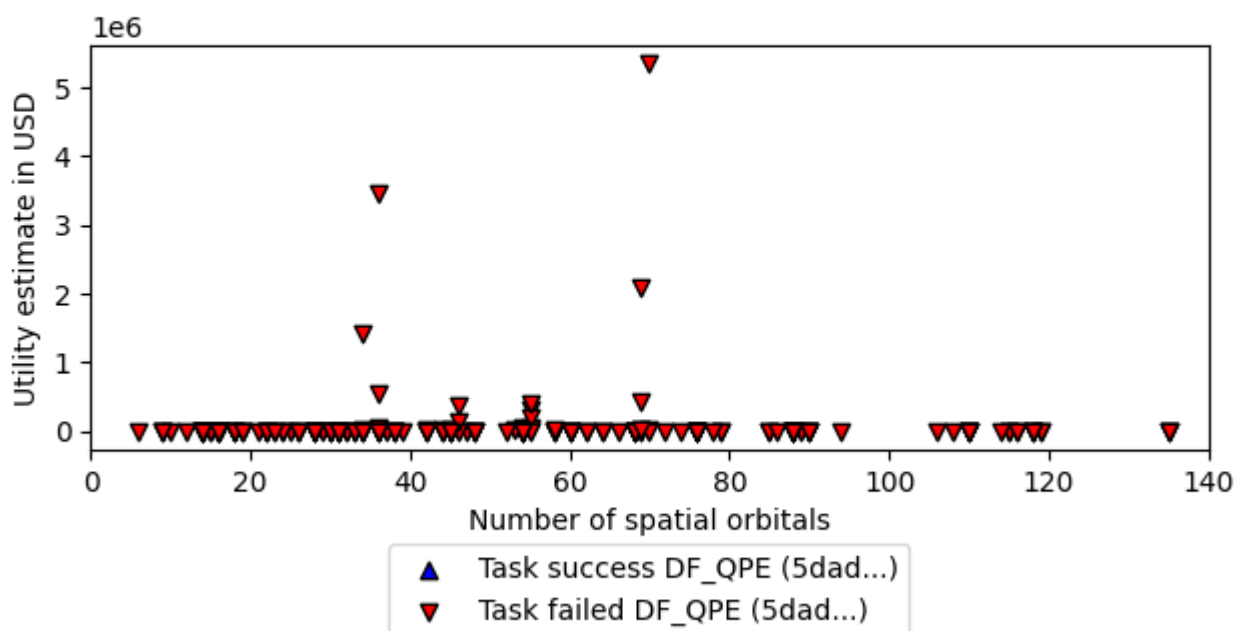




Note: plot only contains attempted tasks.

### Utility capture from DF\_QPE/5dad...

(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



### Solver miniML plot

Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.

### SHAP summary plot

## Solver CISD, 418f060e-496b-4024-8d2d-9b1f8791e76d

solver\_uuid:418f060e-496b-4024-8d2d-9b1f8791e76d

solver\_short\_name:CISD

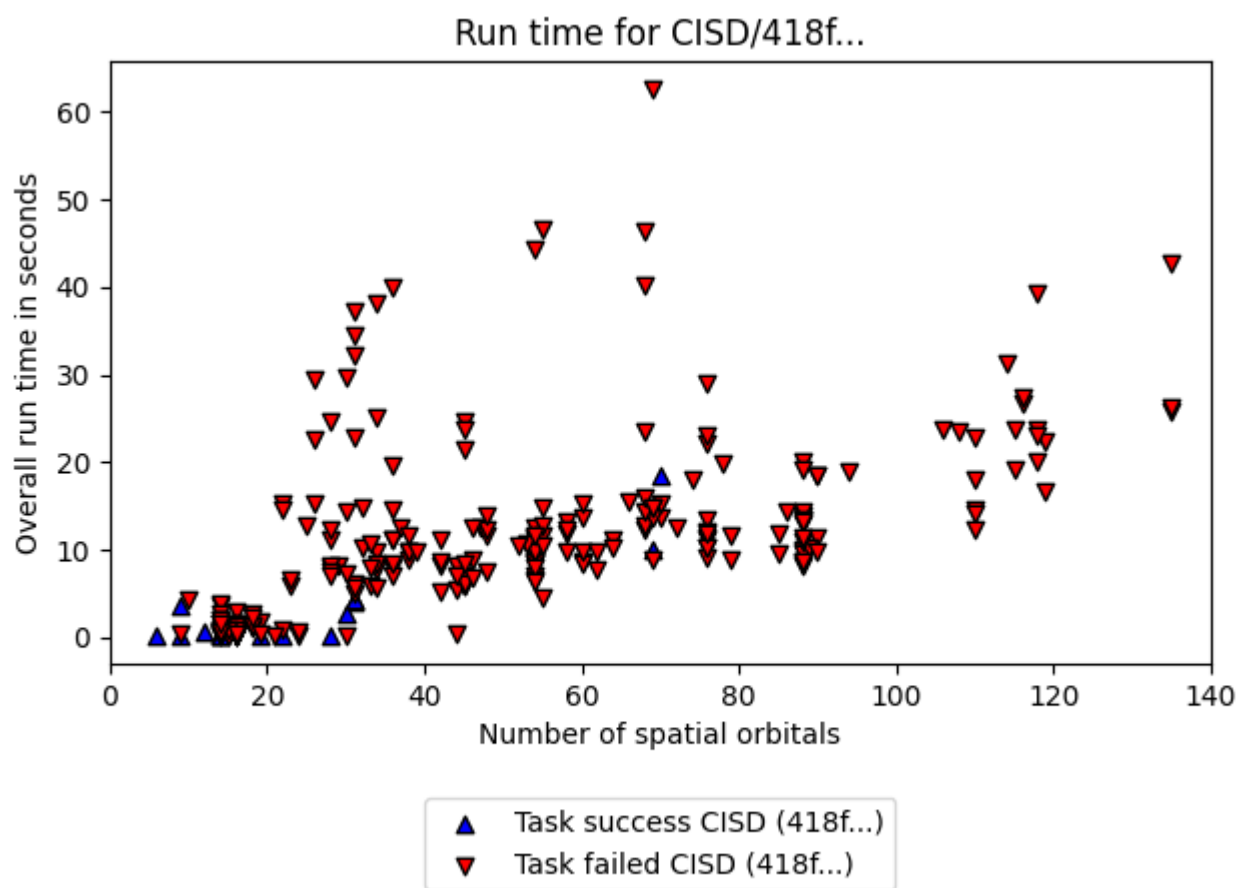
compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

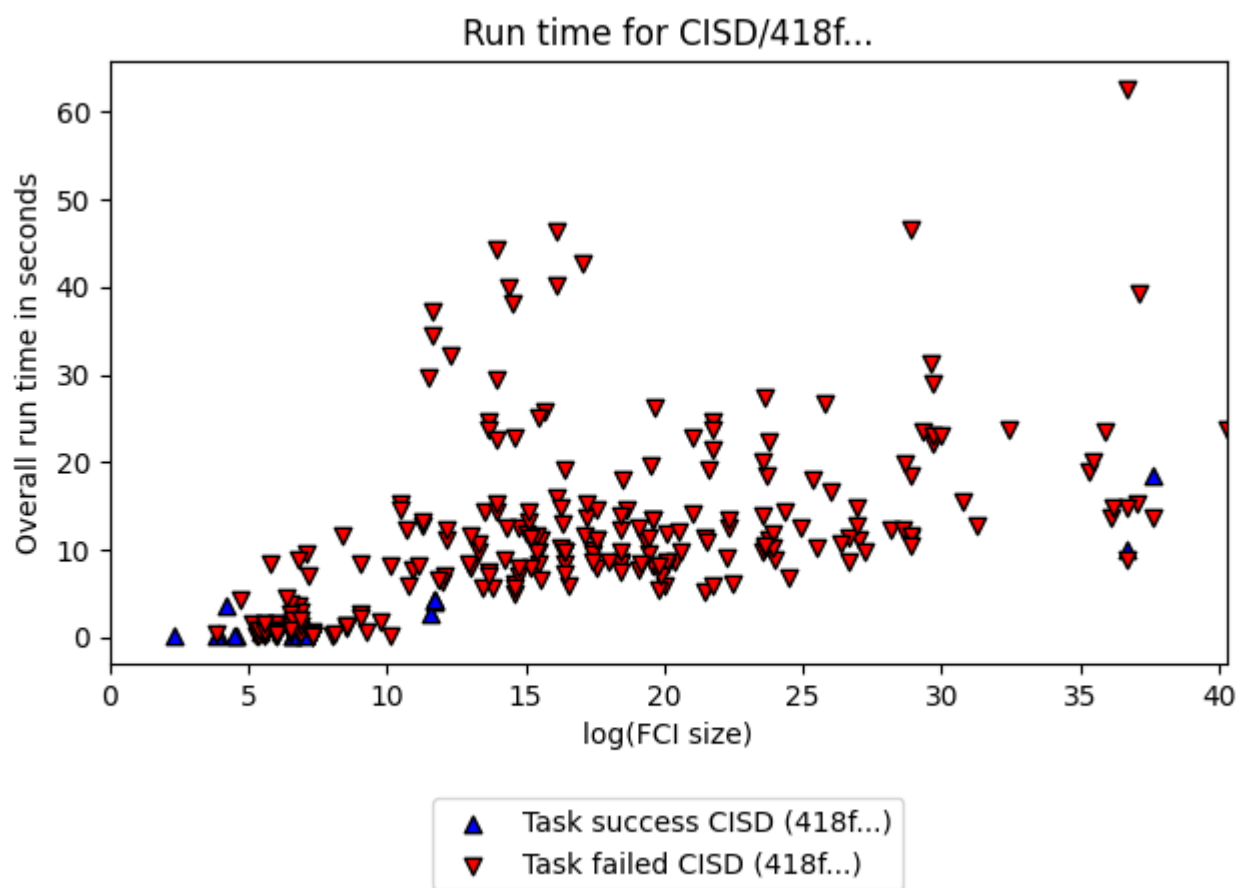
algorithm\_details:CISD

software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: 7fb33e1e-6fb9-4789-9936-ce8b272fbae7  
creation\_timestamp: 2025-01-28T21:50:06.833854+00:00  
number\_of\_problem\_instances: 84  
number\_of\_problem\_instances\_attempted: 84  
number\_of\_problem\_instances\_solved: 9  
number\_of\_tasks: 276  
number\_of\_tasks\_attempted: 276  
number\_of\_tasks\_solved: 17  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 276  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 17  
max\_run\_time\_of\_attempted\_tasks: 62.58296537399292  
sum\_of\_run\_time\_of\_attempted\_tasks: 2929.870177745819  
solvability\_ratio: 0.003  
f1\_score: [0.9782608695652174, 0.85]  
ml\_metrics\_calculator\_version: 1



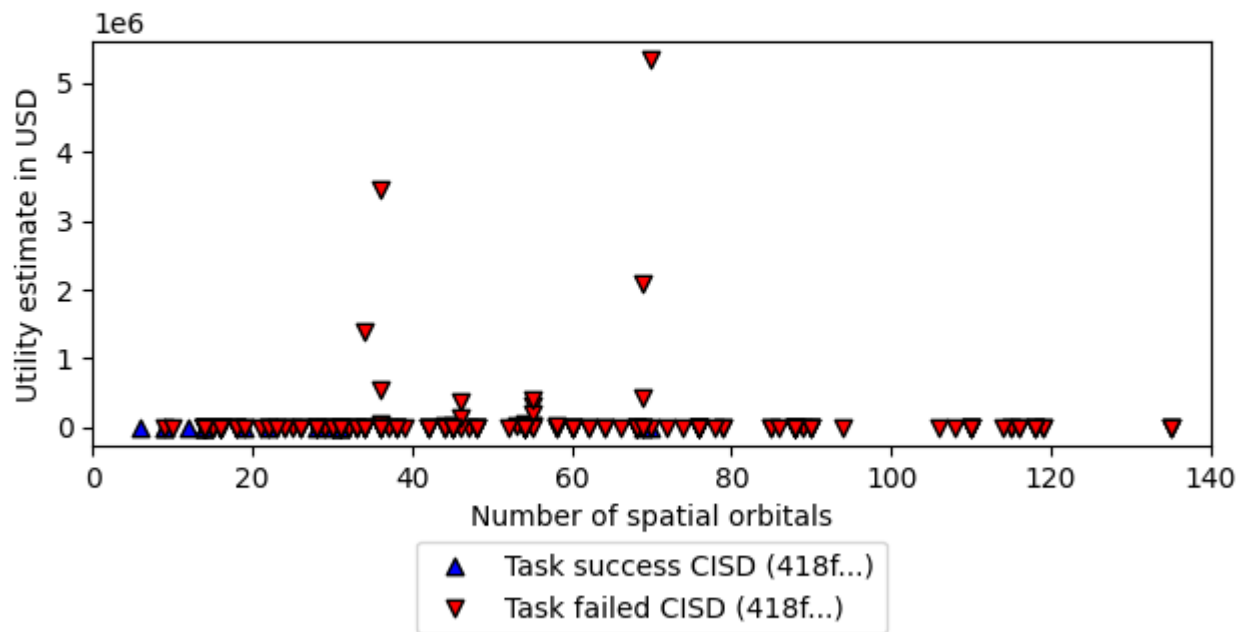
Note: plot only contains attempted tasks.

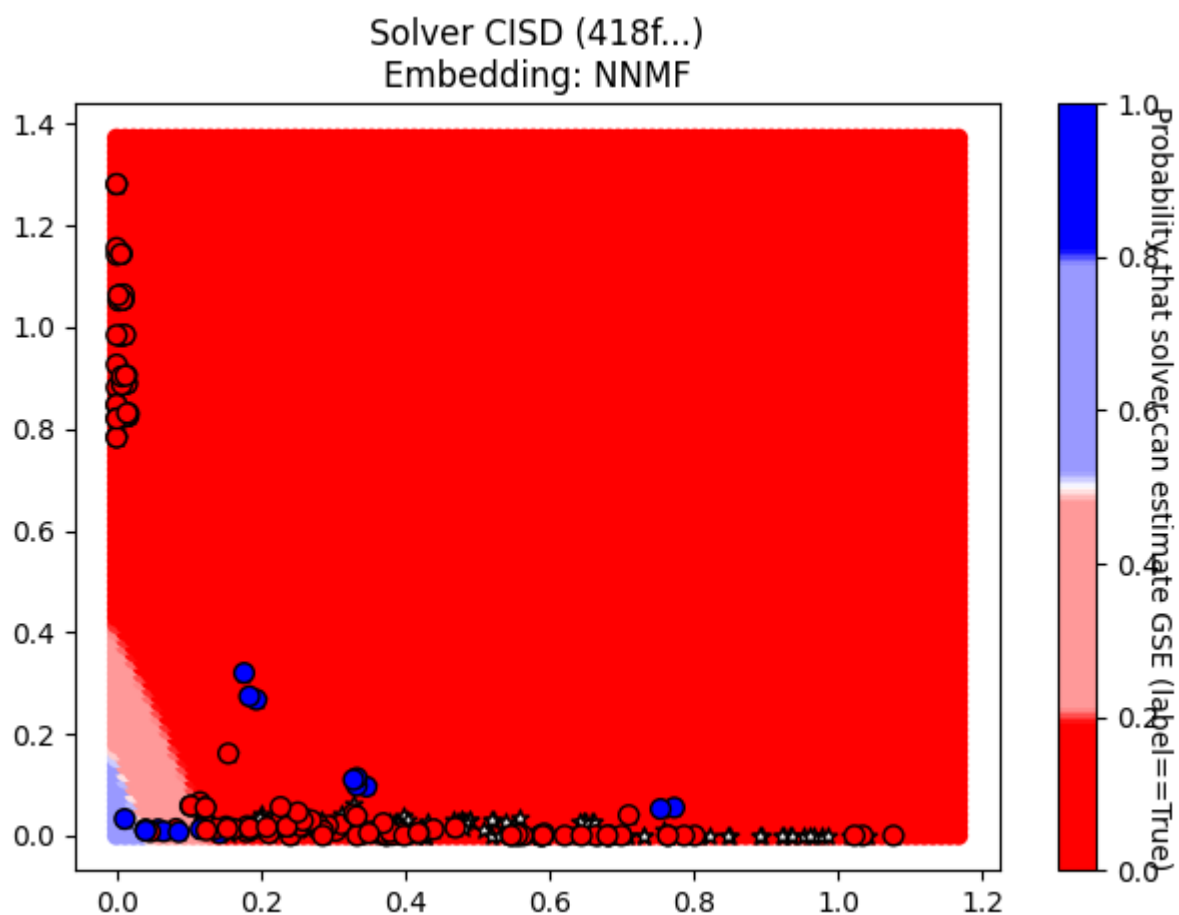


Note: plot only contains attempted tasks.

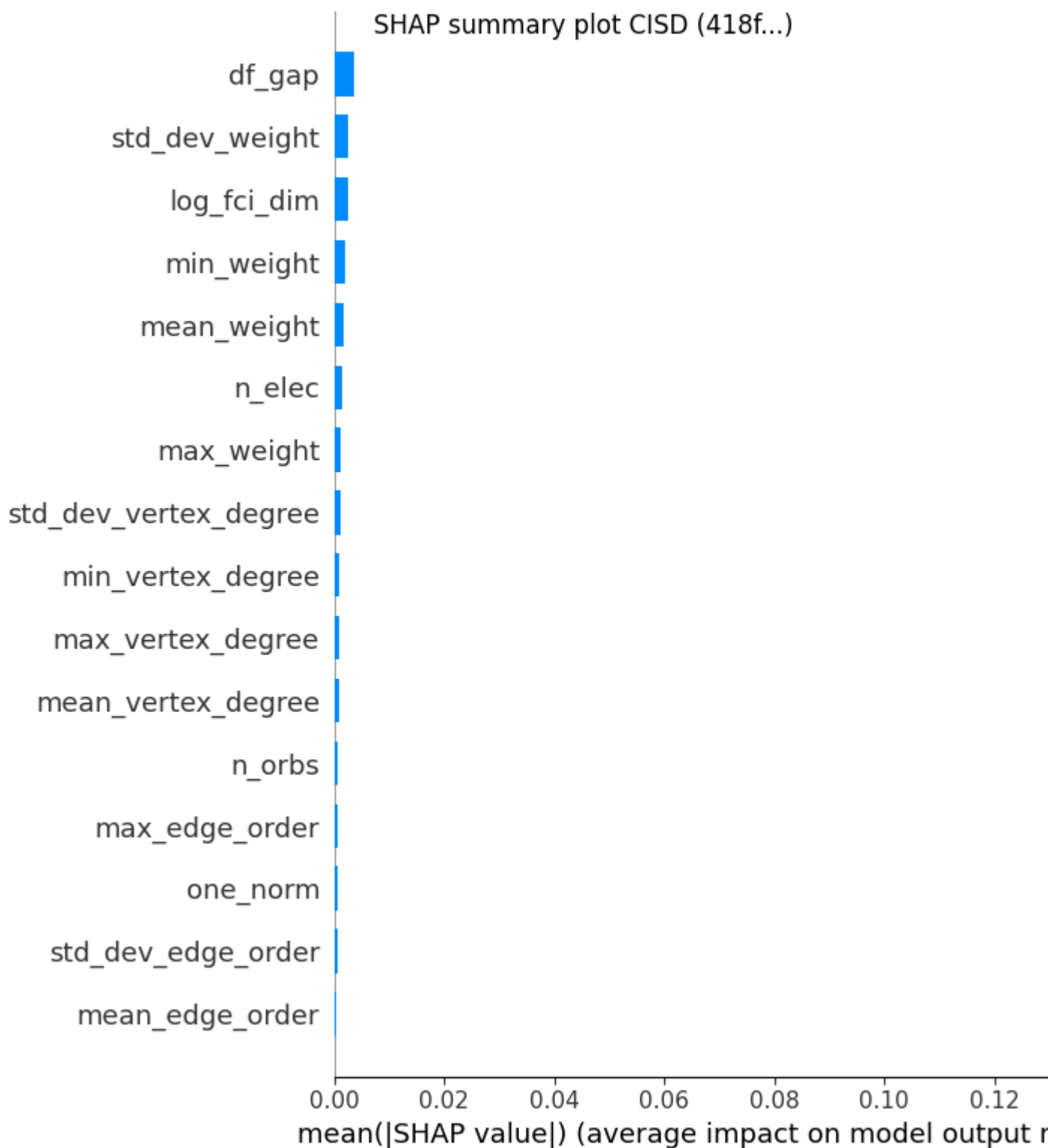
### Utility capture from CISD/418f...

(captured:  $\$4.8\text{e-}03/1.5\text{e+}07$ , approximately  $3.2\text{e-}08\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878**

solver\_uuid:c09217e6-d0f7-4b0f-81c4-79210b7ac878

solver\_short\_name:CCSD(T)



compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:CCSD(T)

software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: 12e14154-4351-464f-a933-e85f088cfe47

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 79

number\_of\_problem\_instances\_solved: 19

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 264

number\_of\_tasks\_solved: 71

number\_of\_tasks\_solved\_within\_run\_time\_limit: 264

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 71

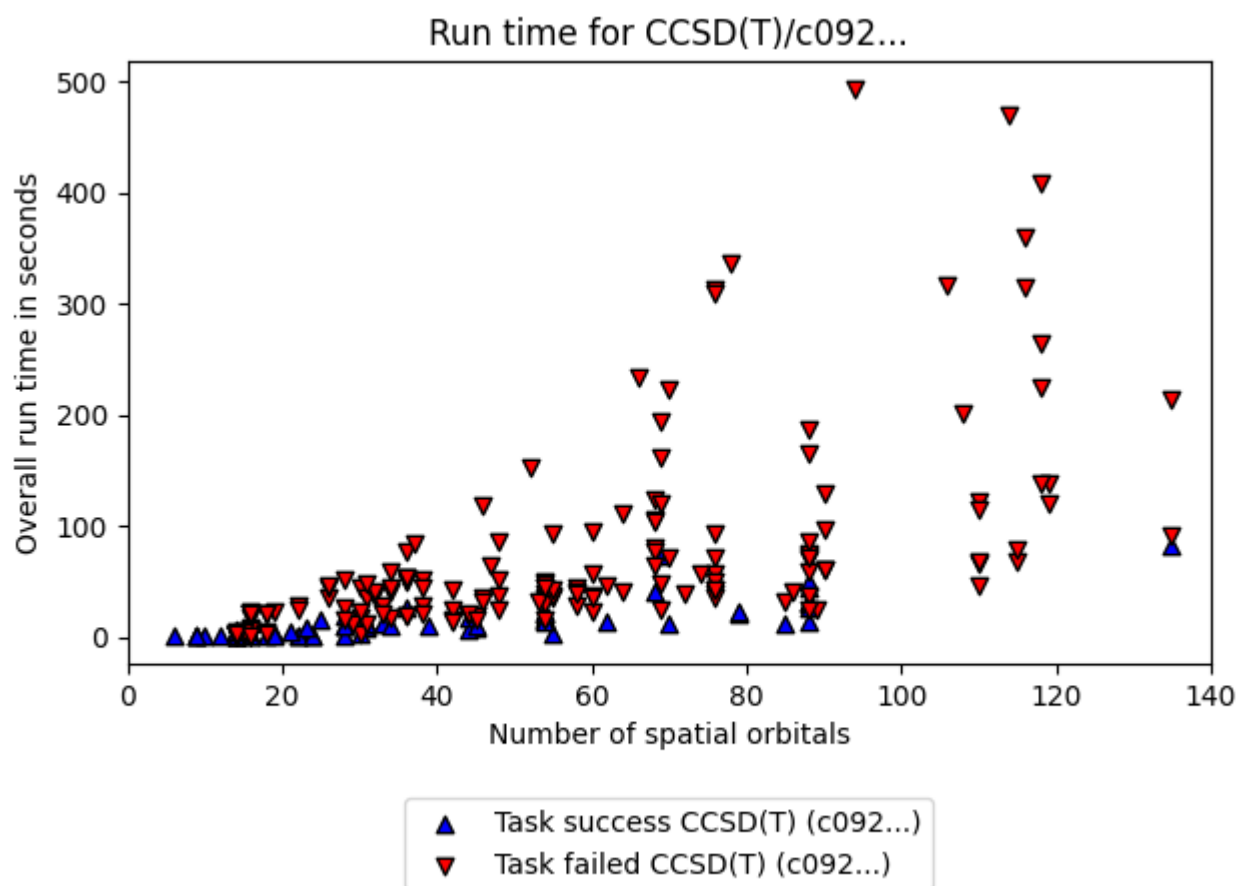
max\_run\_time\_of\_attempted\_tasks: 493.4080808162689

sum\_of\_run\_time\_of\_attempted\_tasks: 13199.317583084106

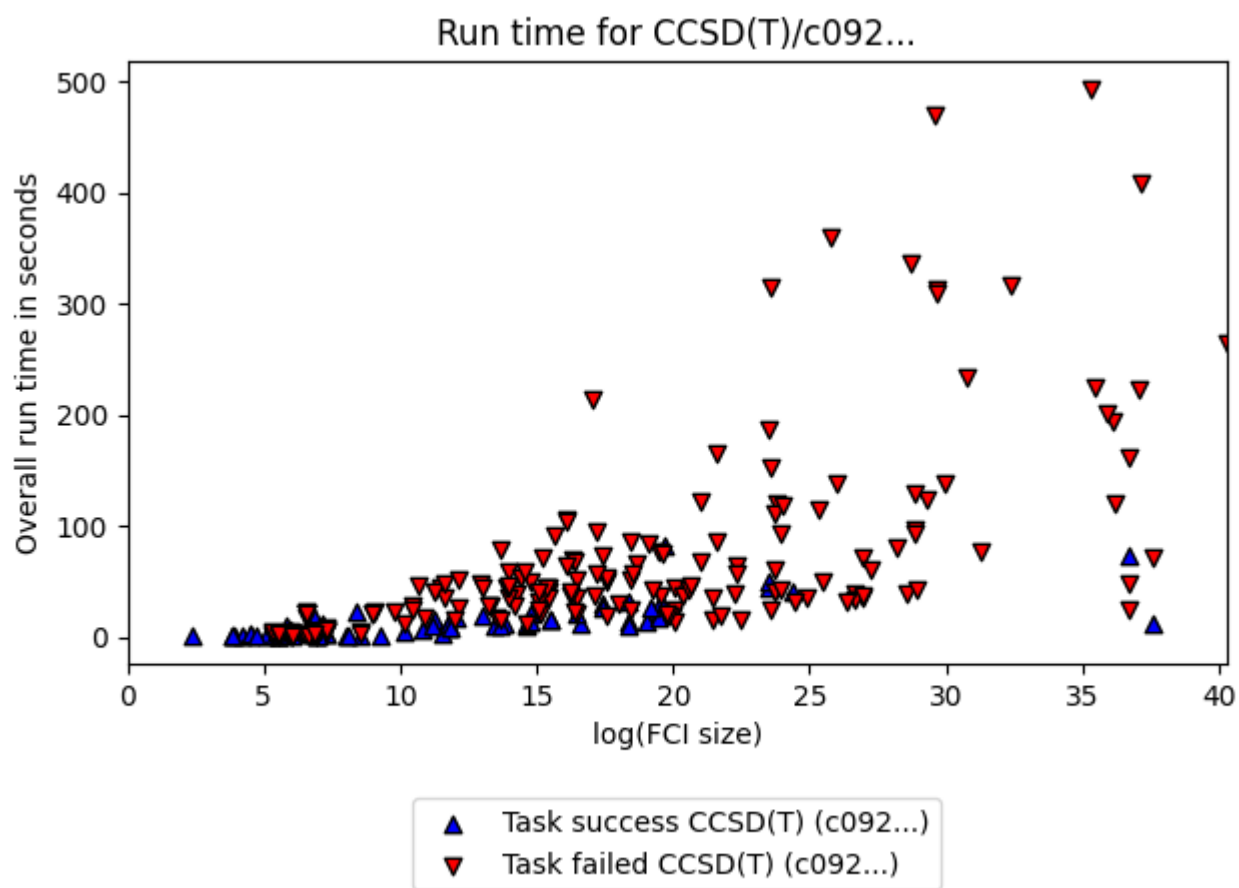
solvability\_ratio: 0.8102

f1\_score: [0.8695652173913043, 0.864516129032258]

ml\_metrics\_calculator\_version: 1



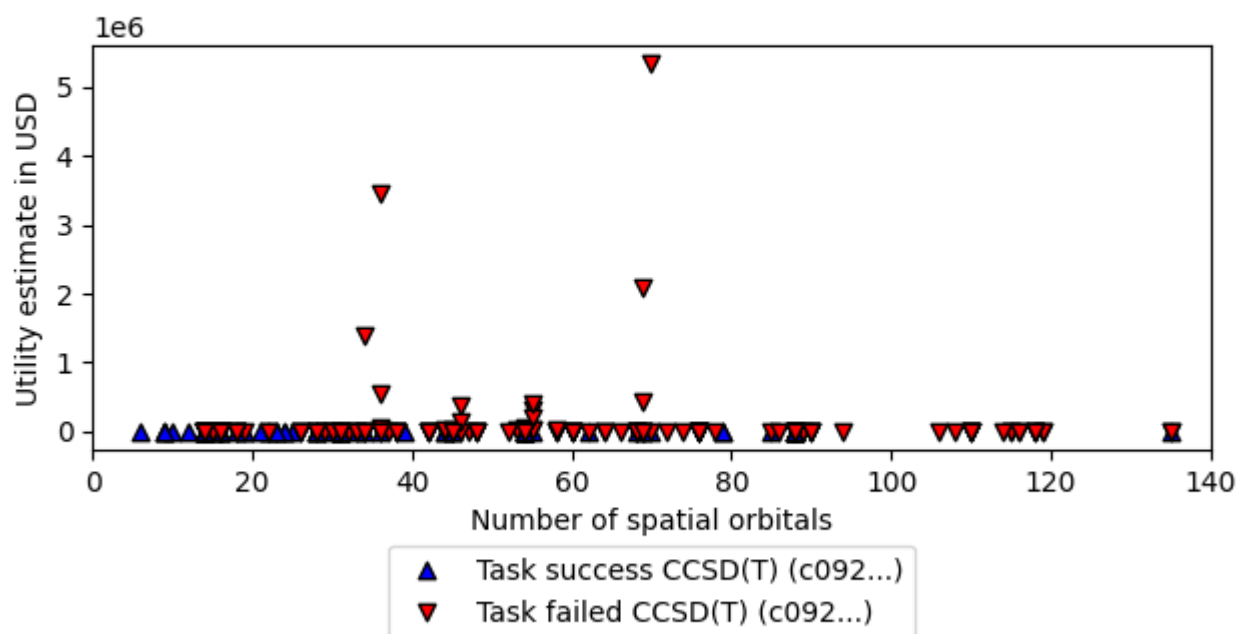
Note: plot only contains attempted tasks.

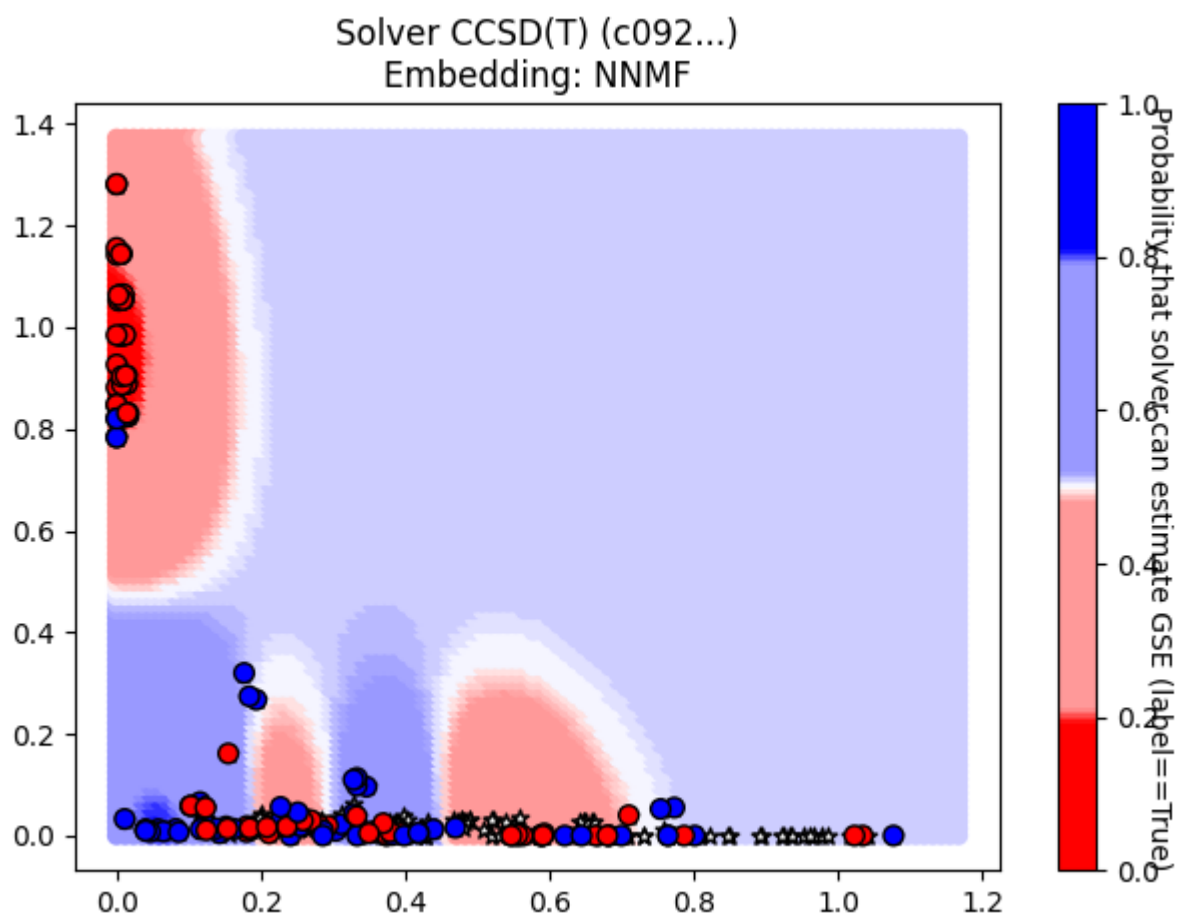


Note: plot only contains attempted tasks.

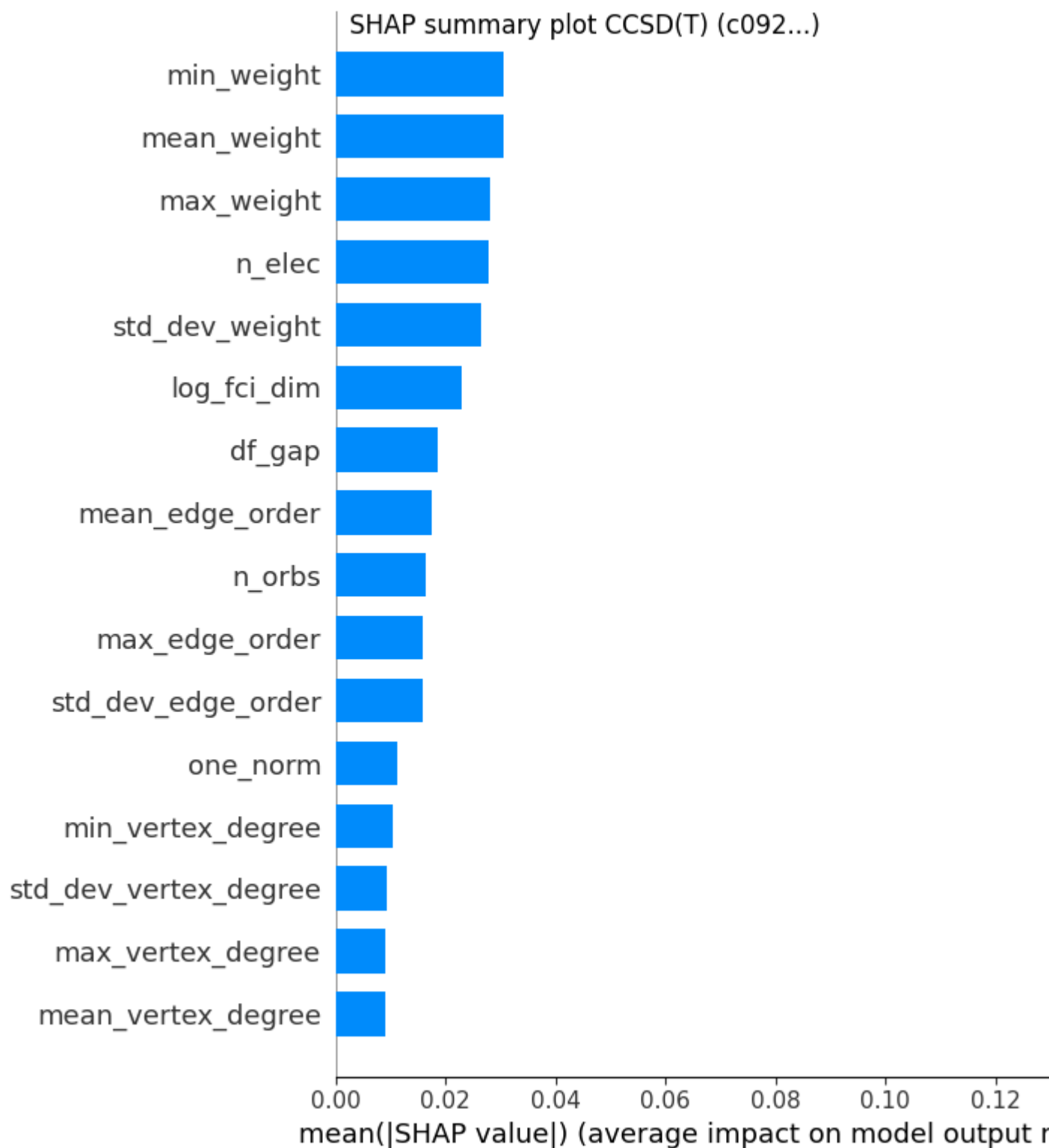
### Utility capture from CCSD(T)/c092...

(captured:  $\$1.8\text{e}+02/1.5\text{e}+07$ , approximately  $1.2\text{e}-03\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012**

solver\_uuid:5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

solver\_short\_name:HF

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:Hartree Fock

software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: 3abe001b-2d7c-4661-9a22-e418c72af383

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 84

number\_of\_problem\_instances\_solved: 5

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 276

number\_of\_tasks\_solved: 5

number\_of\_tasks\_solved\_within\_run\_time\_limit: 276

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 5

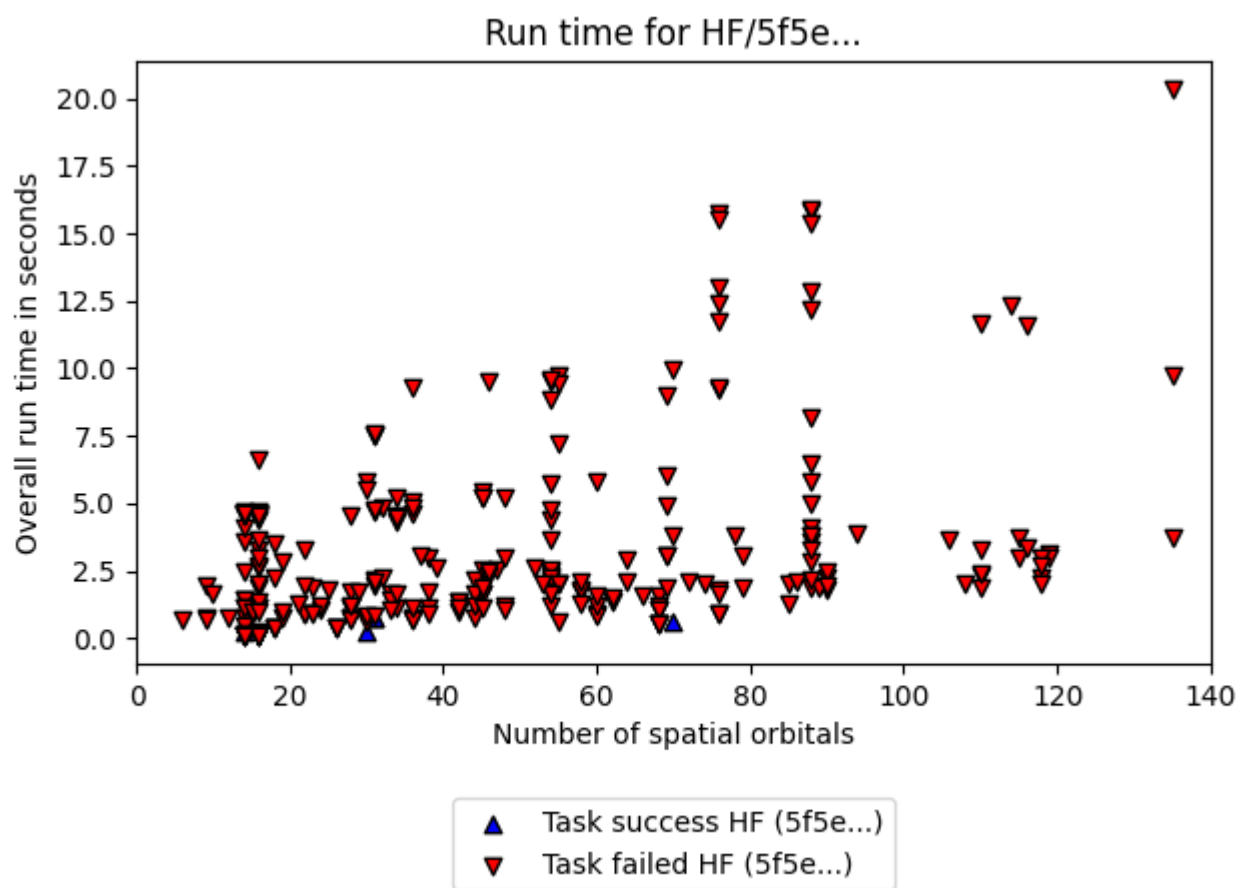
max\_run\_time\_of\_attempted\_tasks: 20.338801622390747

sum\_of\_run\_time\_of\_attempted\_tasks: 906.4860525131226

solvability\_ratio: 0.0

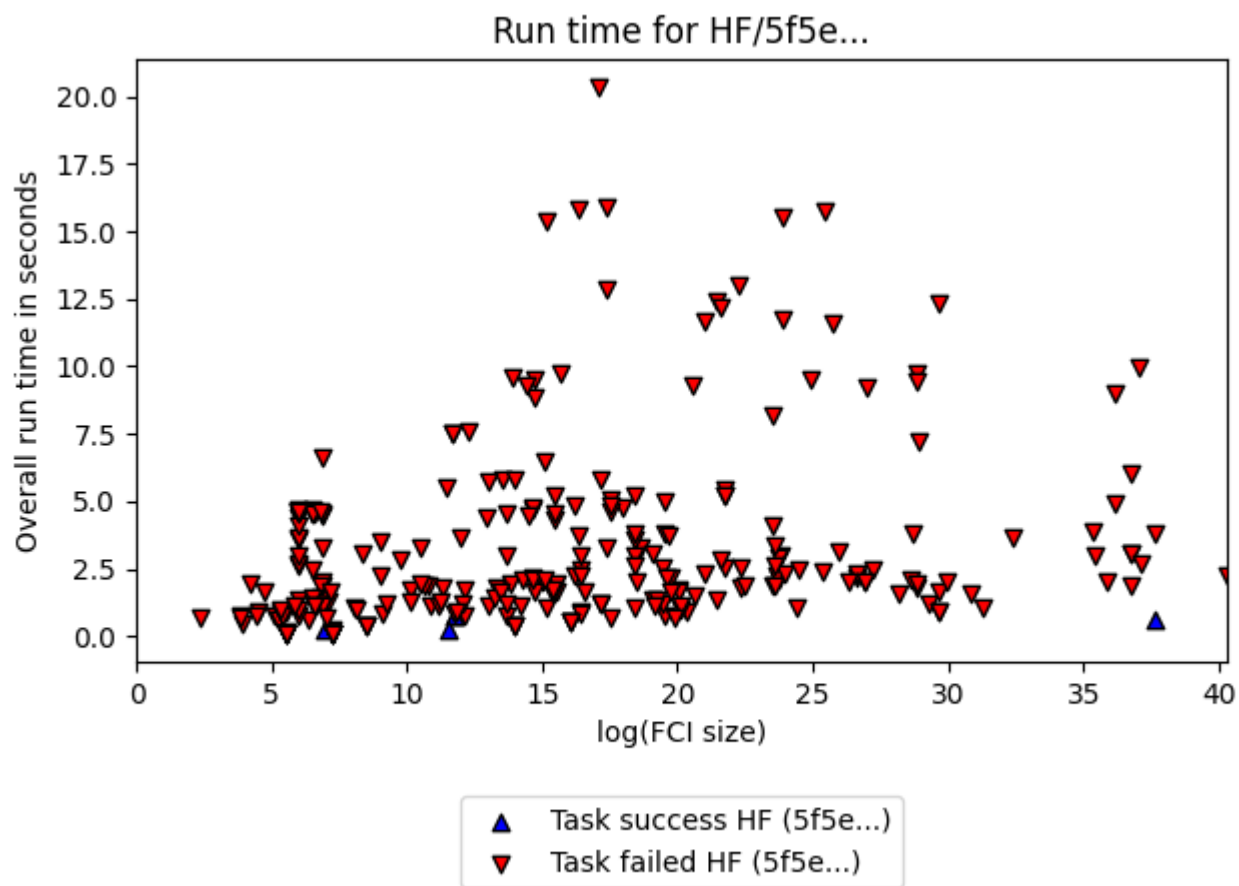
f1\_score: [0.9867549668874173, 0.7142857142857143]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

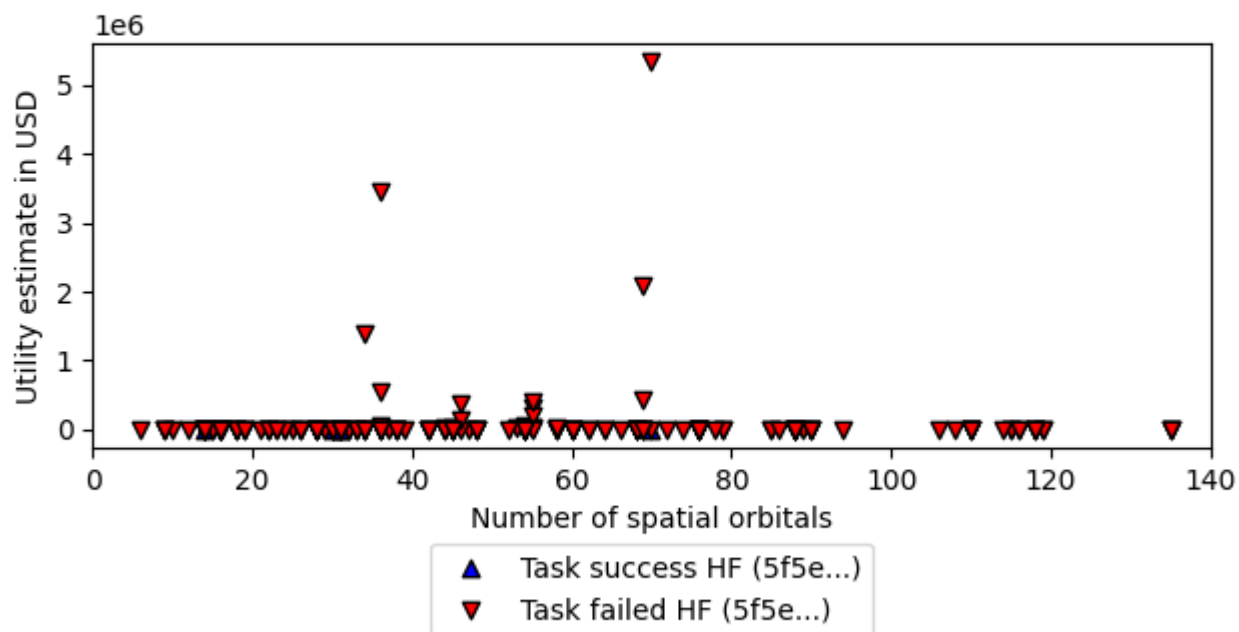


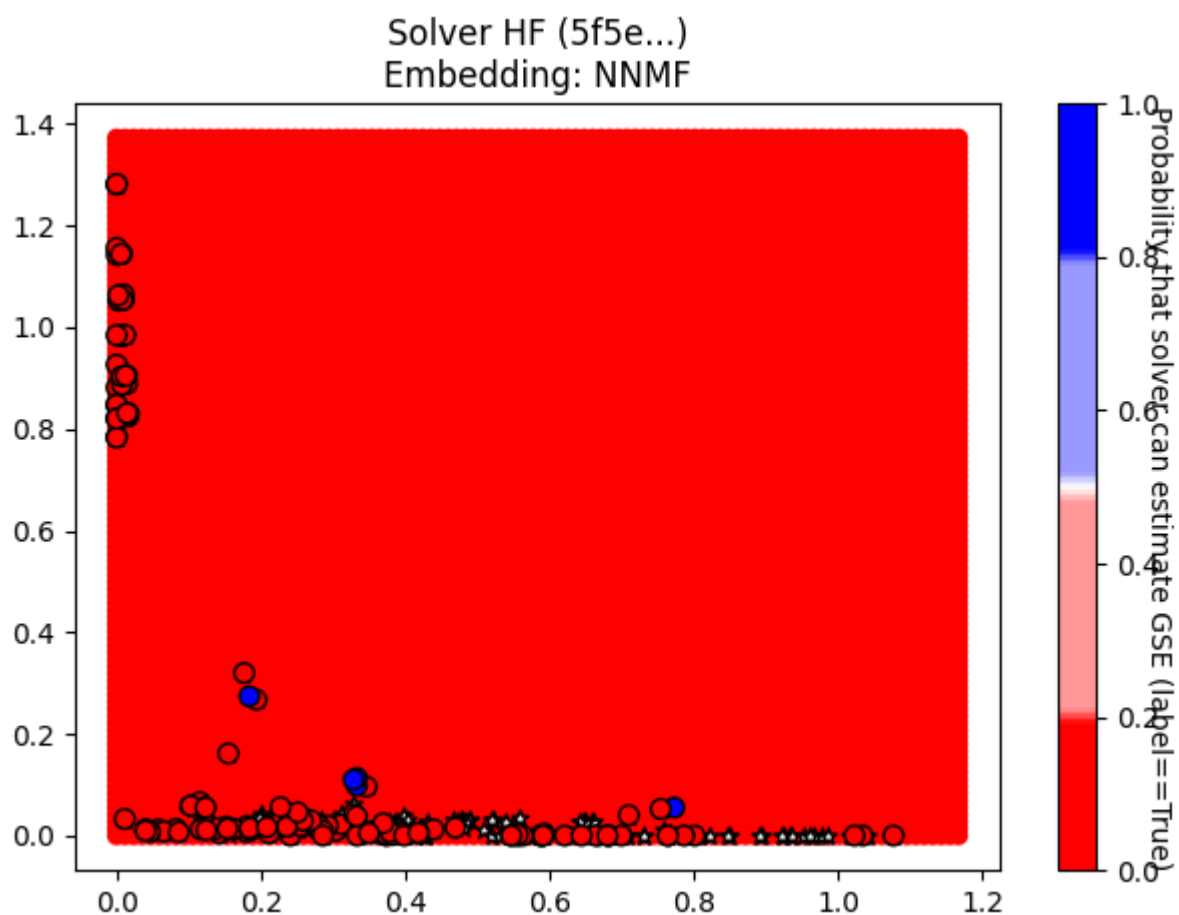


Note: plot only contains attempted tasks.

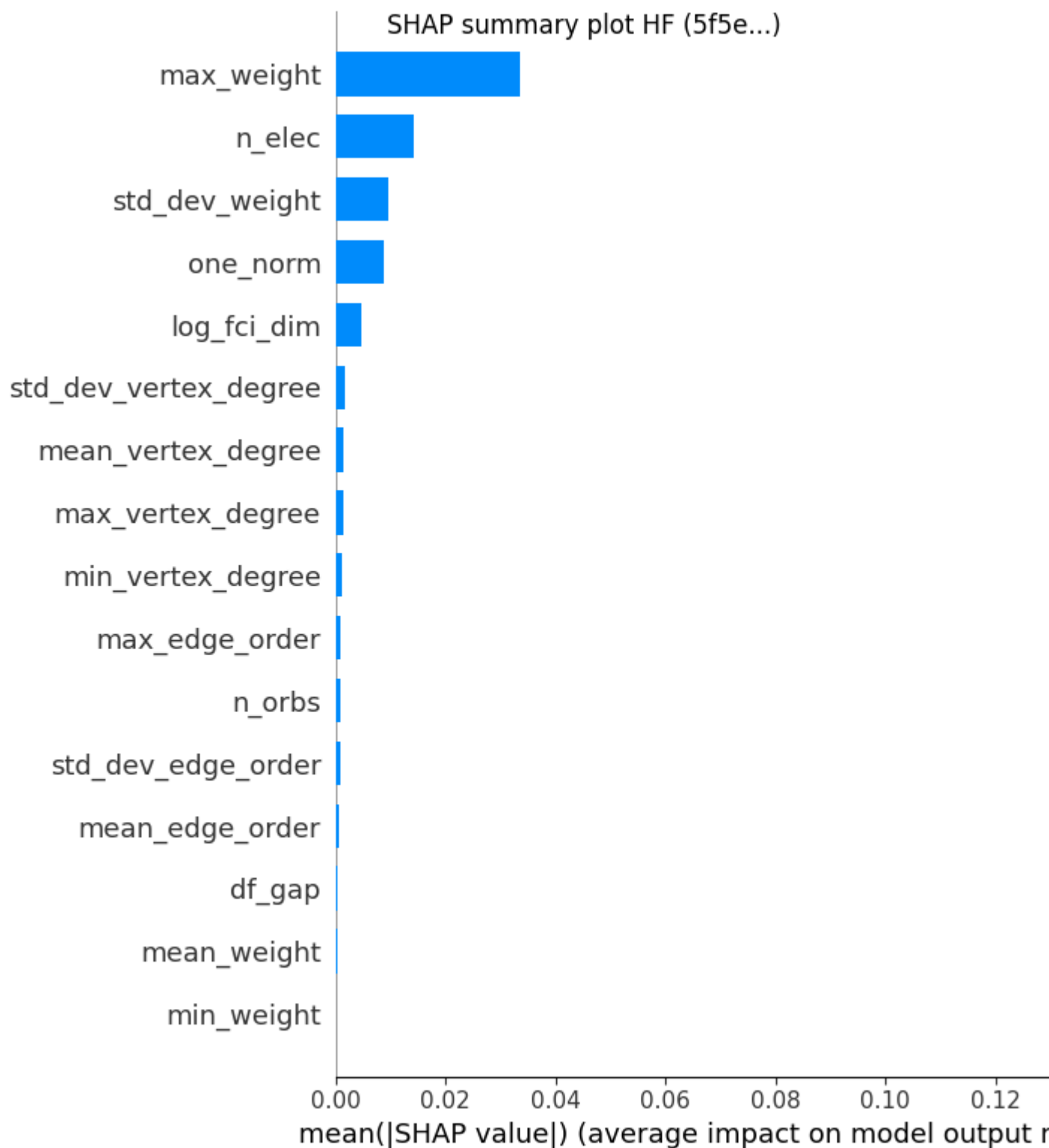
### Utility capture from HF/5f5e...

(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aec2**

solver\_uuid:b420358b-5def-41e6-8c5d-b9d93b6aec2

solver\_short\_name:MP2

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:MP2

software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: d1774265-c873-46bf-b518-670a2a9a9b77

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 81

number\_of\_problem\_instances\_solved: 5

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 268

number\_of\_tasks\_solved: 5

number\_of\_tasks\_solved\_within\_run\_time\_limit: 268

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 5

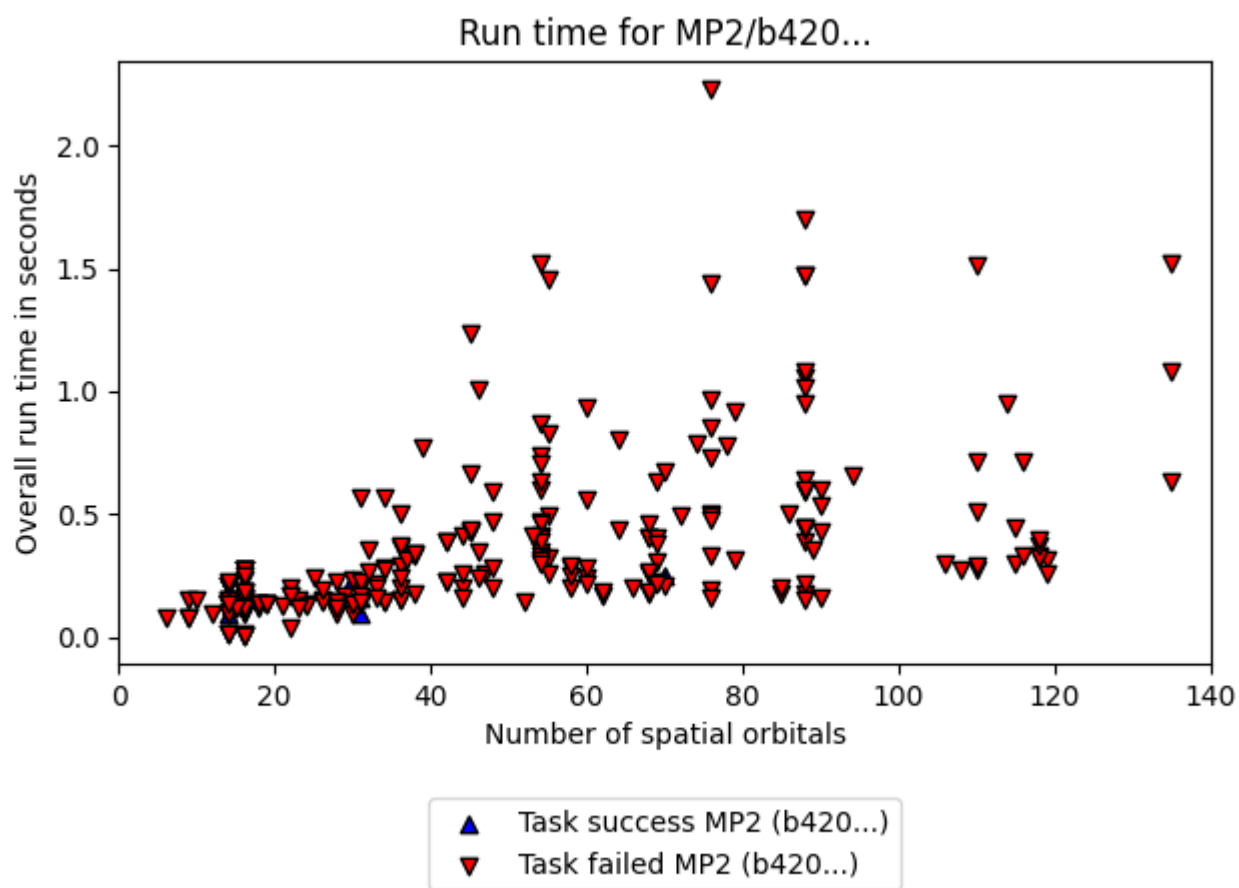
max\_run\_time\_of\_attempted\_tasks: 2.230440139770508

sum\_of\_run\_time\_of\_attempted\_tasks: 94.7442626953125

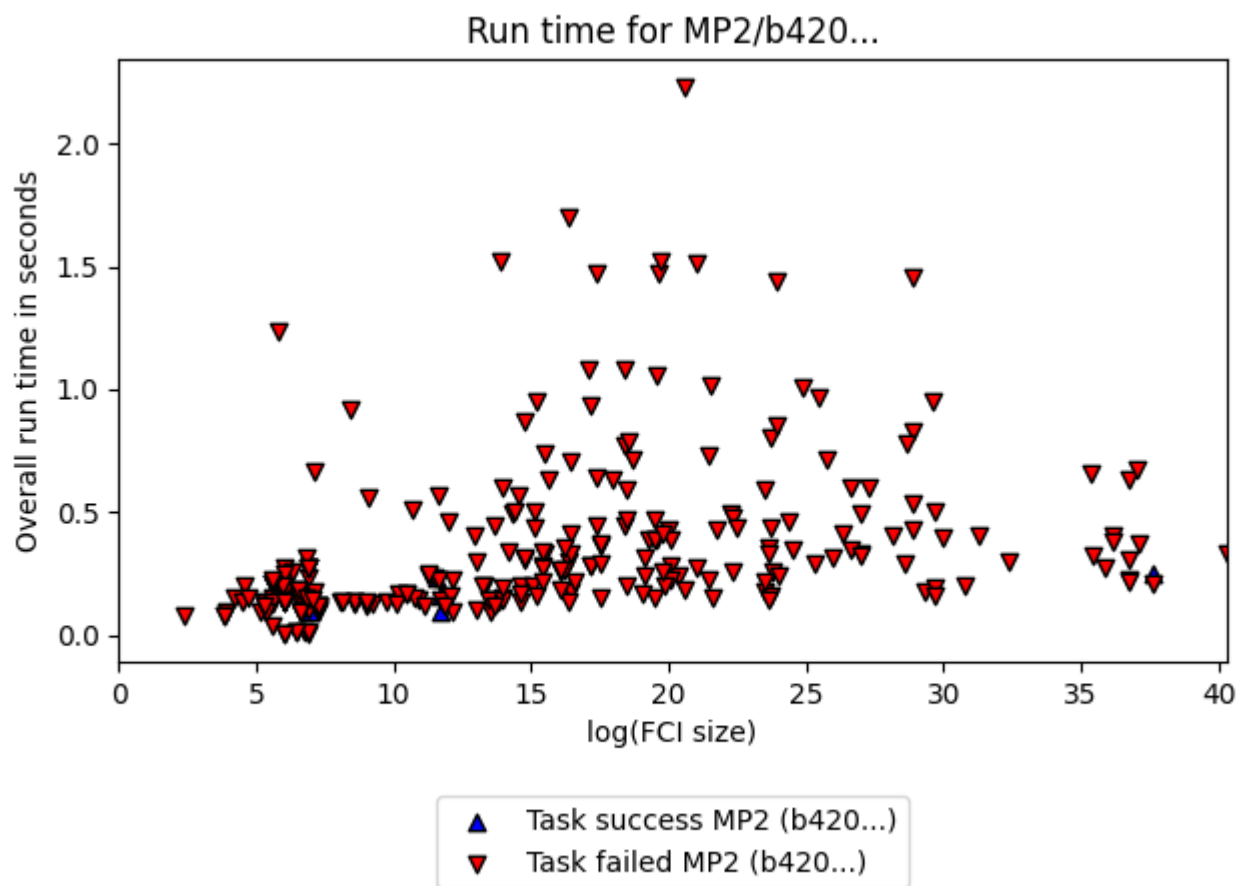
solvability\_ratio: 0.0

f1\_score: [0.9867549668874173, 0.7142857142857143]

ml\_metrics\_calculator\_version: 1



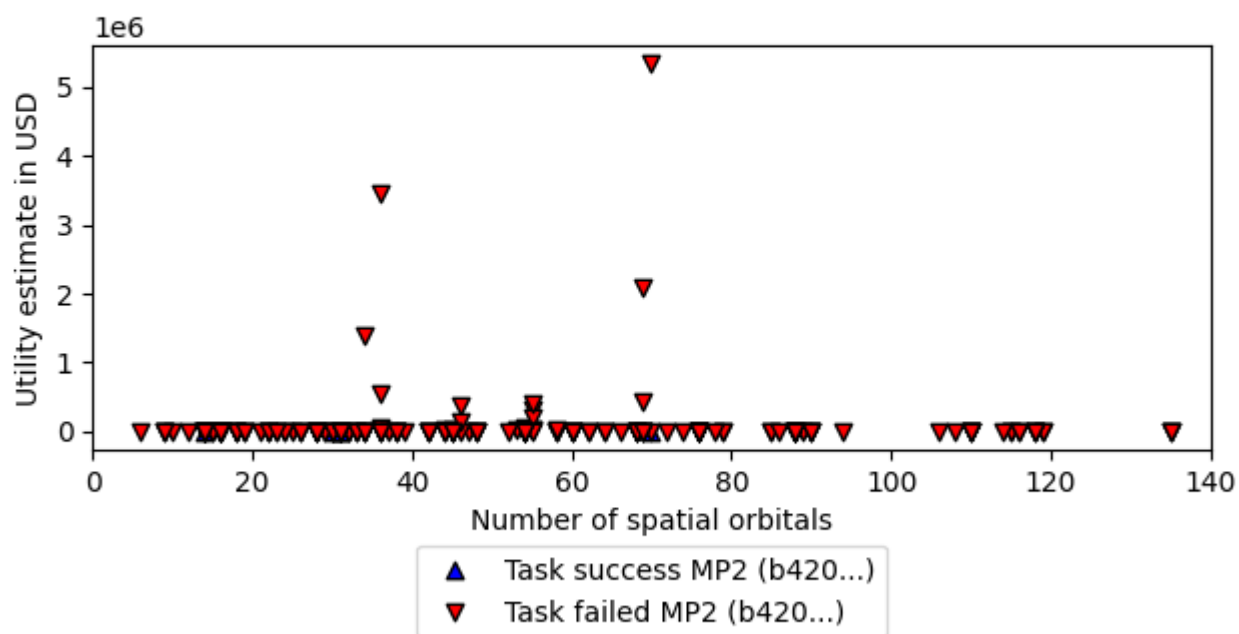
Note: plot only contains attempted tasks.



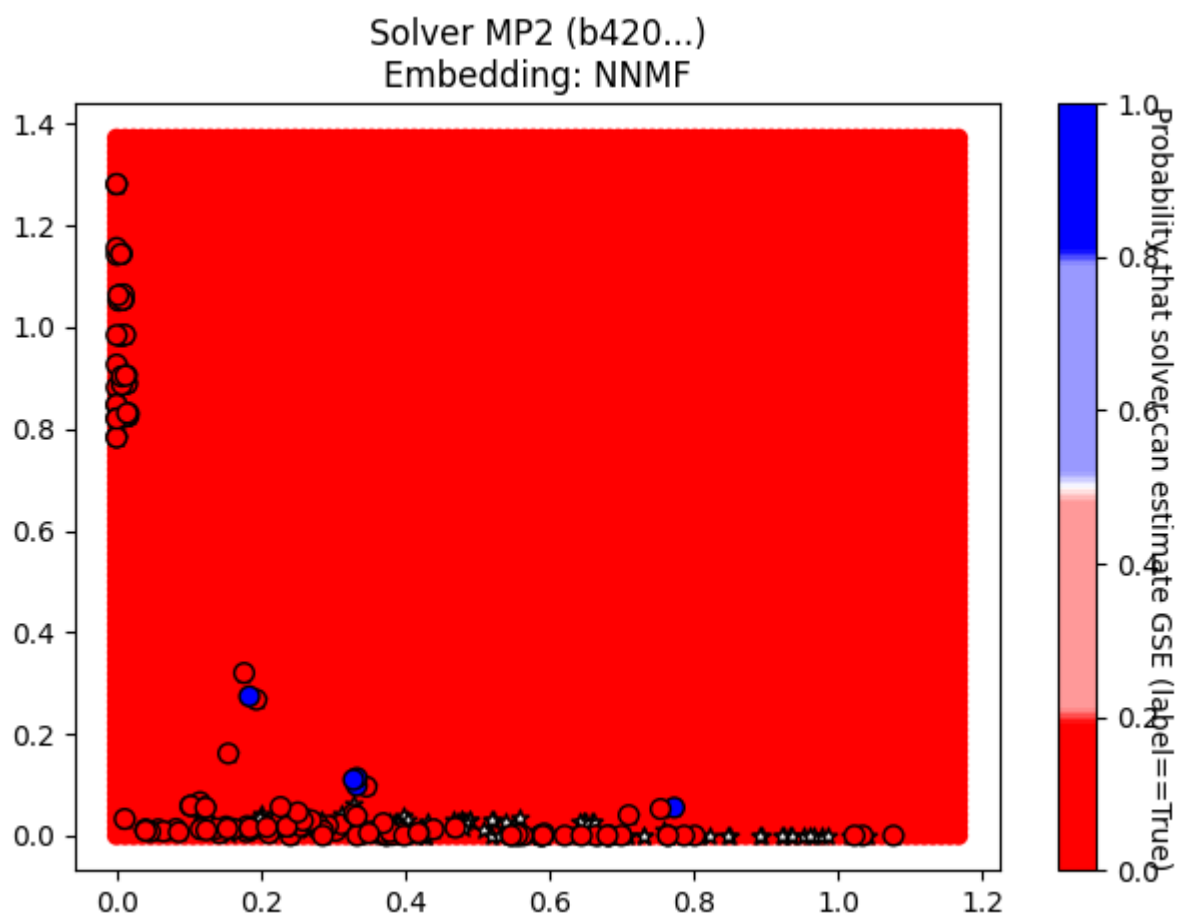
Note: plot only contains attempted tasks.

# Utility capture from MP2/b420...

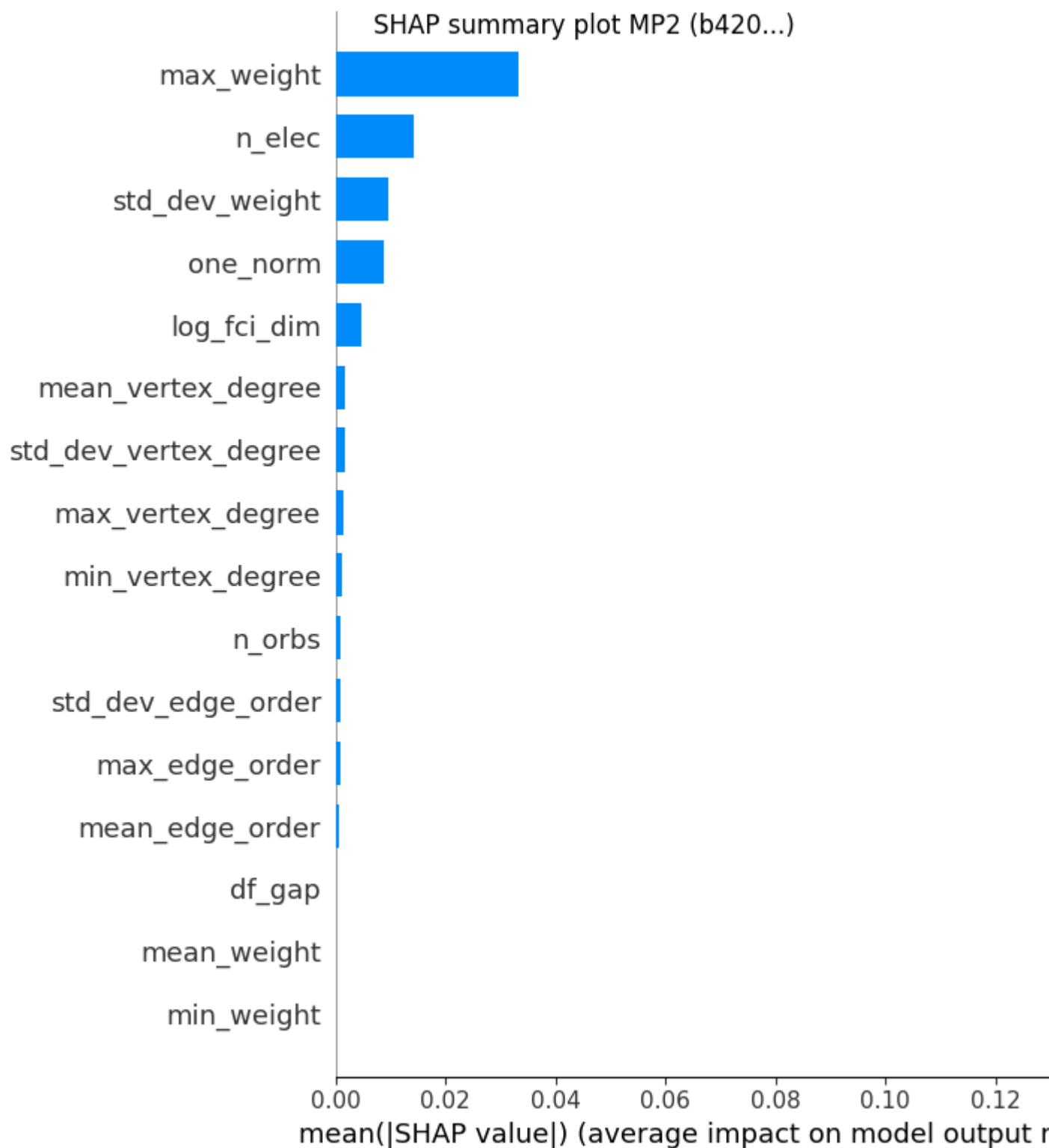
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)







Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa**

solver\_uuid:0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

solver\_short\_name:CCSD

compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}

algorithm\_details:CCSD

software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: 3b4570f3-f224-4fec-857b-4725857548ac

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 79

number\_of\_problem\_instances\_solved: 10

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 264

number\_of\_tasks\_solved: 24

number\_of\_tasks\_solved\_within\_run\_time\_limit: 264

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 24

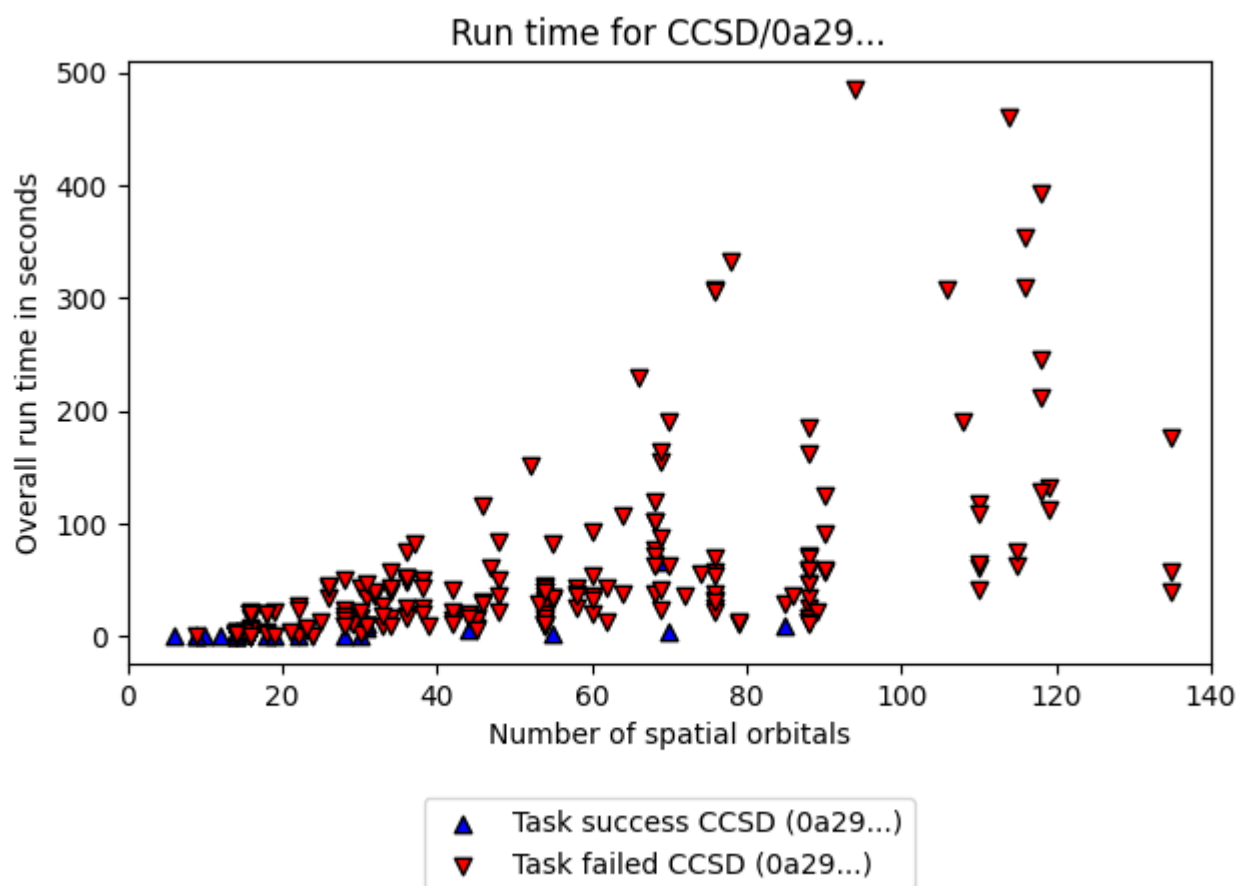
max\_run\_time\_of\_attempted\_tasks: 485.1982181072235

sum\_of\_run\_time\_of\_attempted\_tasks: 12252.72845697403

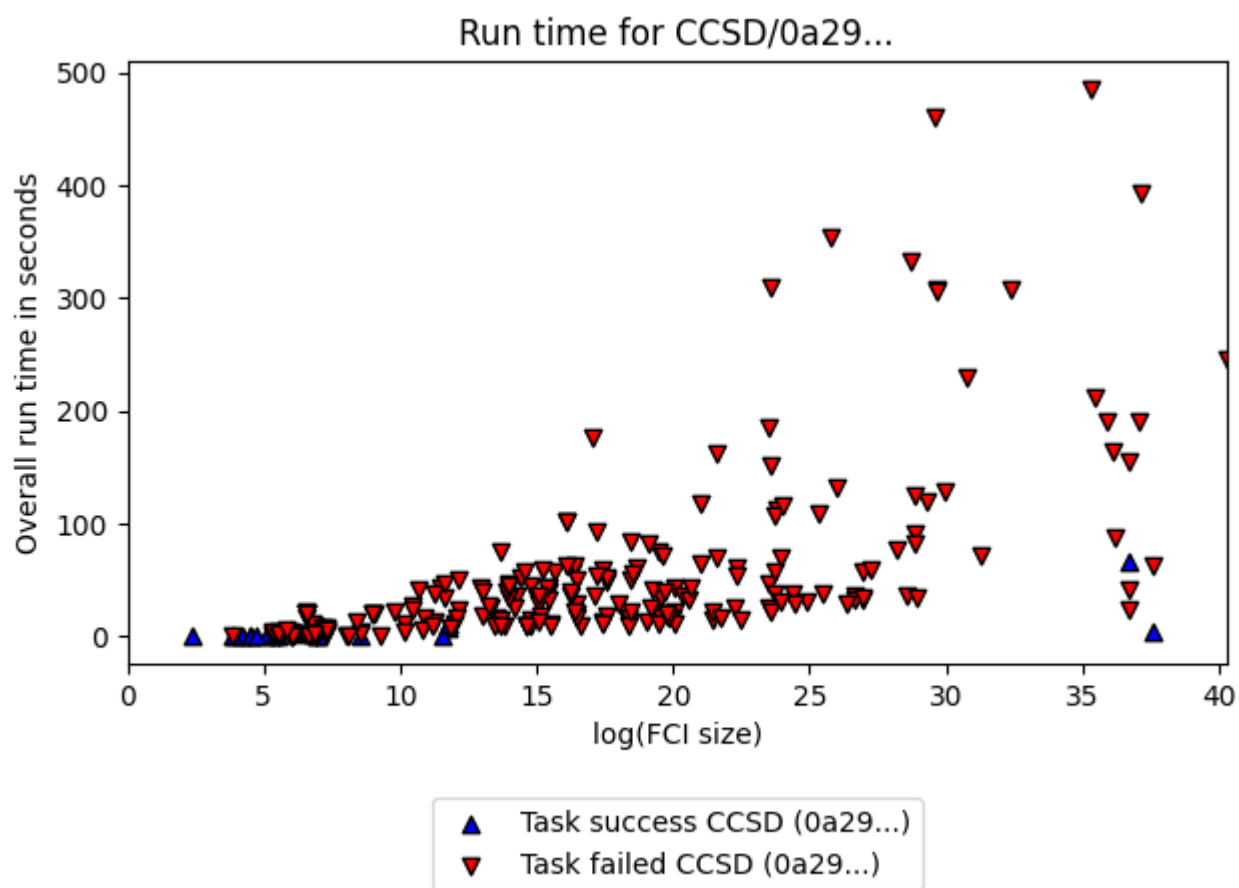
solvability\_ratio: 0.0197

f1\_score: [0.9886792452830189, 0.9411764705882353]

ml\_metrics\_calculator\_version: 1



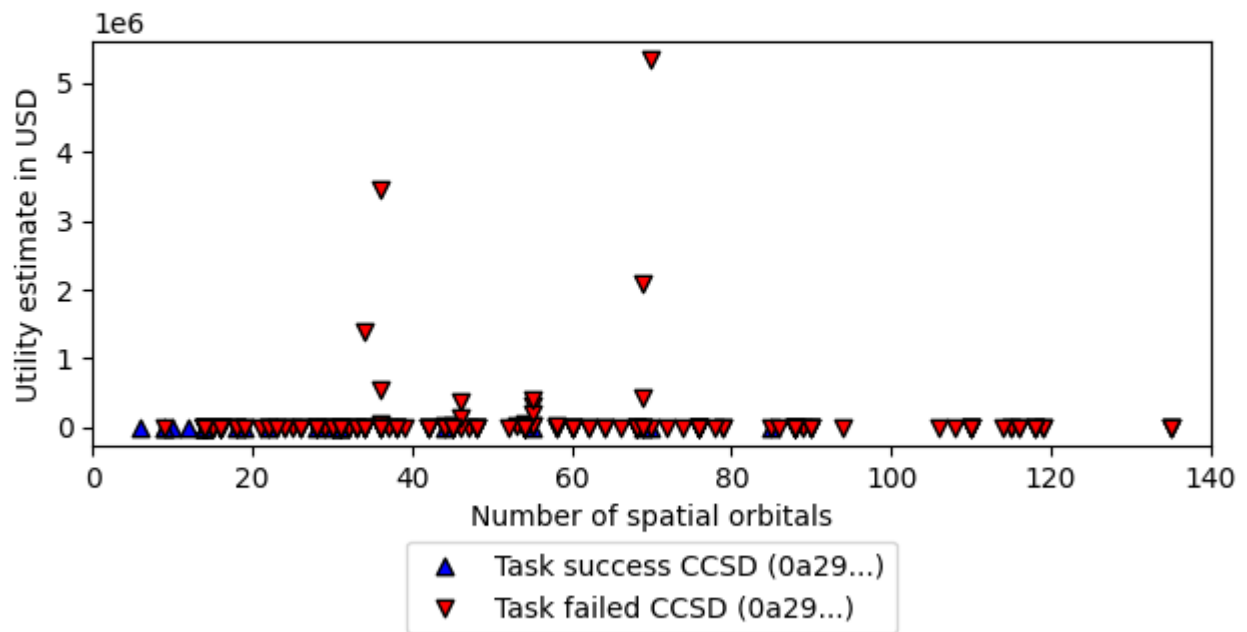
Note: plot only contains attempted tasks.

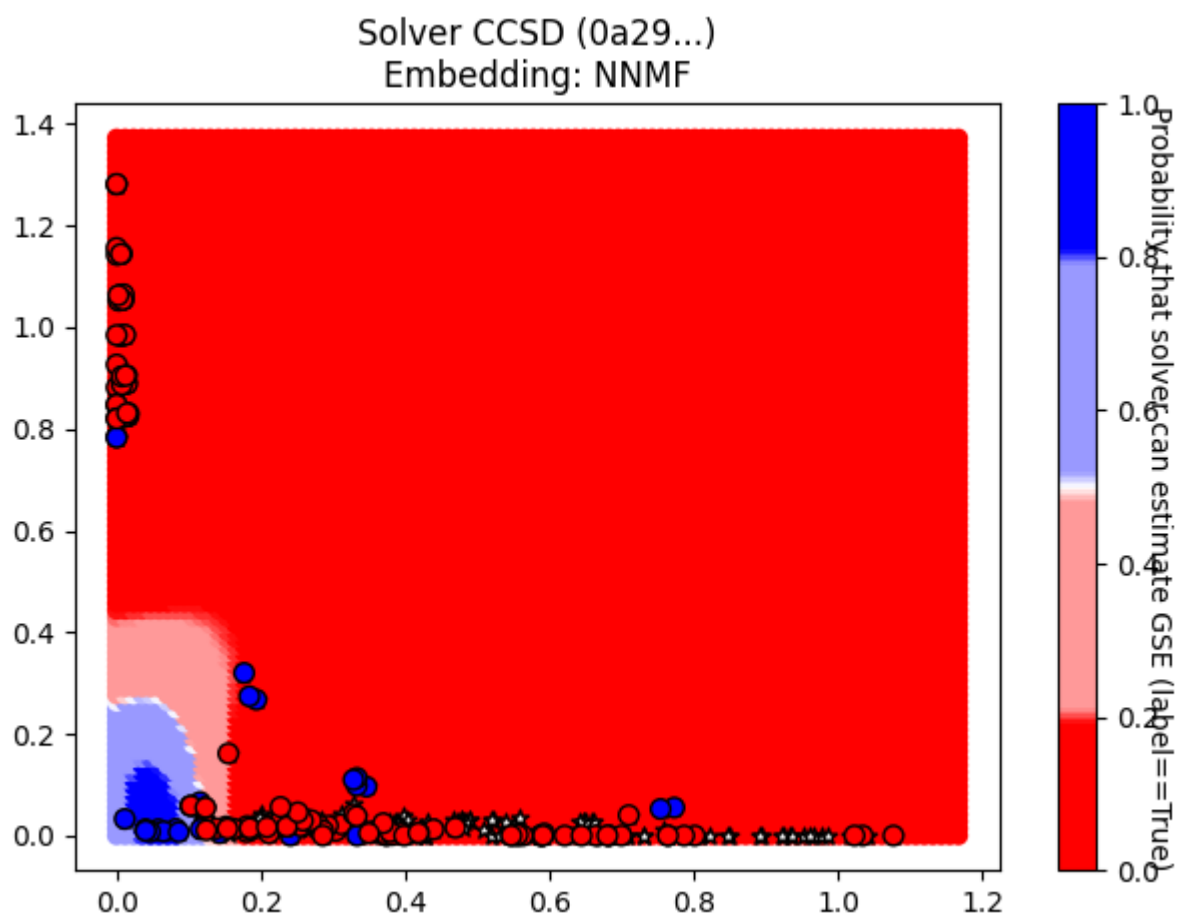


Note: plot only contains attempted tasks.

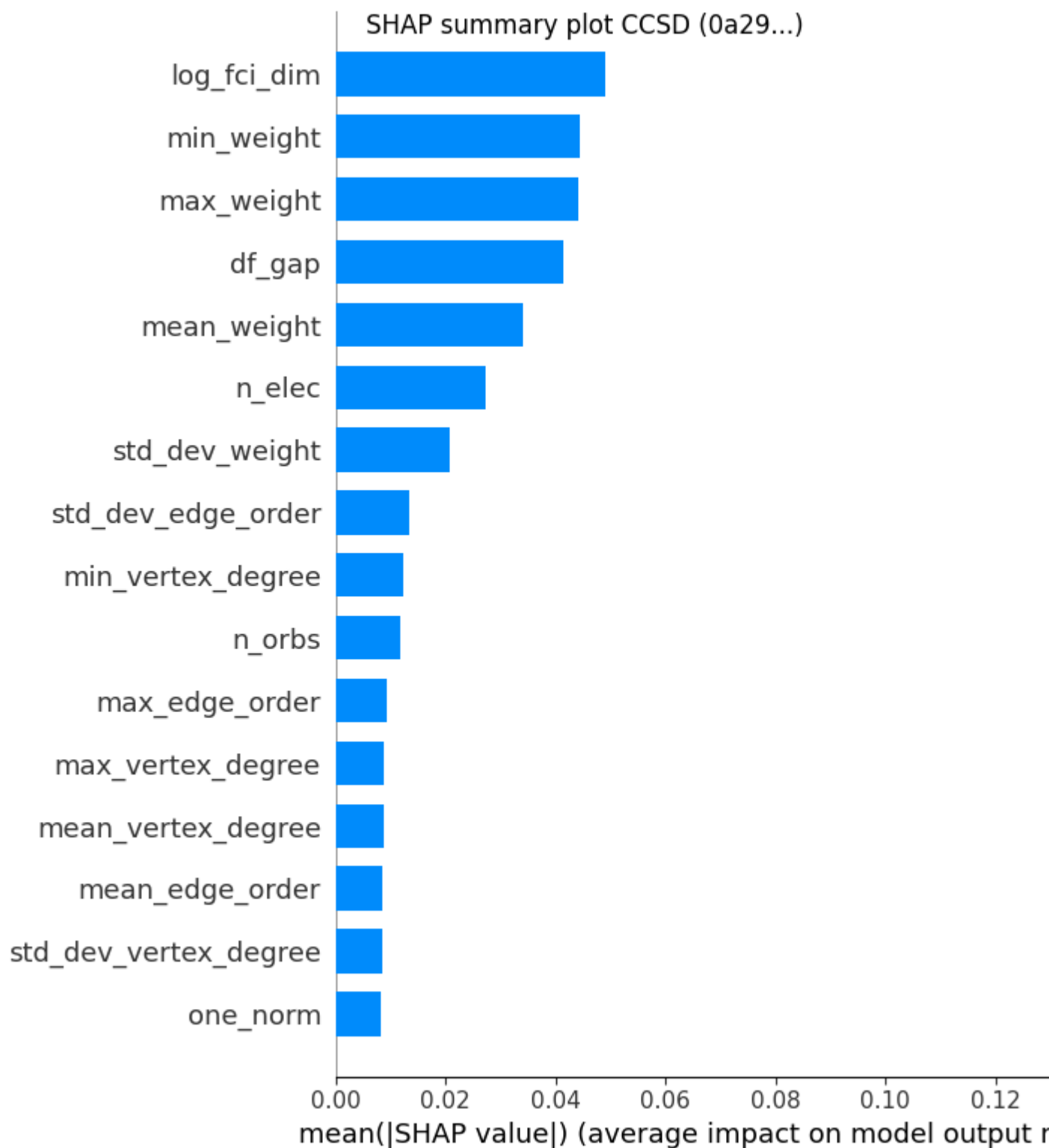
# Utility capture from CCSD/0a29...

(captured:  $\$2.1\text{e-}02/1.5\text{e+}07$ , approximately  $1.4\text{e-}07\%$ )





Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



**Solver DMRG\_Niagara\_cluster\_lowest\_energy,  
16537433-9f4c-4eae-a65d-787dc3b35b59**

solver\_uuid:16537433-9f4c-4eae-a65d-787dc3b35b59

solver\_short\_name:DMRG\_Niagara\_cluster\_lowest\_energy



compute\_hardware\_type:classical\_computer

classical\_hardware\_details: {'computing\_environment\_name': 'Niagara Cluster, Compute Canada', 'cpu\_description': '40 Intel "Skylake" cores at 2.4 GHz or 40 Intel "CascadeLake" cores at 2.5 GHz', 'ram\_available\_gb': '202 GB (188 GiB)', 'clock\_speed': '2.4 GHz or 2.5 GHz', 'total\_num\_cores': 40}

algorithm\_details:DMRG with the lowest variational energy obtained so far.

software\_details:Block2 v0.5.3rc16 with dmrghandler, commit version d603fdc6409fc194a416aa3a519362d5d91790d9 or later.

performance\_metrics\_uuid: 98ee23bd-16f7-402a-9818-f1ffc399ac74

creation\_timestamp: 2025-01-28T21:50:06.833854+00:00

number\_of\_problem\_instances: 84

number\_of\_problem\_instances\_attempted: 84

number\_of\_problem\_instances\_solved: 9

number\_of\_tasks: 276

number\_of\_tasks\_attempted: 276

number\_of\_tasks\_solved: 112

number\_of\_tasks\_solved\_within\_run\_time\_limit: 276

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 112

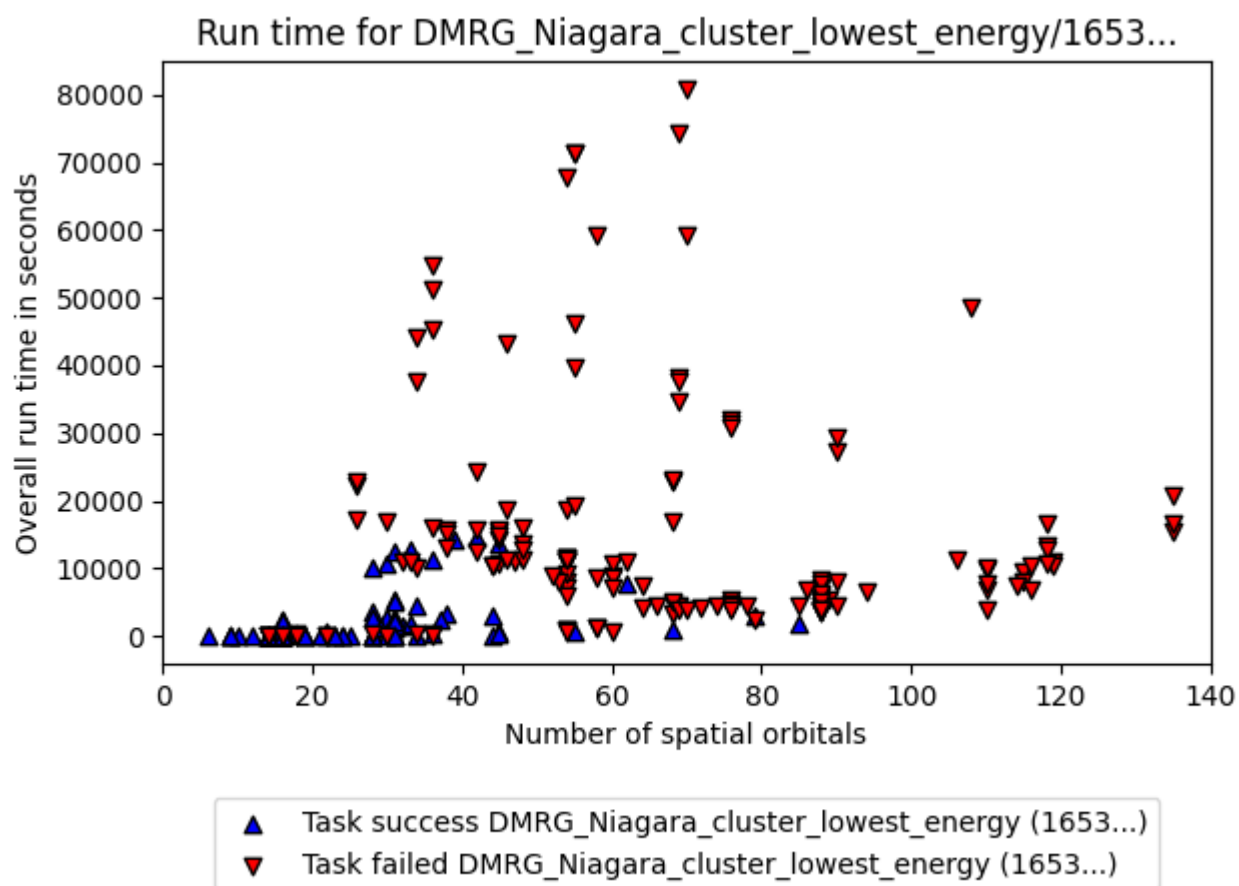
max\_run\_time\_of\_attempted\_tasks: 80820.729907066

sum\_of\_run\_time\_of\_attempted\_tasks: 2471726.9051446947

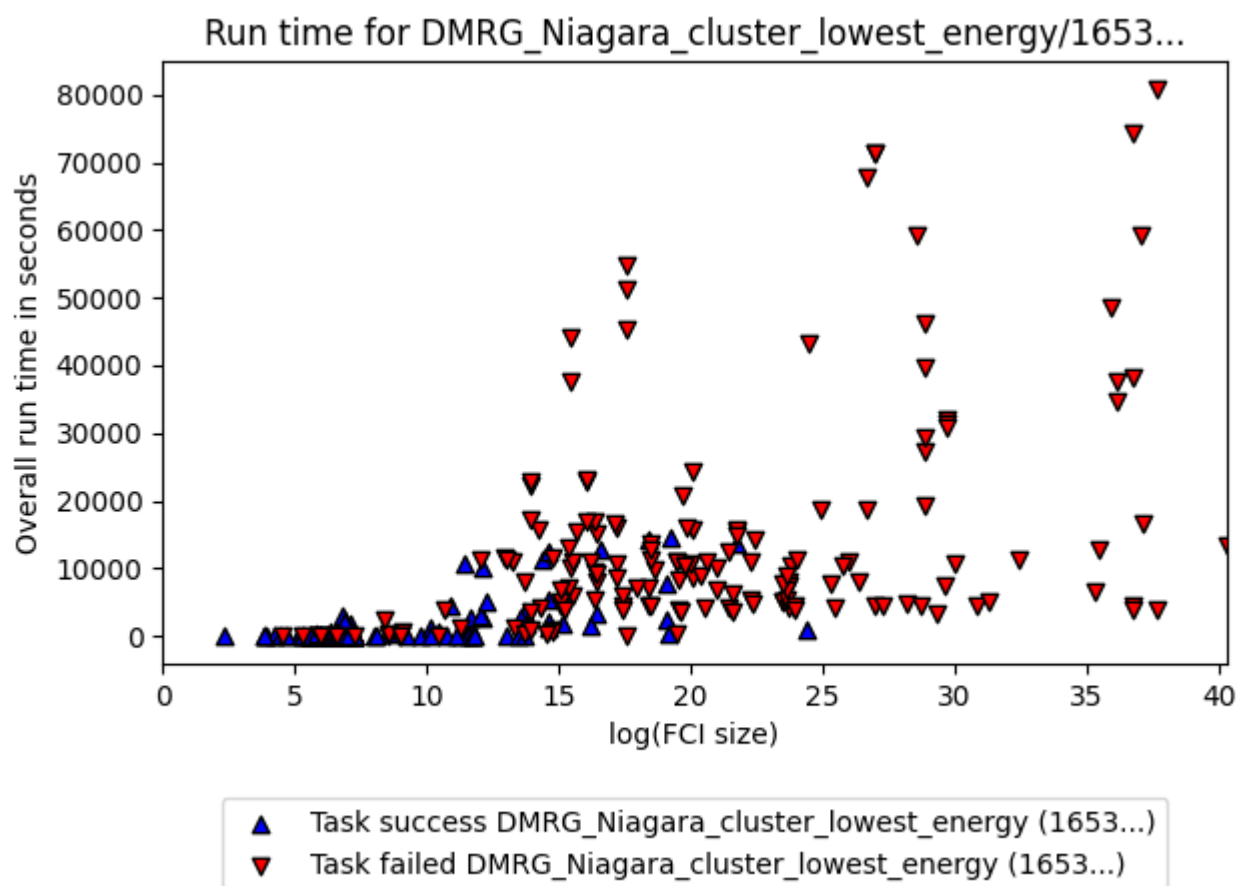
solvability\_ratio: 0.6106

f1\_score: [0.9662921348314607, 0.986784140969163]

ml\_metrics\_calculator\_version: 1



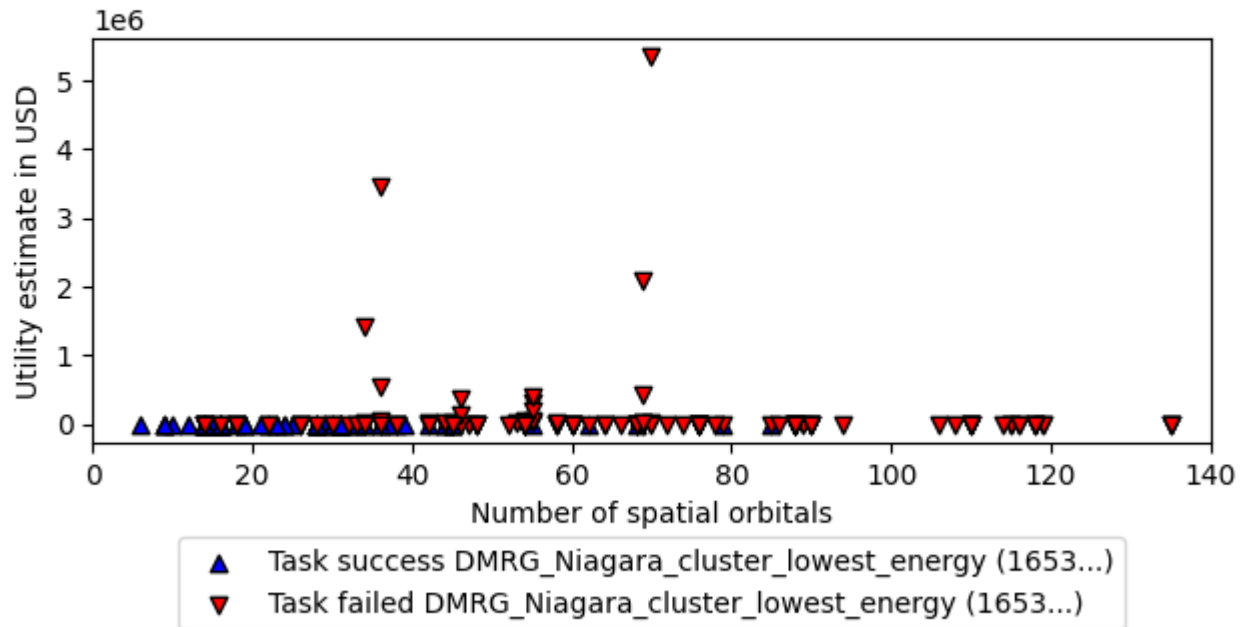
Note: plot only contains attempted tasks.

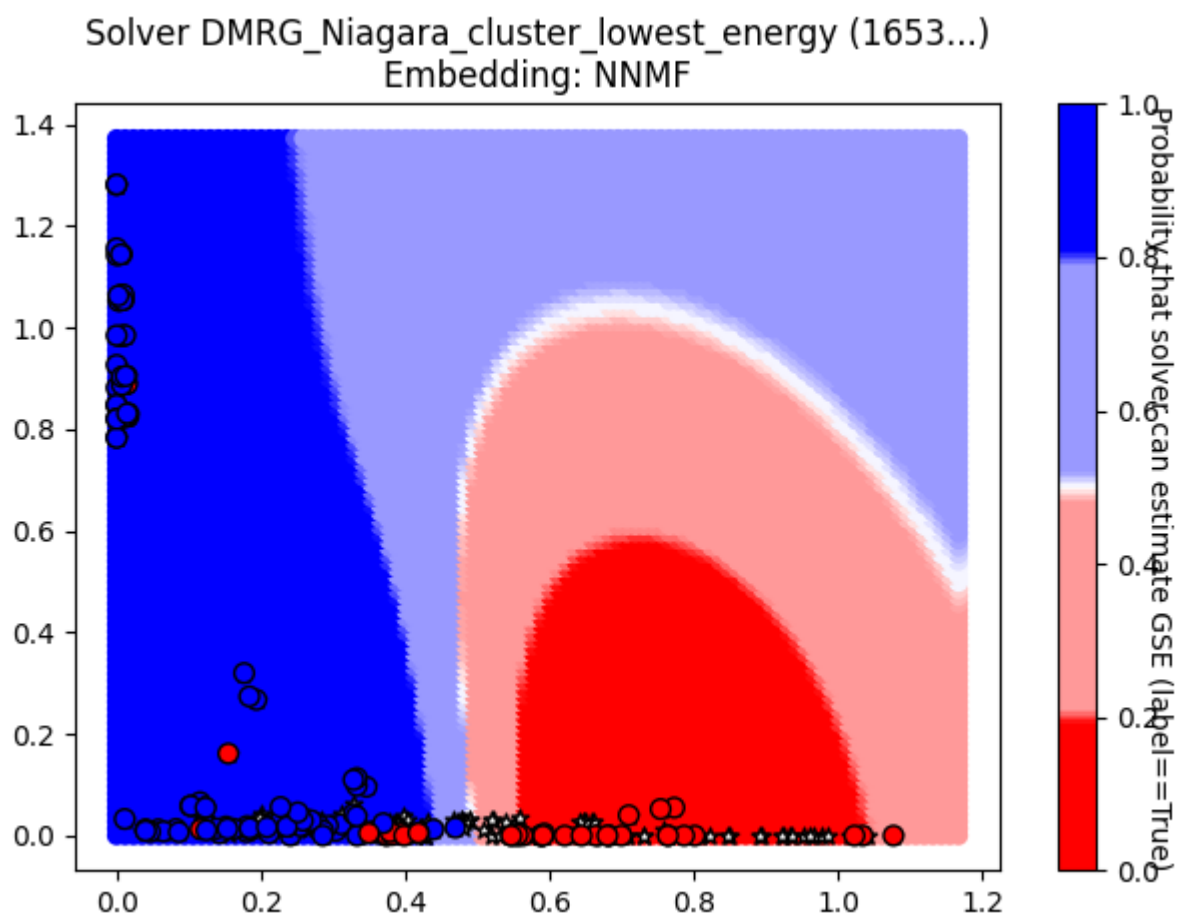


Note: plot only contains attempted tasks.

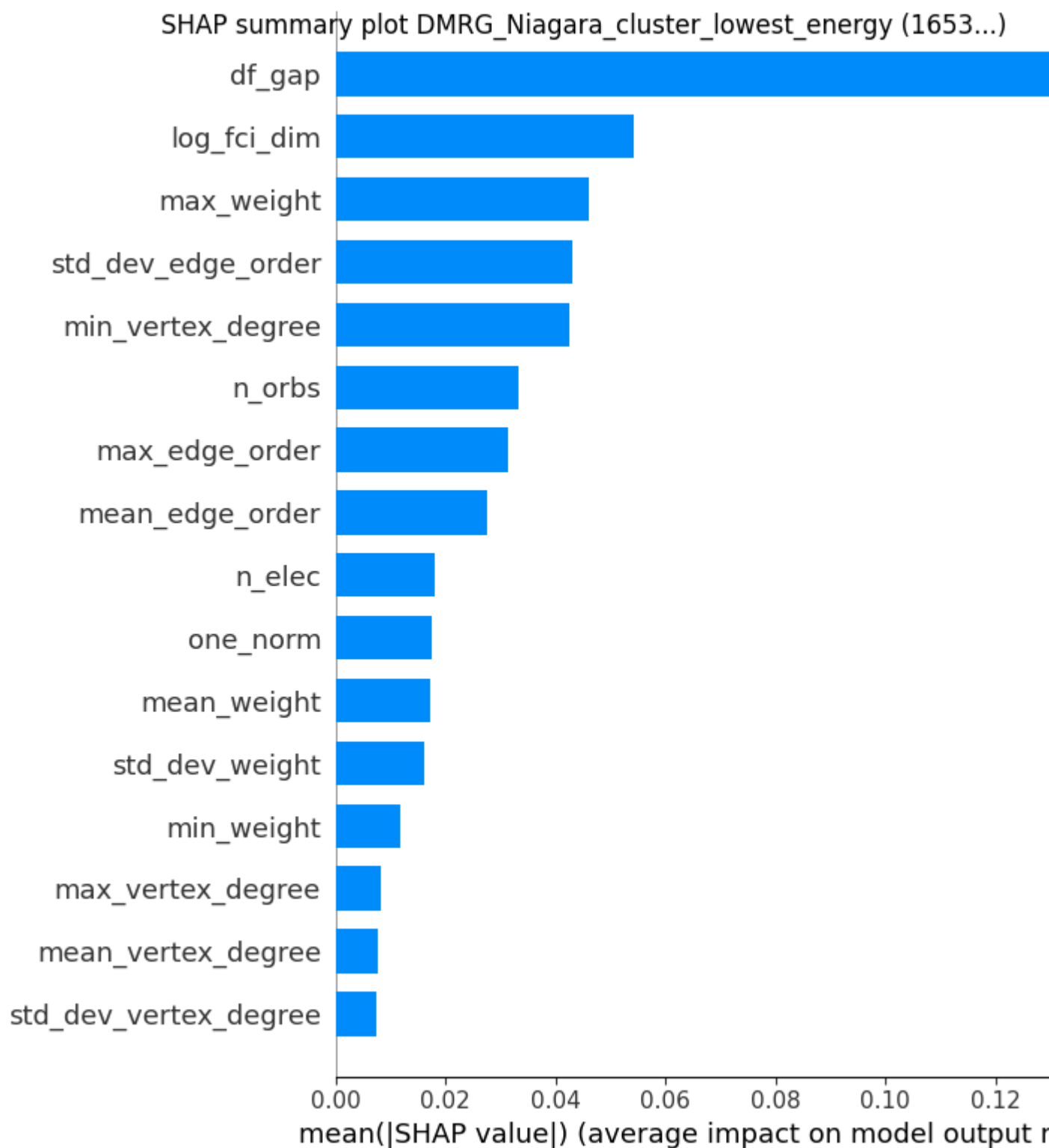
Utility capture from DMRG\_Niagara\_cluster\_lowest\_energy/1653..

(captured:  $\$8.0\text{e}+02/1.5\text{e}+07$ , approximately  $5.3\text{e}-03\%$ )

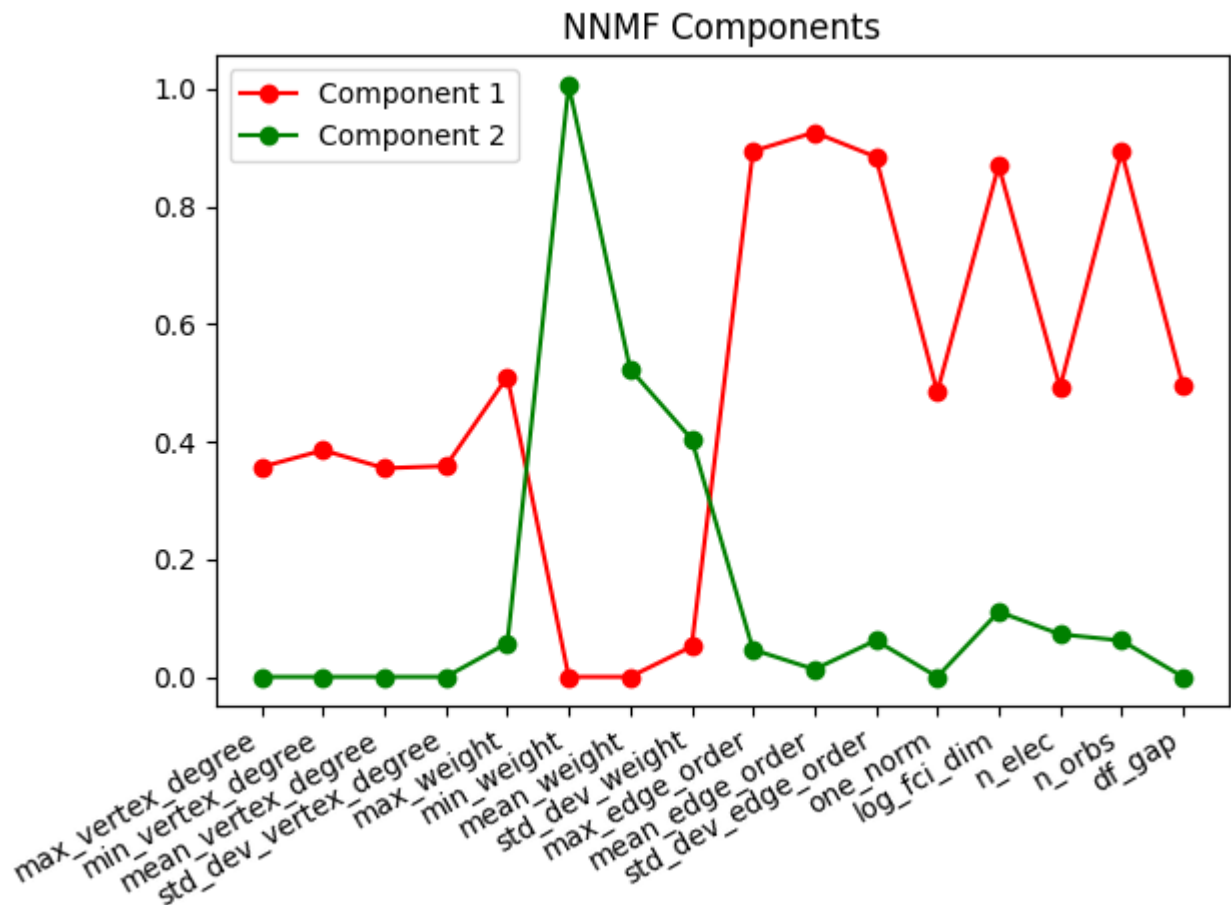




Note: attempted may be True or False. Tasks with a reference\_energy can be labeled as solved or failed-to-solve. A task with a reference\_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference\_energy.



# Non-negative matrix factorization (ML latent space)



Features: ['max\_vertex\_degree', 'min\_vertex\_degree', 'mean\_vertex\_degree', 'std\_dev\_vertex\_degree', 'max\_weight', 'min\_weight', 'mean\_weight', 'std\_dev\_weight', 'max\_edge\_order', 'mean\_edge\_order', 'std\_dev\_edge\_order', 'one\_norm', 'log\_fci\_dim', 'n\_elec', 'n\_orbs', 'df\_gap']

Component 1: [0.35690922 0.38545468 0.35487749 0.35852601  
0.51063391 0.0 0.0515893 0.89395573 0.92611292 0.88423213  
0.48450204 0.86941452 0.49234596 0.89376327 0.49515561]

Component 2: [0.0 0.0 0.0 0.0 0.05747991 1.00601694 0.52355998 0.4045106  
0.04642006 0.0127596 0.06203818 0.0 0.11068966 0.07250786 0.06174321  
0.]