

# GSEE Benchmark Standard Report

Report based on data from 2025-01-27T16:43:41.107794+00:00

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

Input data: Hamiltonian\_features.csv, last modified Mon Jan 27 11:42:37 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: Mon Jan 27 11:42:54 2025

## Problem Instance Summary Statistics

number of problem\_instances: 84.

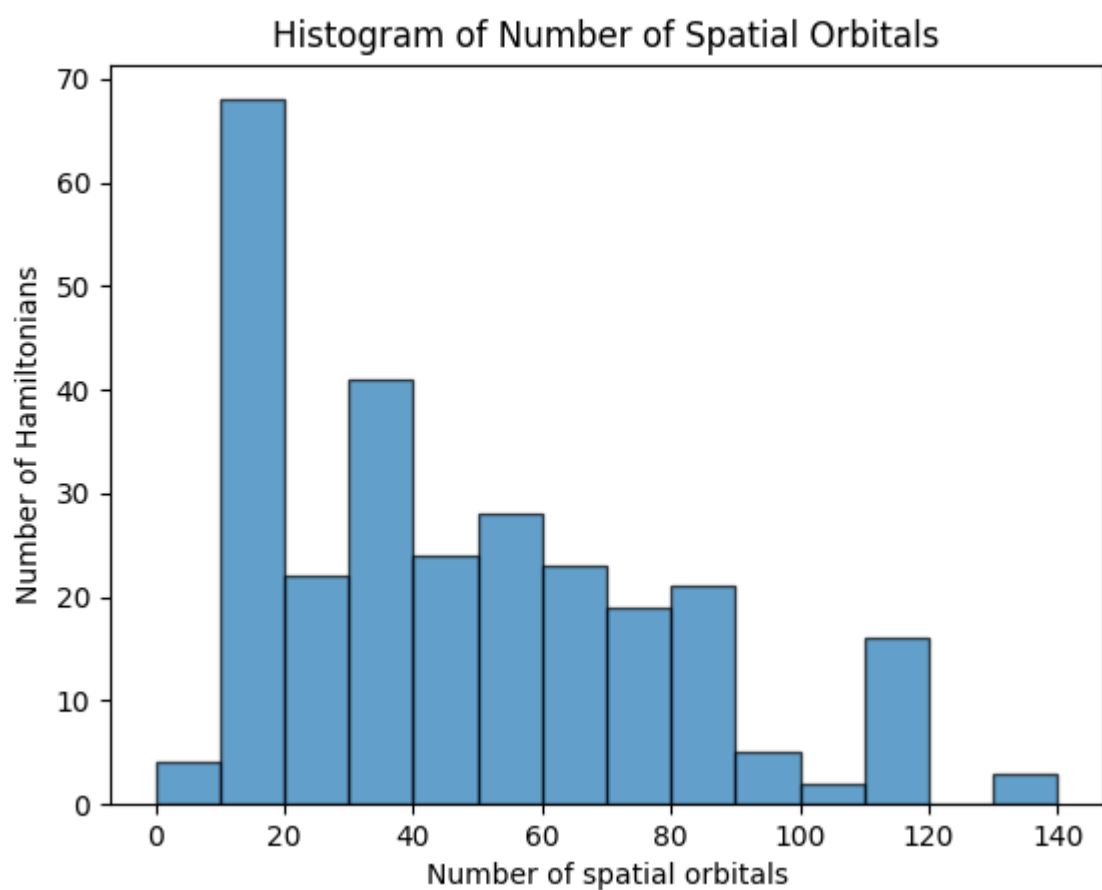
problem\_instance.json with the most tasks: 30 (hubbard\_square/614c4444-a31a-4348-b24d-01040208651c)

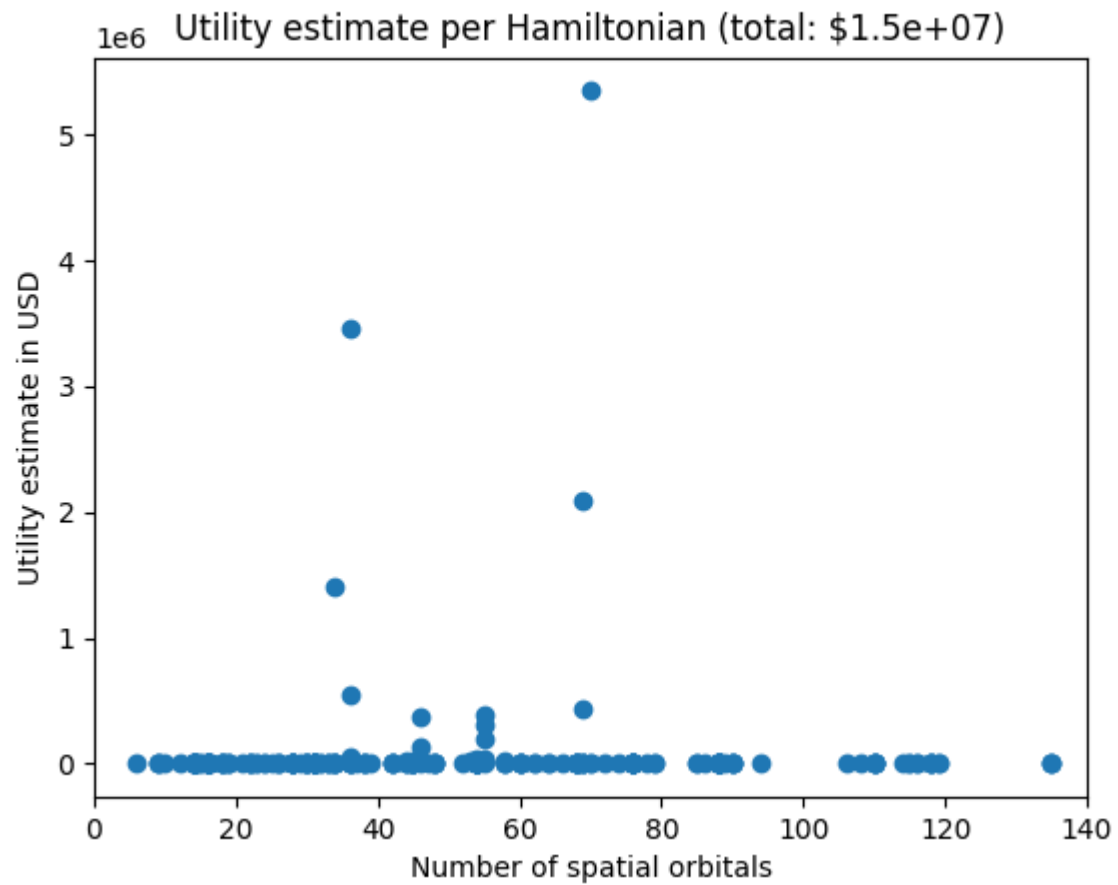
number of Hamiltonians (i.e., tasks) we have features calculated for: 276

minimum number of orbitals: 6

median number of orbitals: 42.0

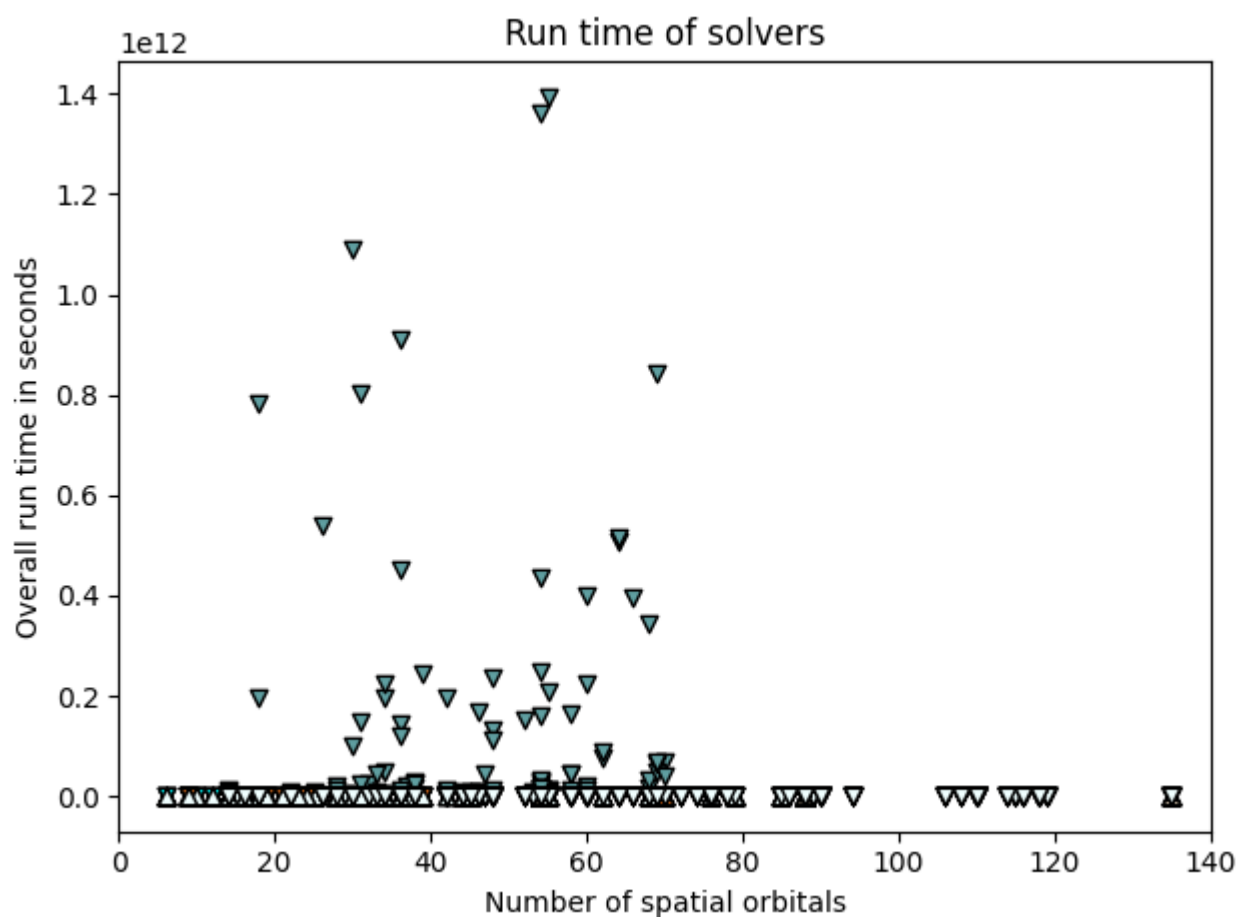
maximum number of orbitals: 135



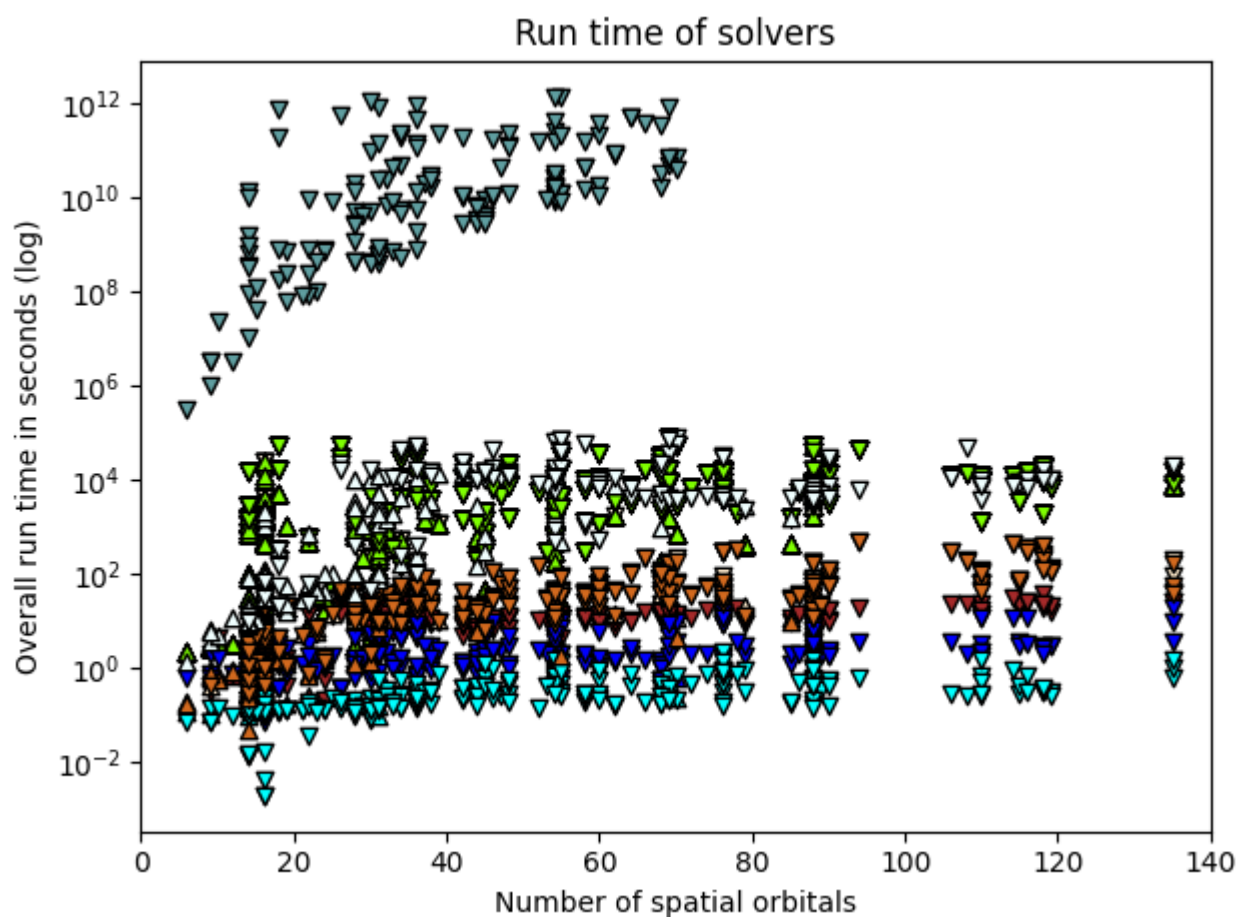


## Solver Summary Statistics

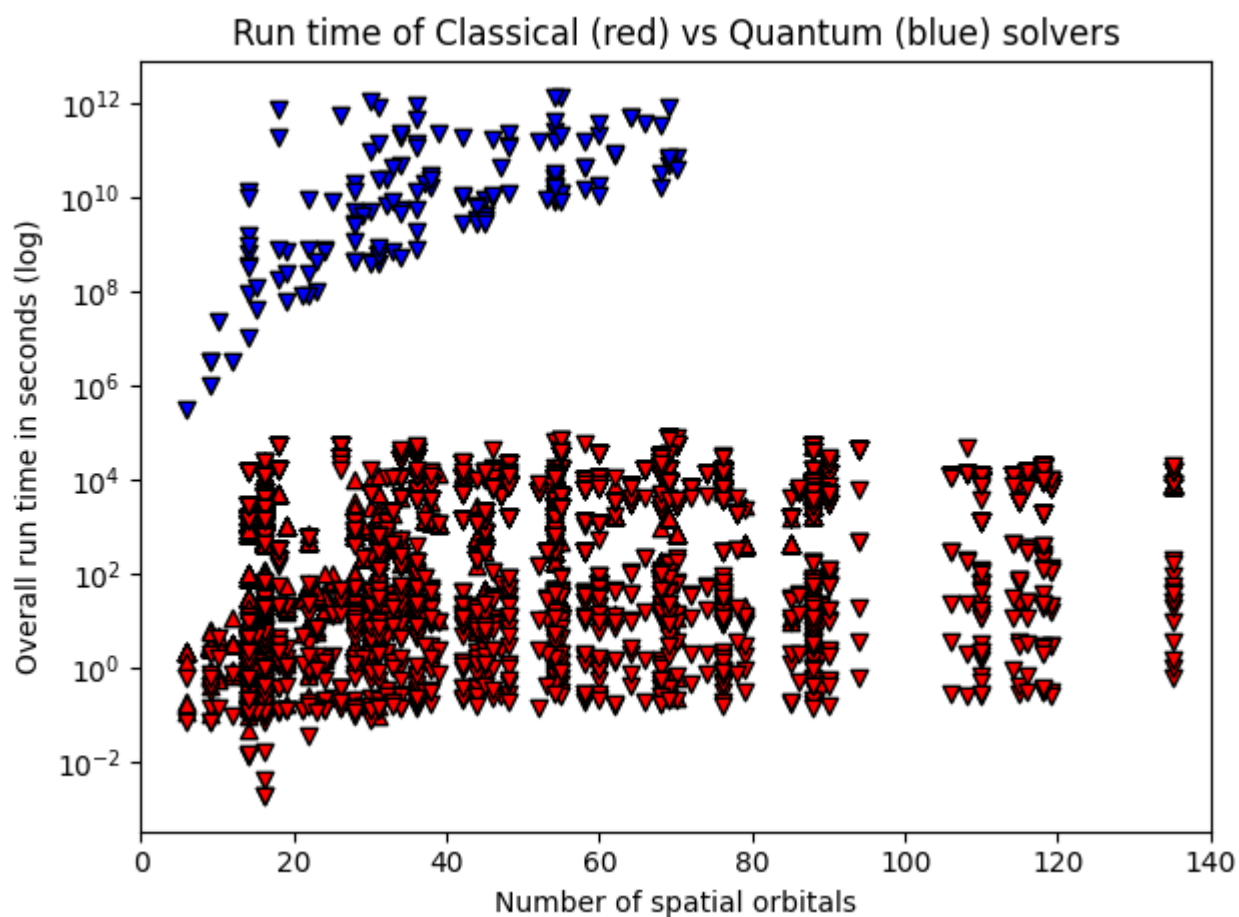
number of unique participating solvers: 16



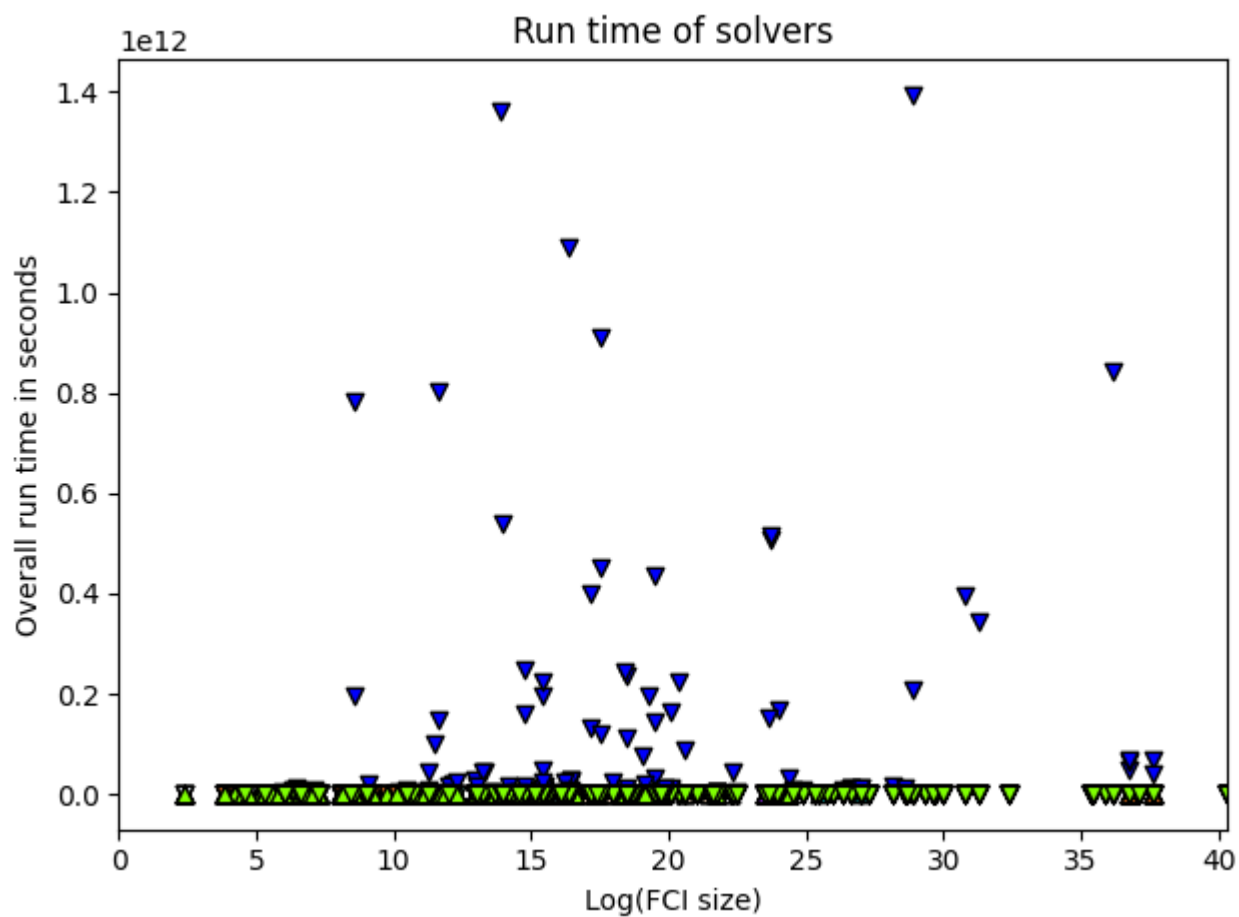
NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.



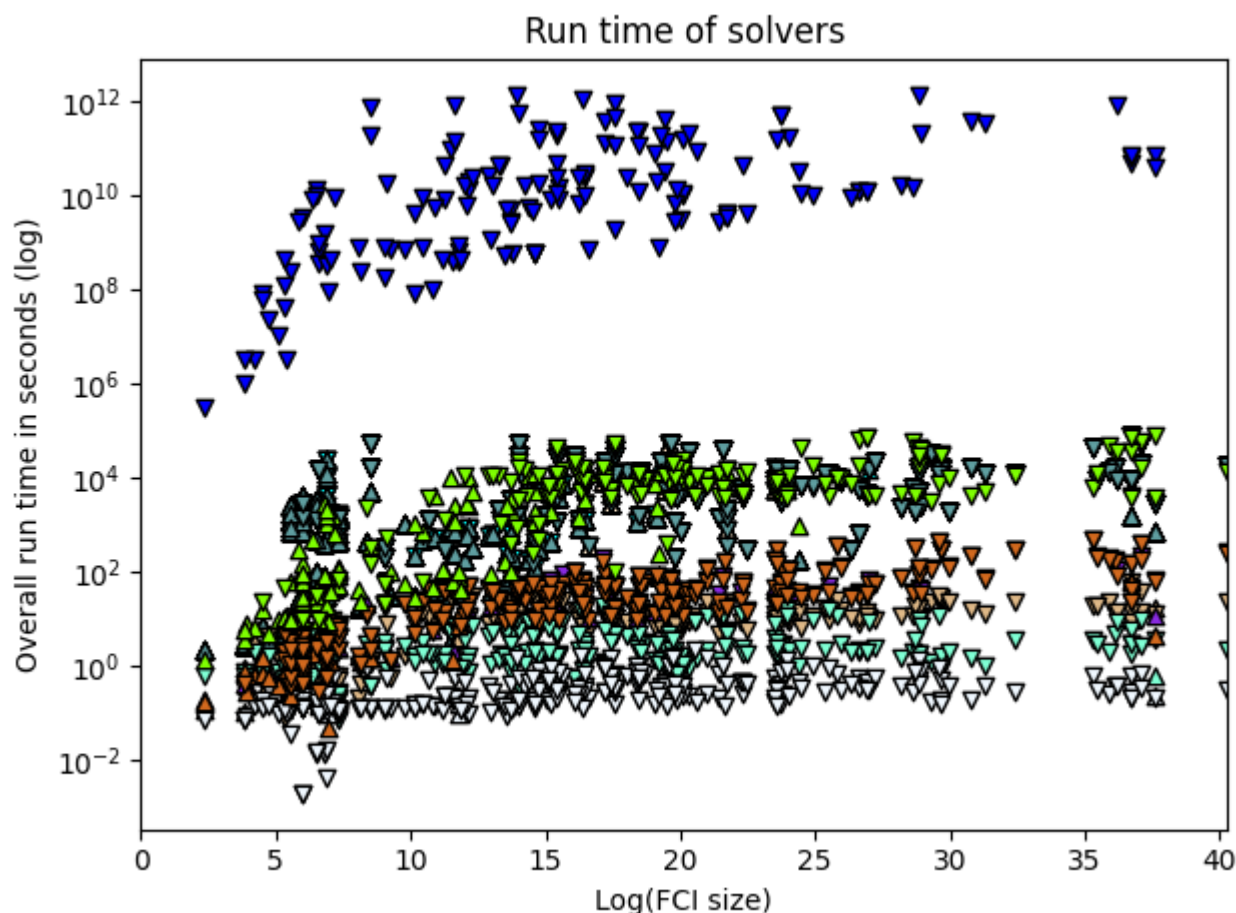
NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.



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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>).

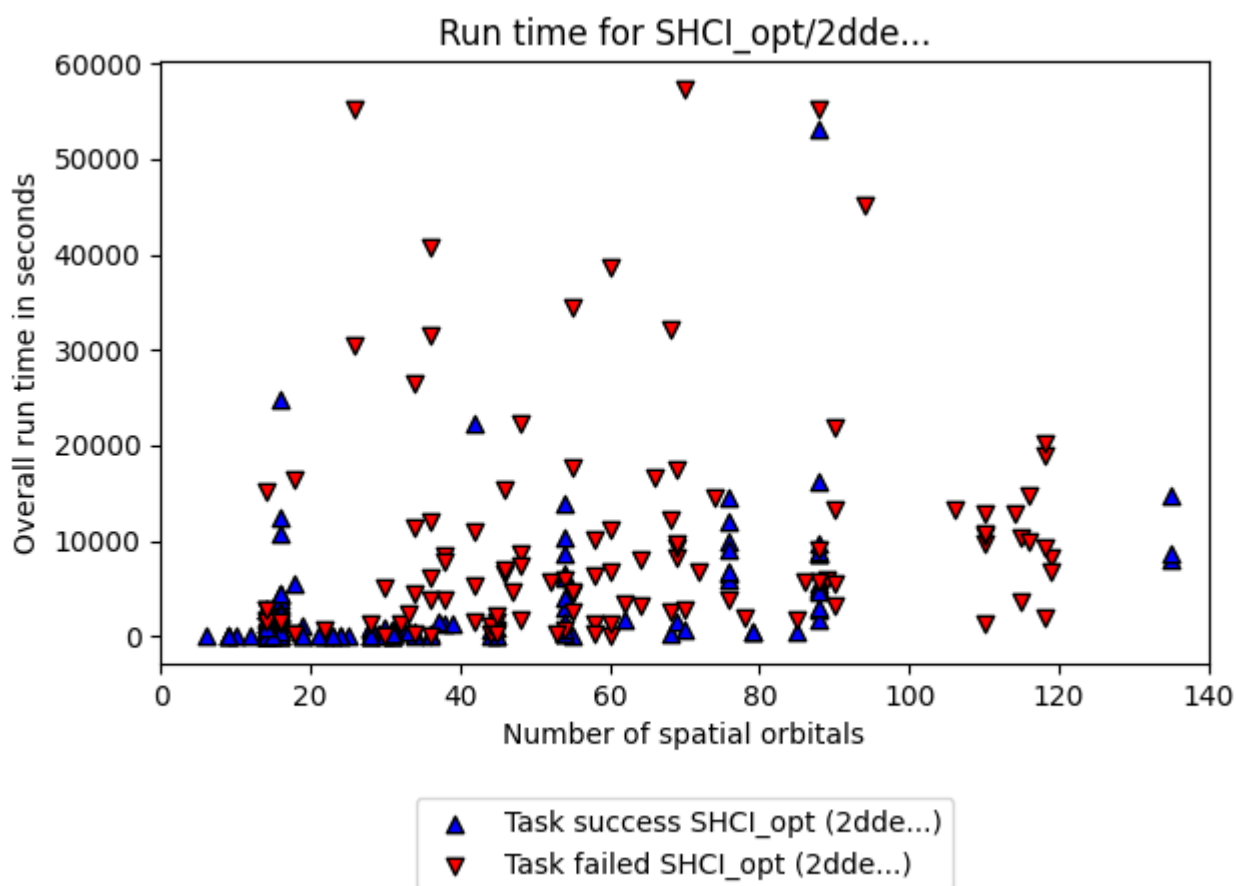
performance\_metrics\_uuid: 431232fa-2c17-4c53-bc08-c53ad727f2d6

creation\_timestamp: 2025-01-27T16:43:41.107794+00:00

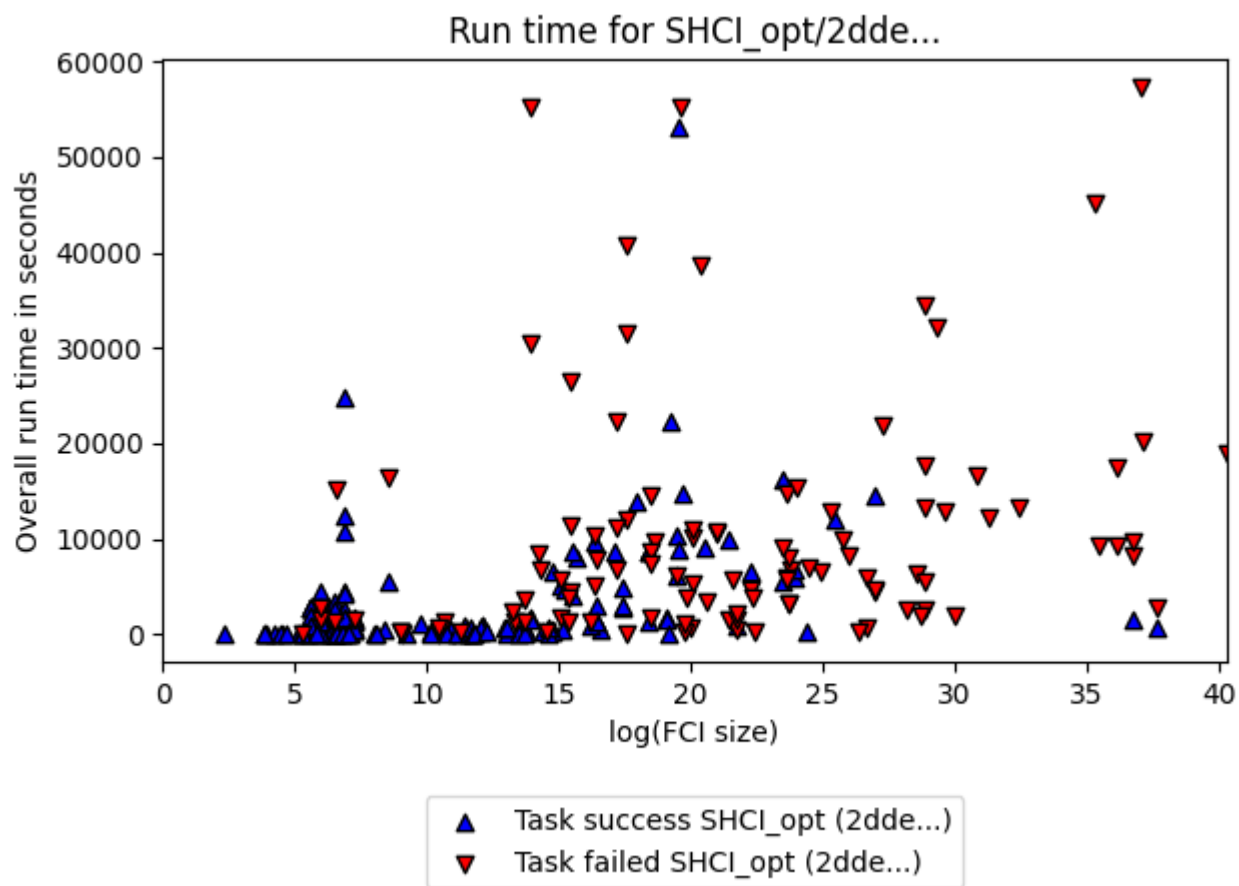
number\_of\_problem\_instances: 84



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



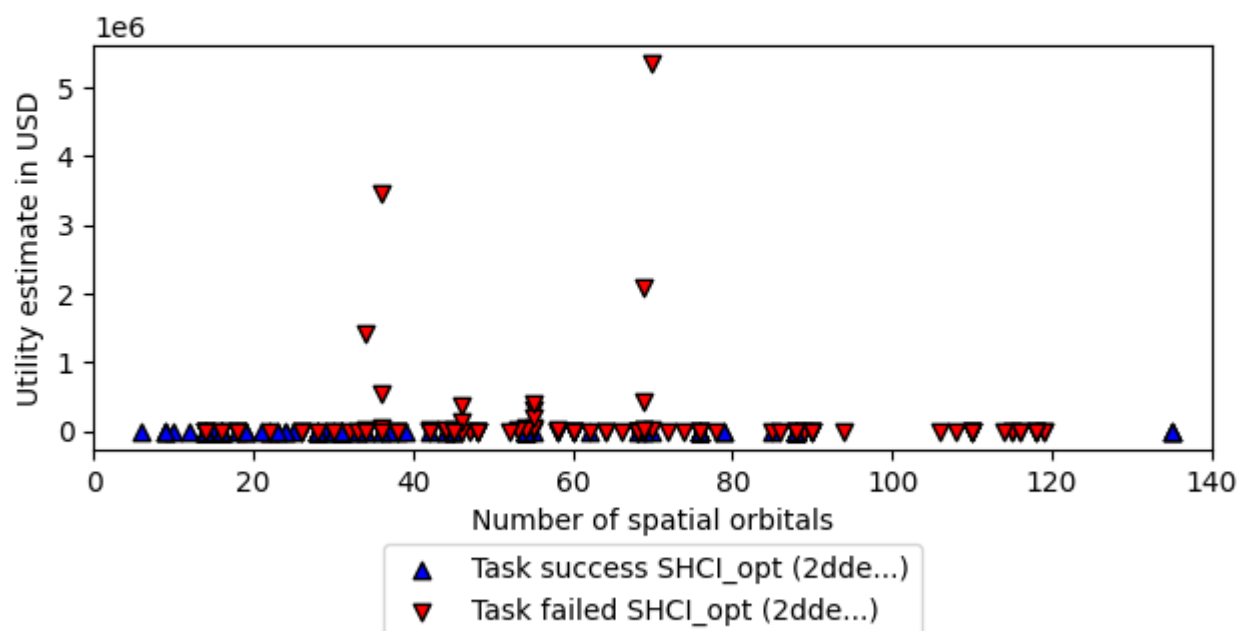
Note: plot only contains attempted tasks.

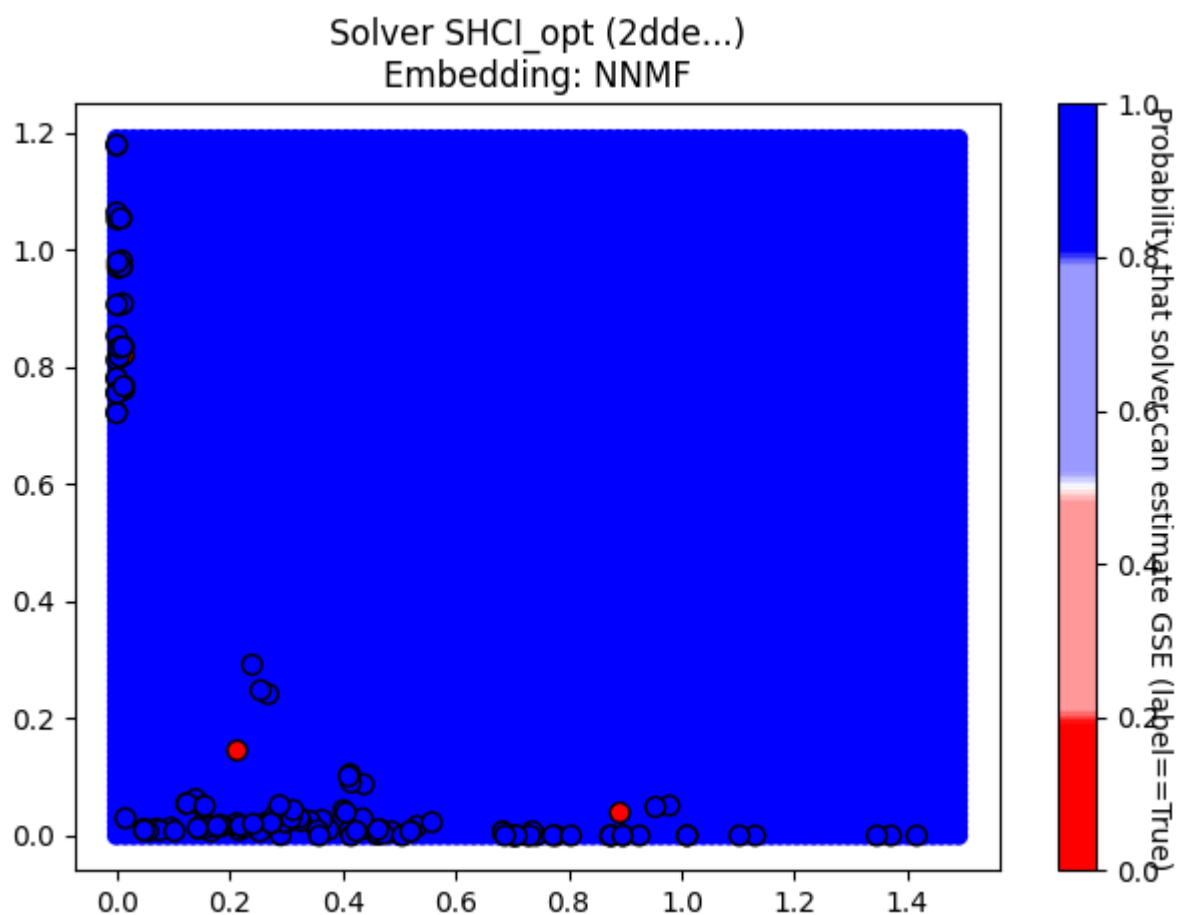


Note: plot only contains attempted tasks.

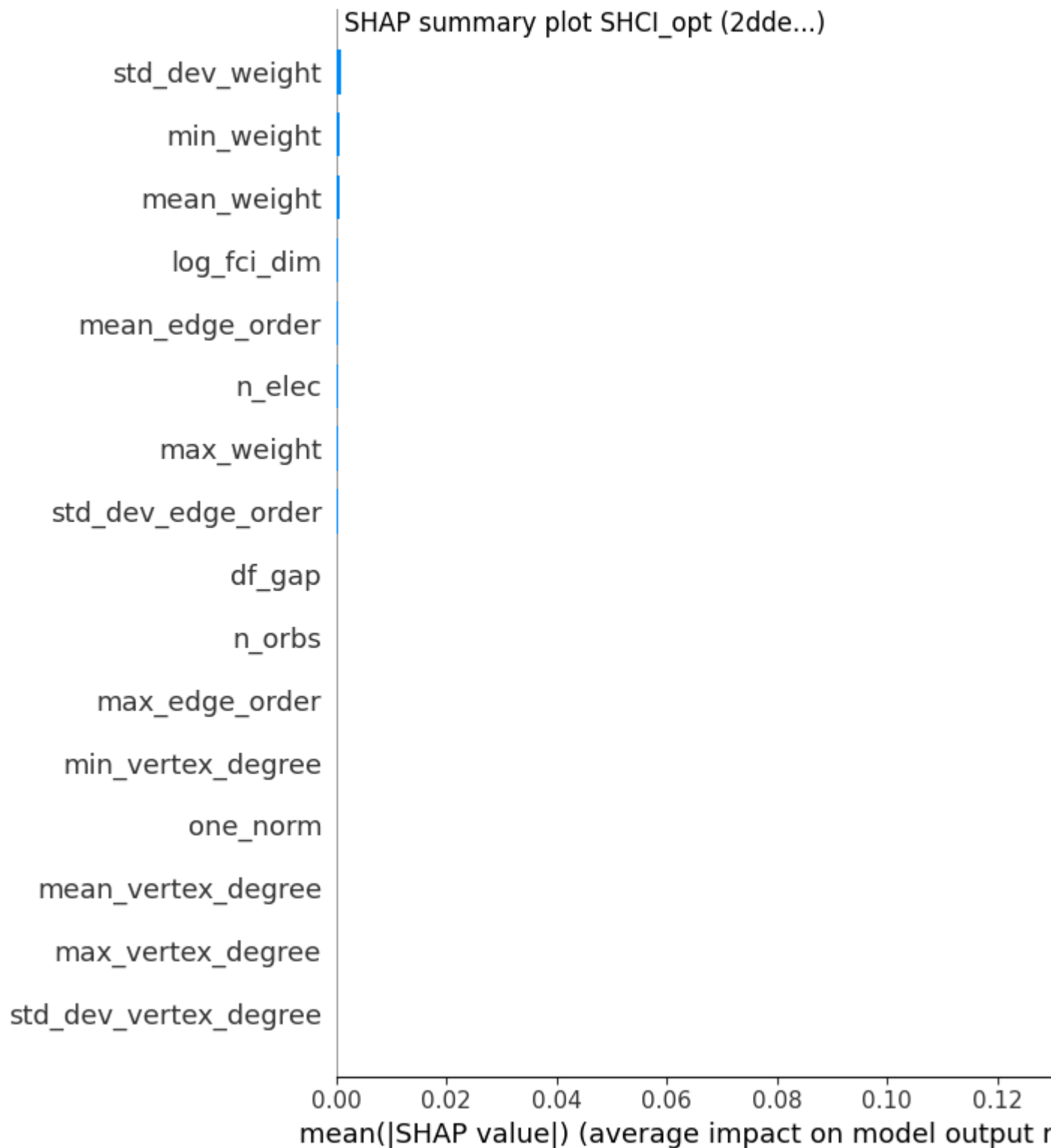
# Utility capture from SHCI\_opt/2dde...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: 137e4b1e-0d98-490e-9b76-7a5025f14ee3

creation\_timestamp: 2025-01-27T16:43:41.107794+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

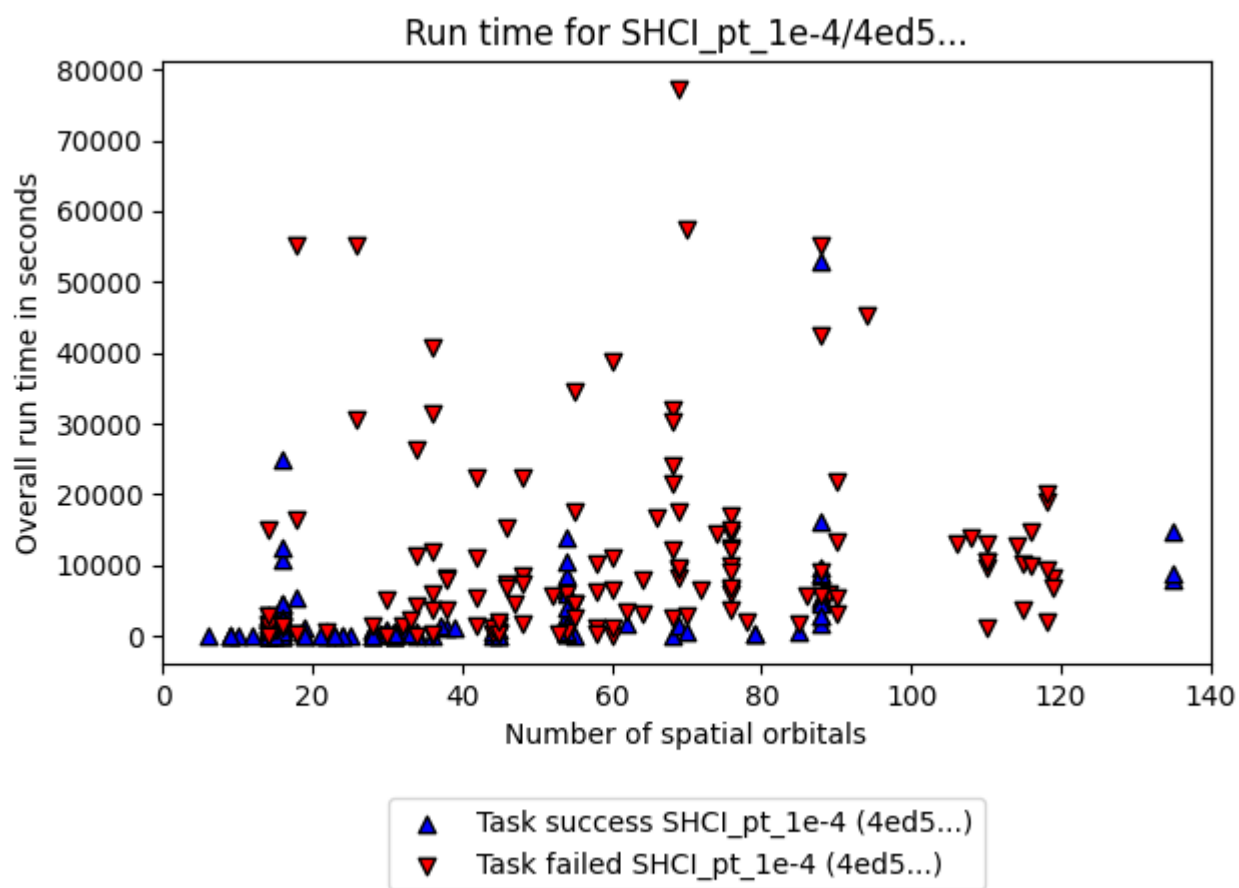
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

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

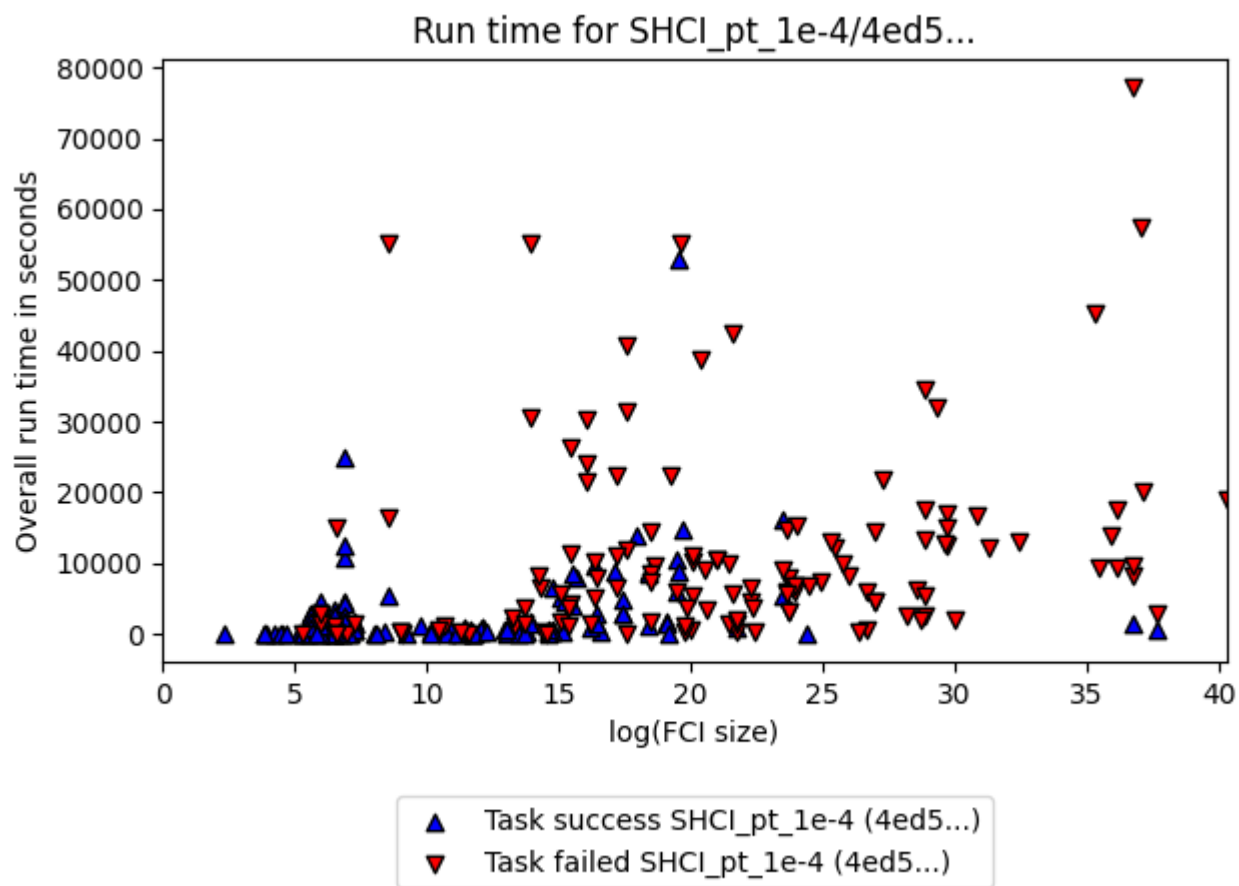
solvability\_ratio: 0.547

f1\_score: [0.8, 0.9750889679715302]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

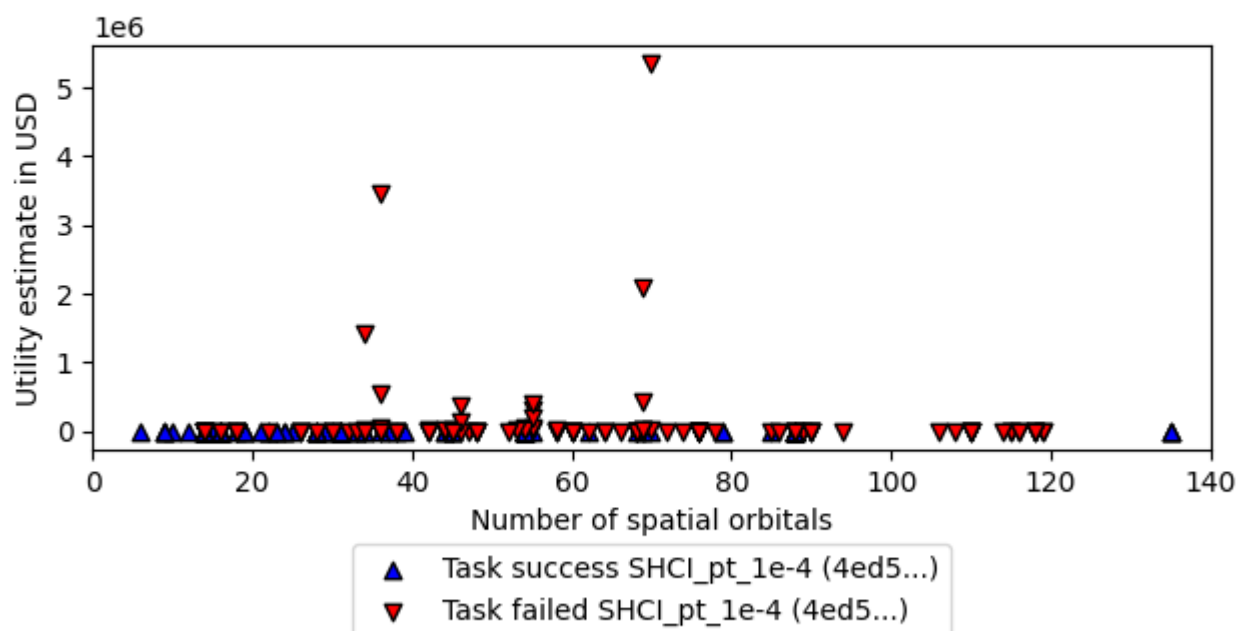


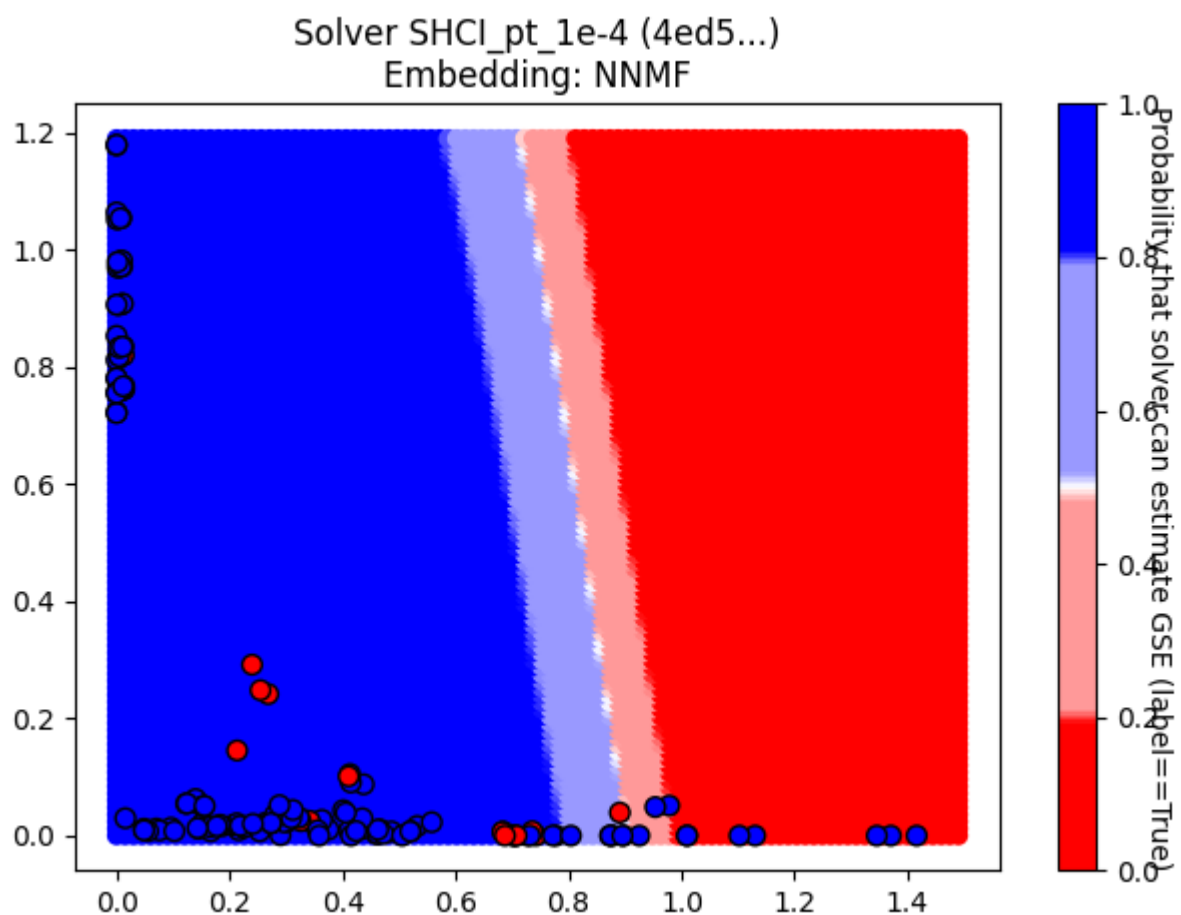
Note: plot only contains attempted tasks.



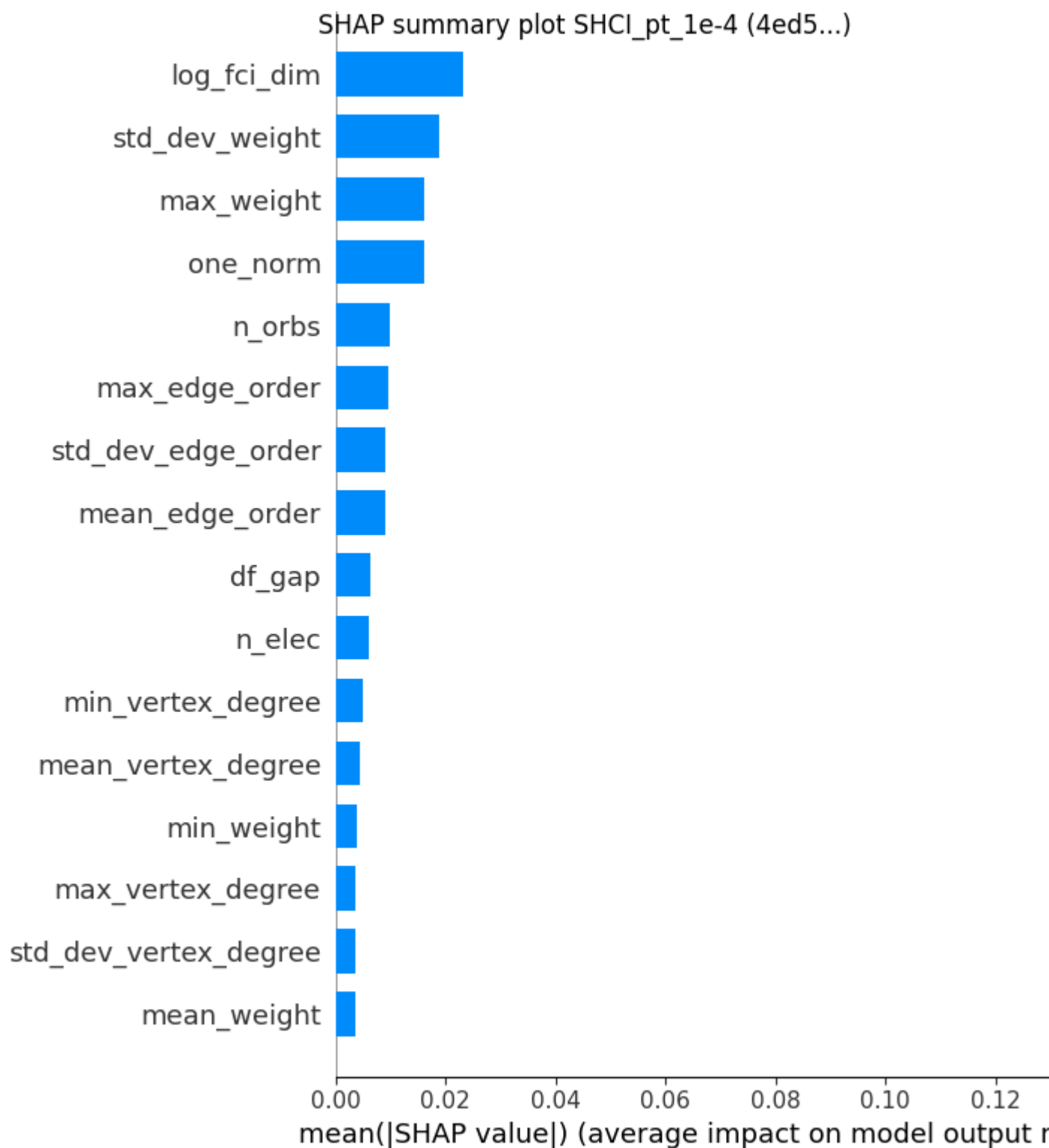
### Utility capture from SHCI\_pt\_1e-4/4ed5...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: e62321ab-6054-4124-b1dc-0abac2ffd112

creation\_timestamp: 2025-01-27T16:43:41.107794+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

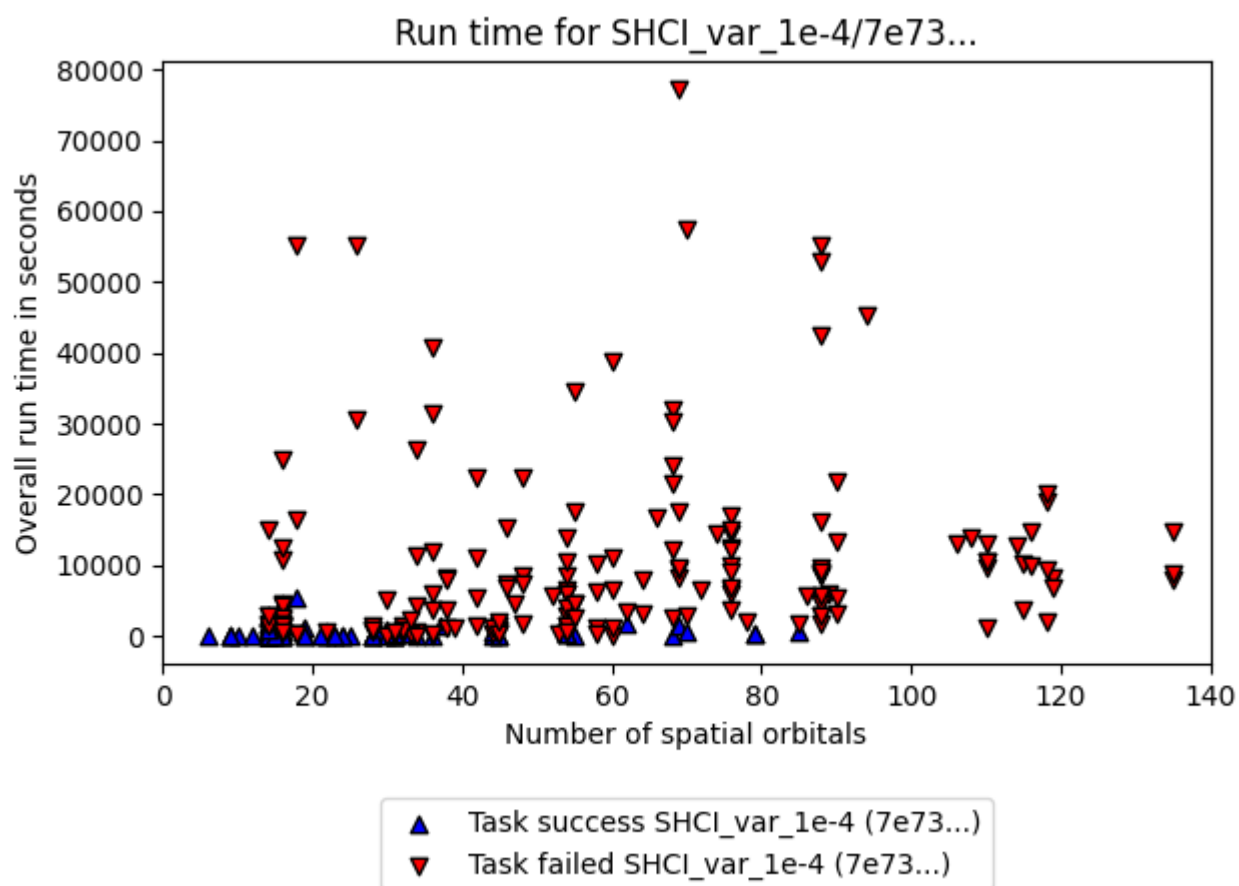
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

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

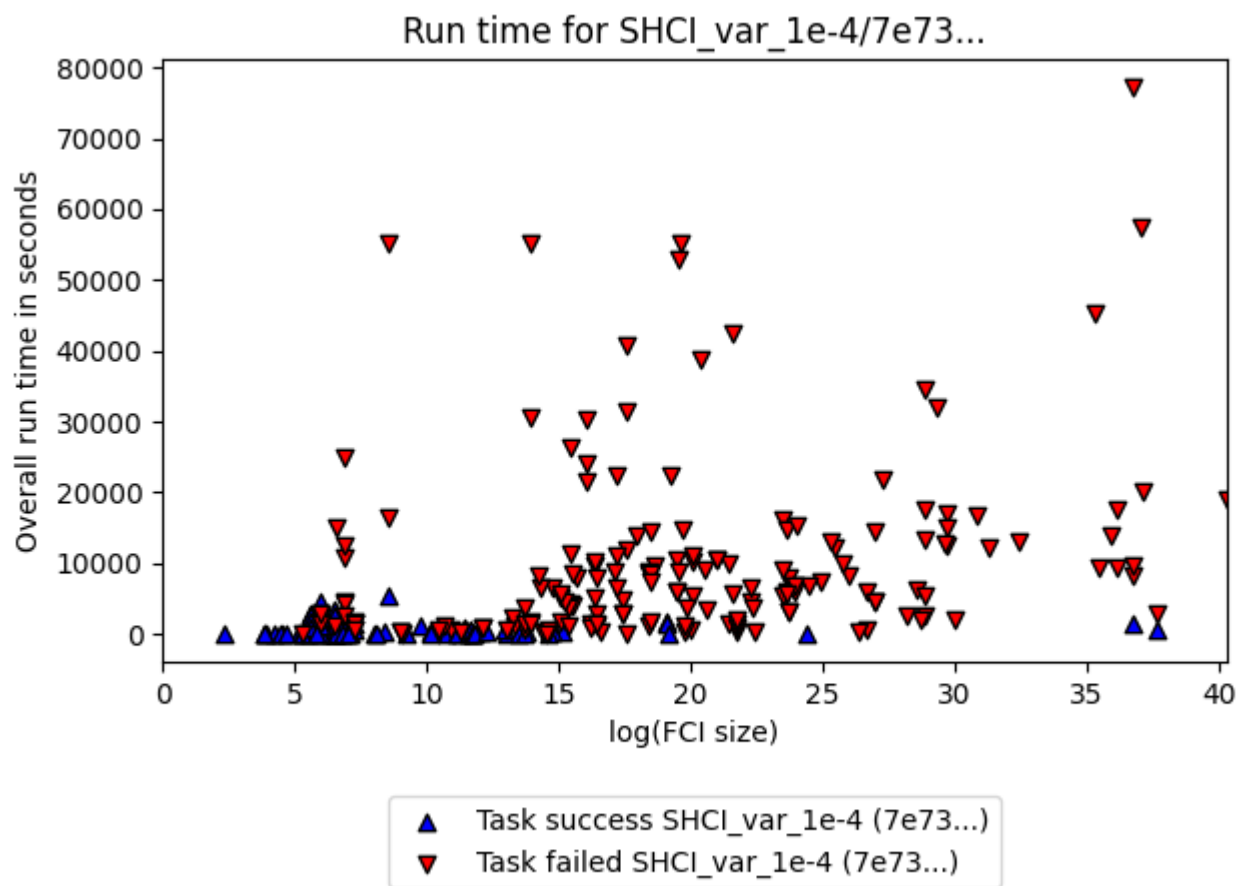
solvability\_ratio: 0.9262

f1\_score: [0.9841269841269841, 0.9894736842105263]

ml\_metrics\_calculator\_version: 1



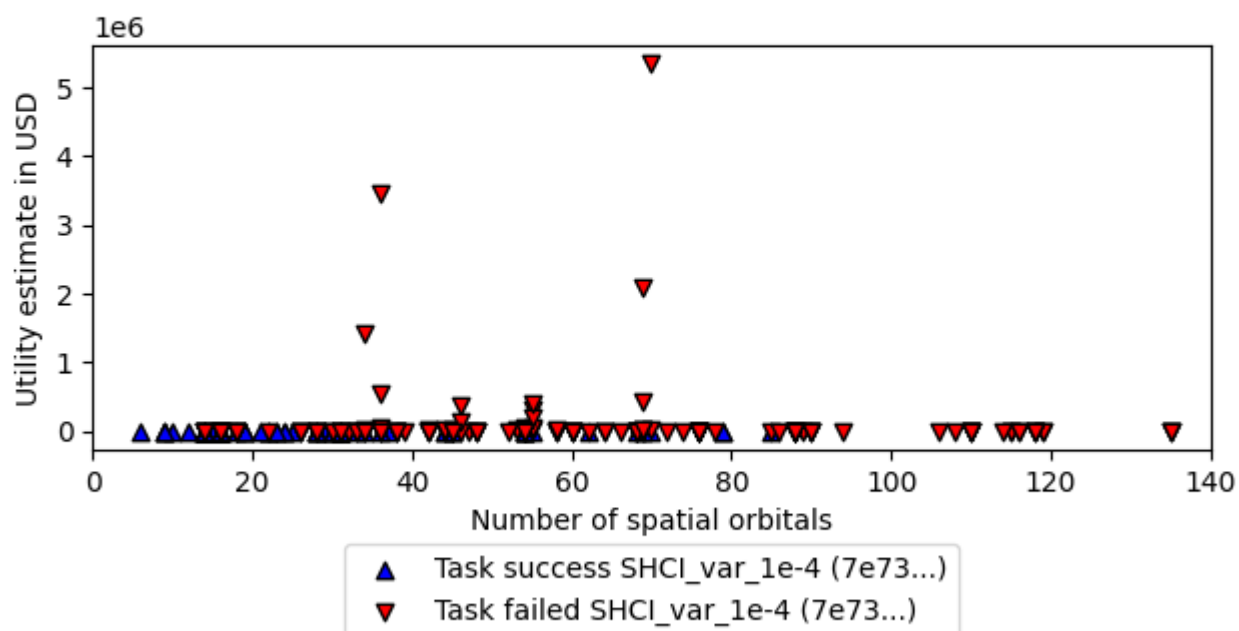
Note: plot only contains attempted tasks.

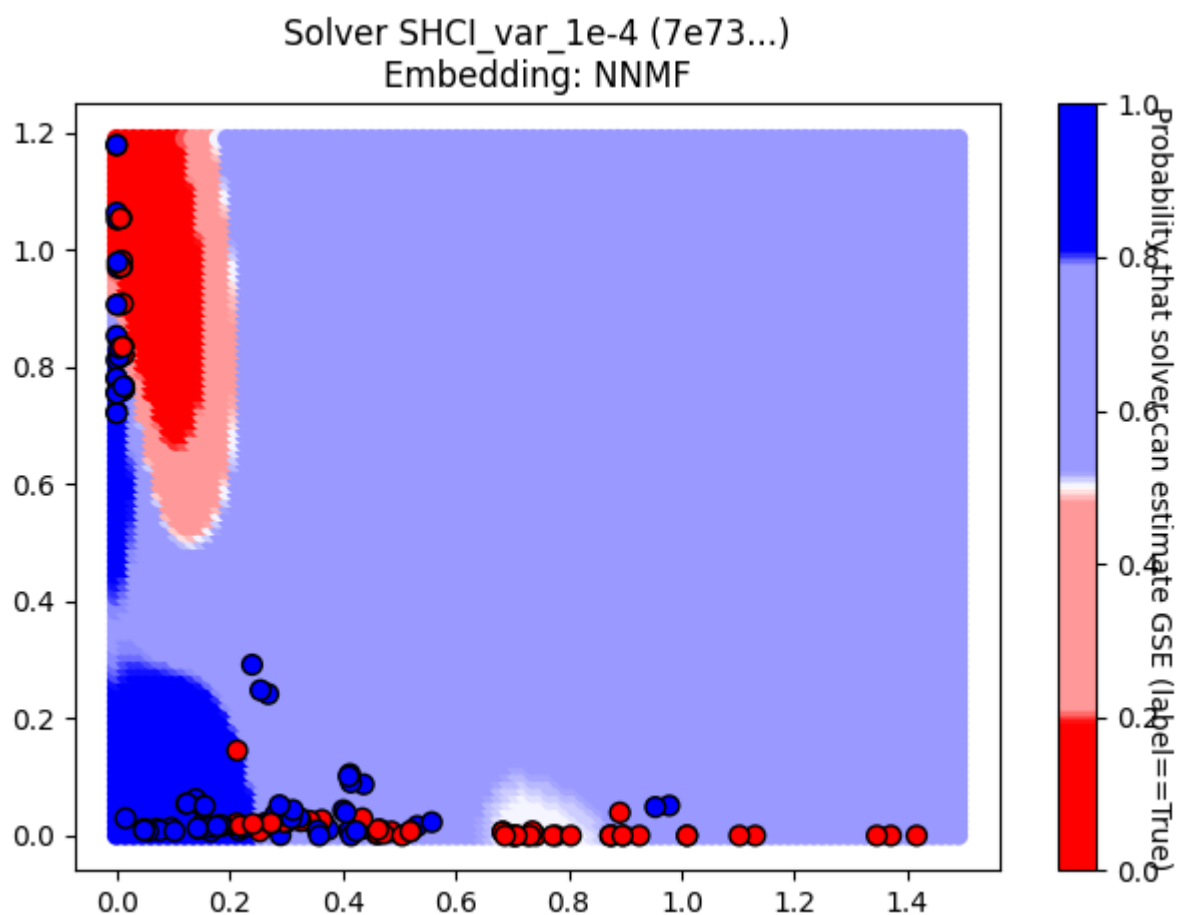


Note: plot only contains attempted tasks.

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

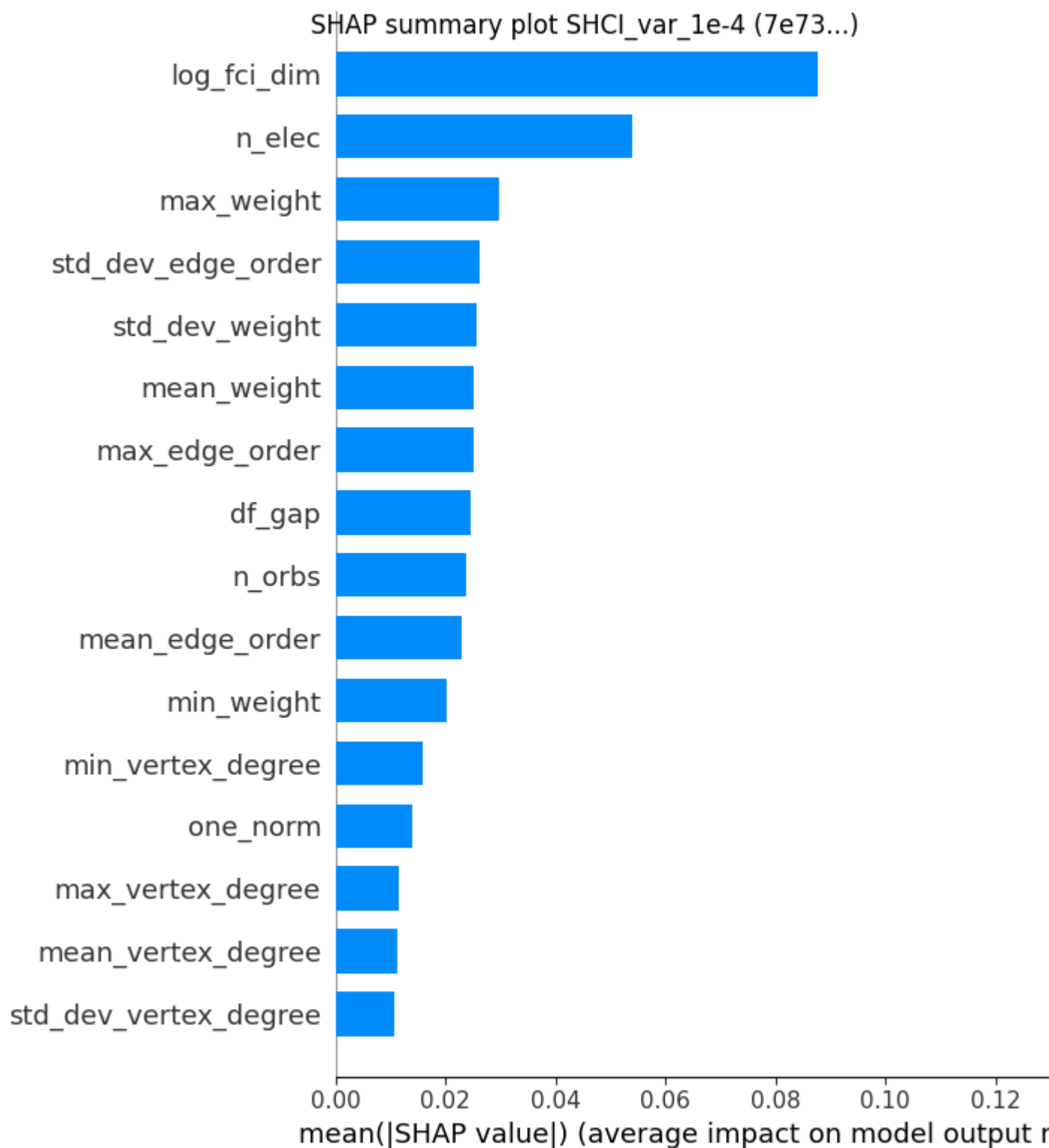
(captured: \$1.0e+02/1.5e+07, approximately 6.8e-04%)





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)





**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: 4e309f75-a220-4ae3-be6e-15b956525b42

creation\_timestamp: 2025-01-27T16:43:41.107794+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

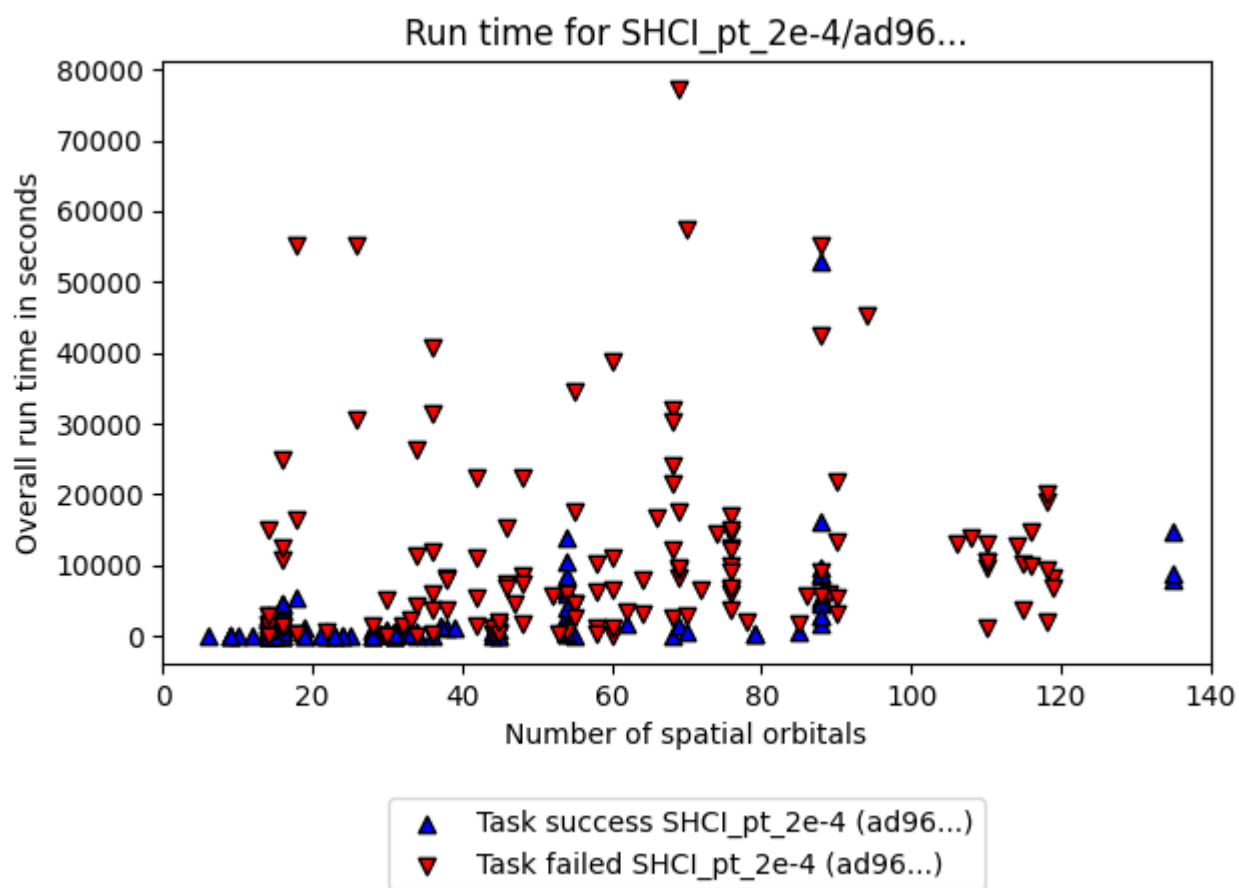
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

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

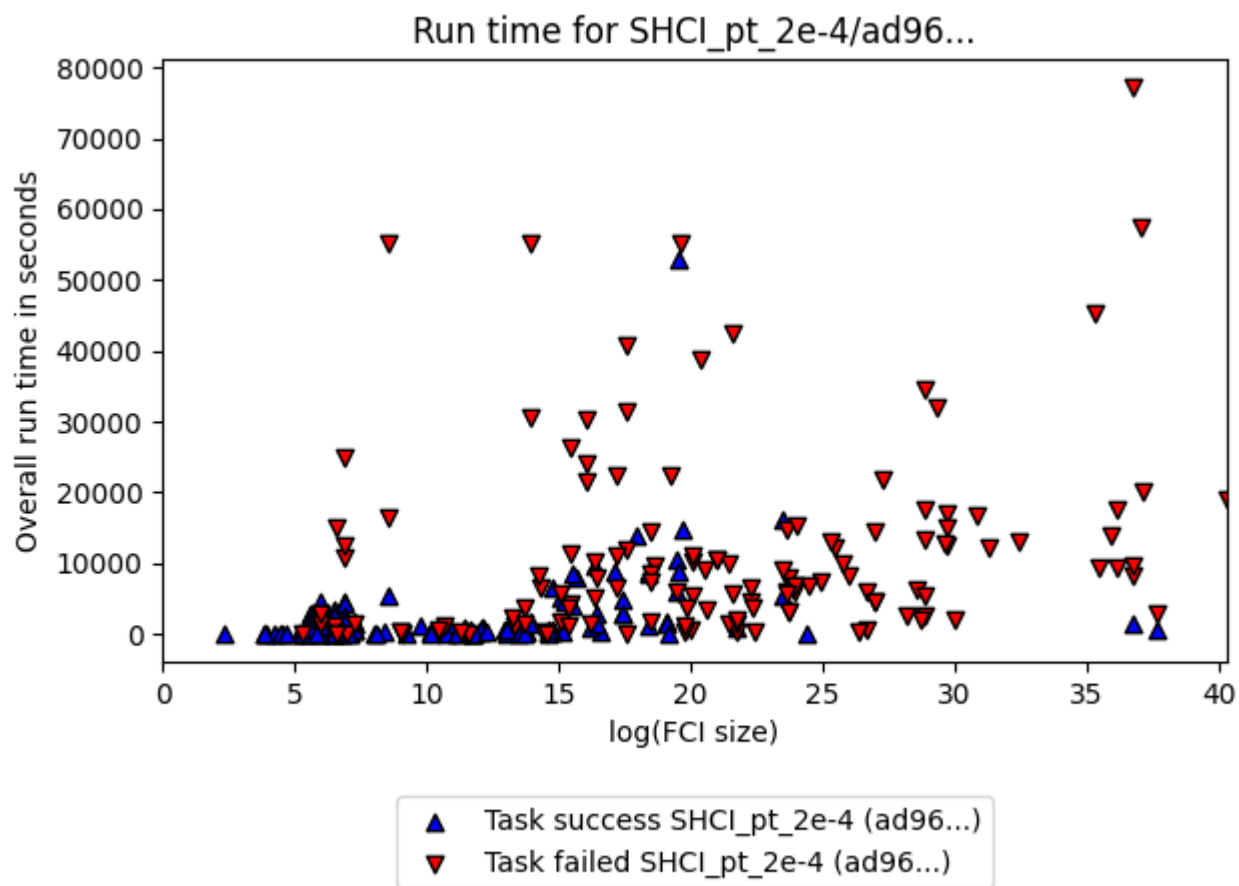
solvability\_ratio: 0.5184

f1\_score: [0.6486486486486487, 0.953405017921147]

ml\_metrics\_calculator\_version: 1



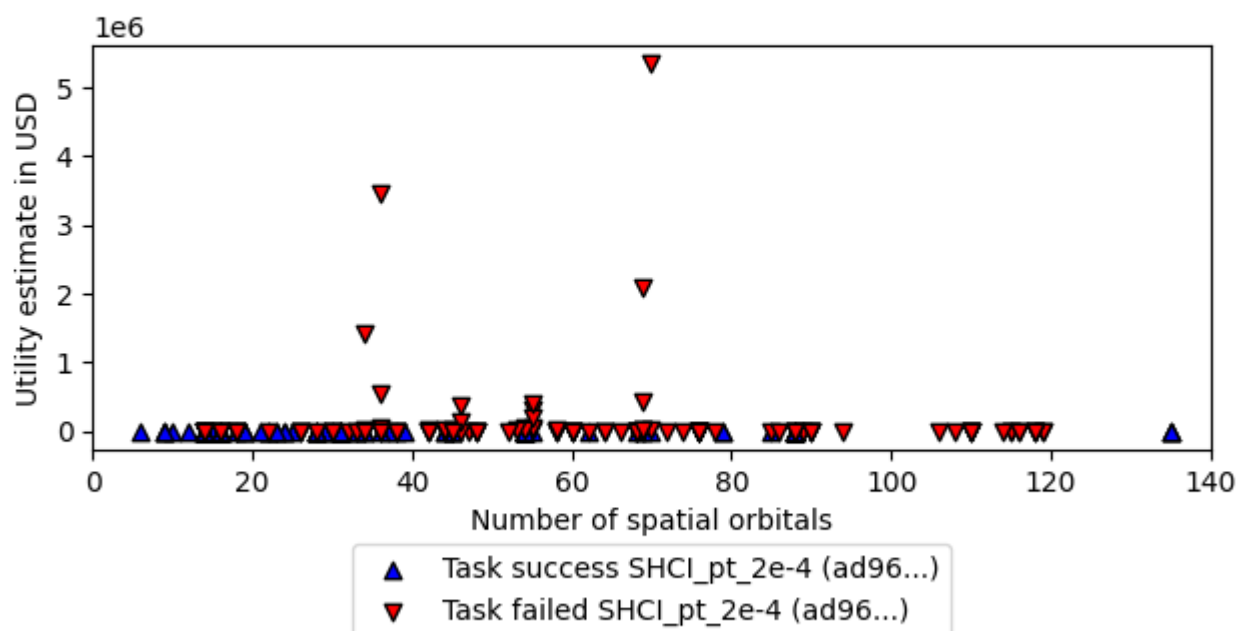
Note: plot only contains attempted tasks.

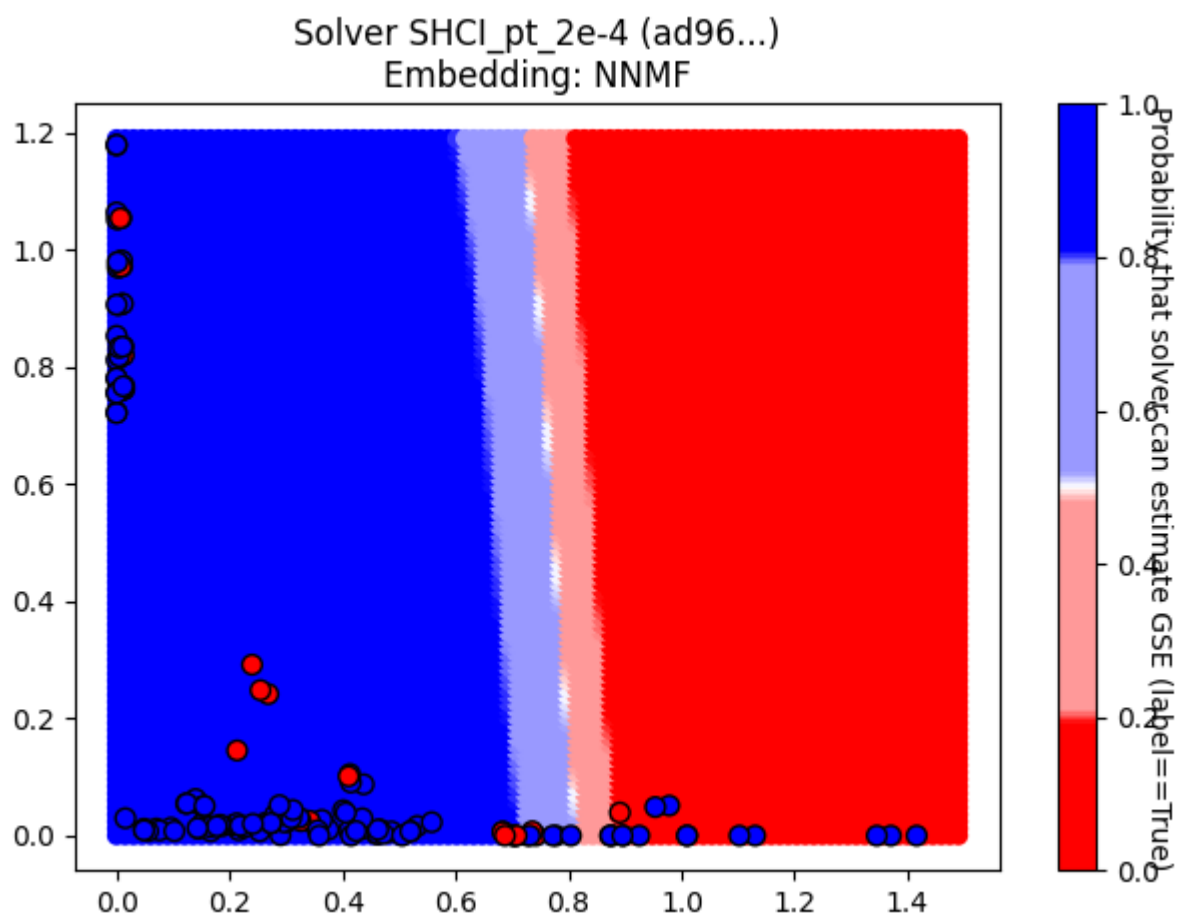


Note: plot only contains attempted tasks.

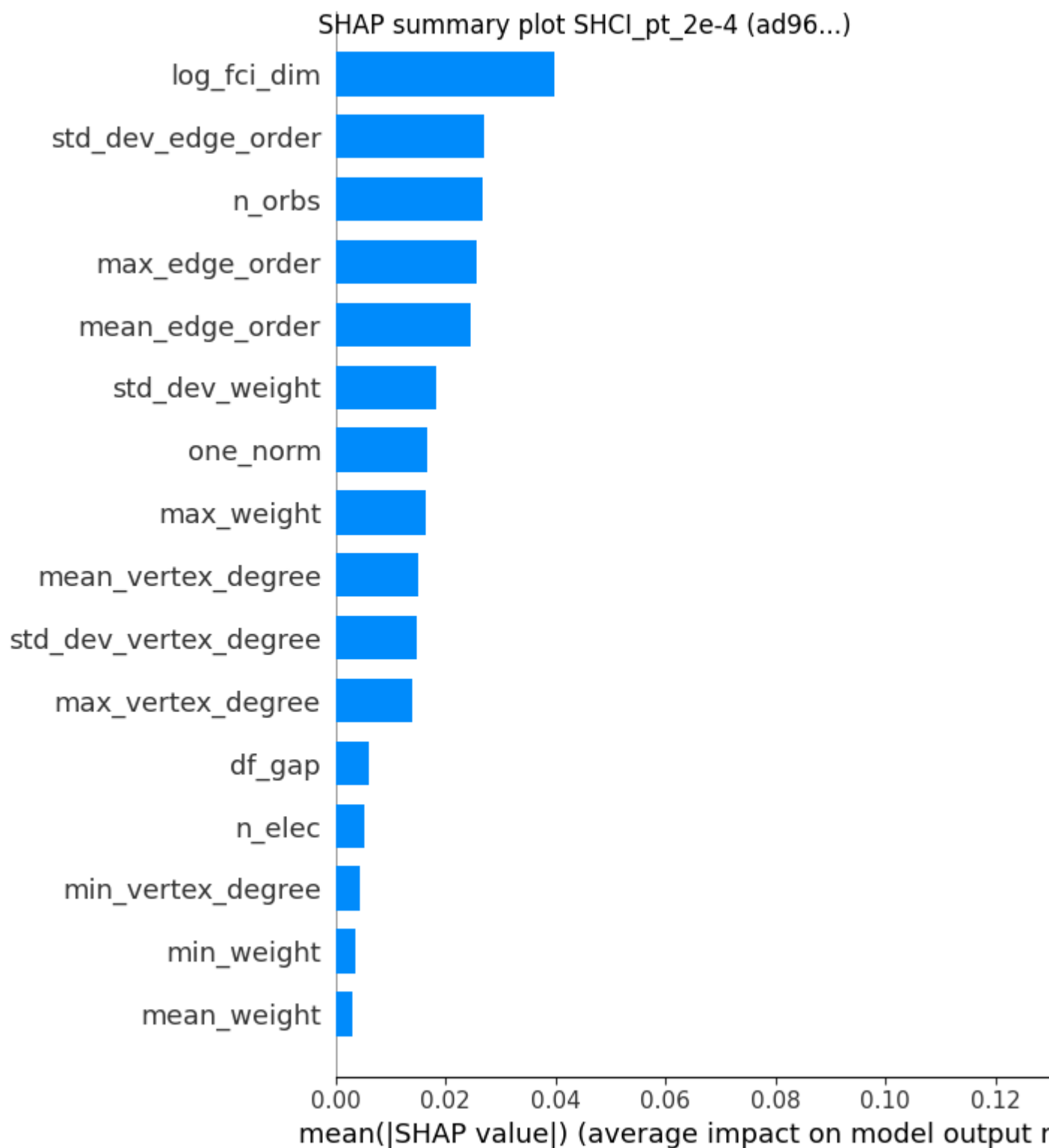
### Utility capture from SHCI\_pt\_2e-4/ad96...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: 85a2e7bb-3417-44b4-8121-e0f9f5e63811

creation\_timestamp: 2025-01-27T16:43:41.107794+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

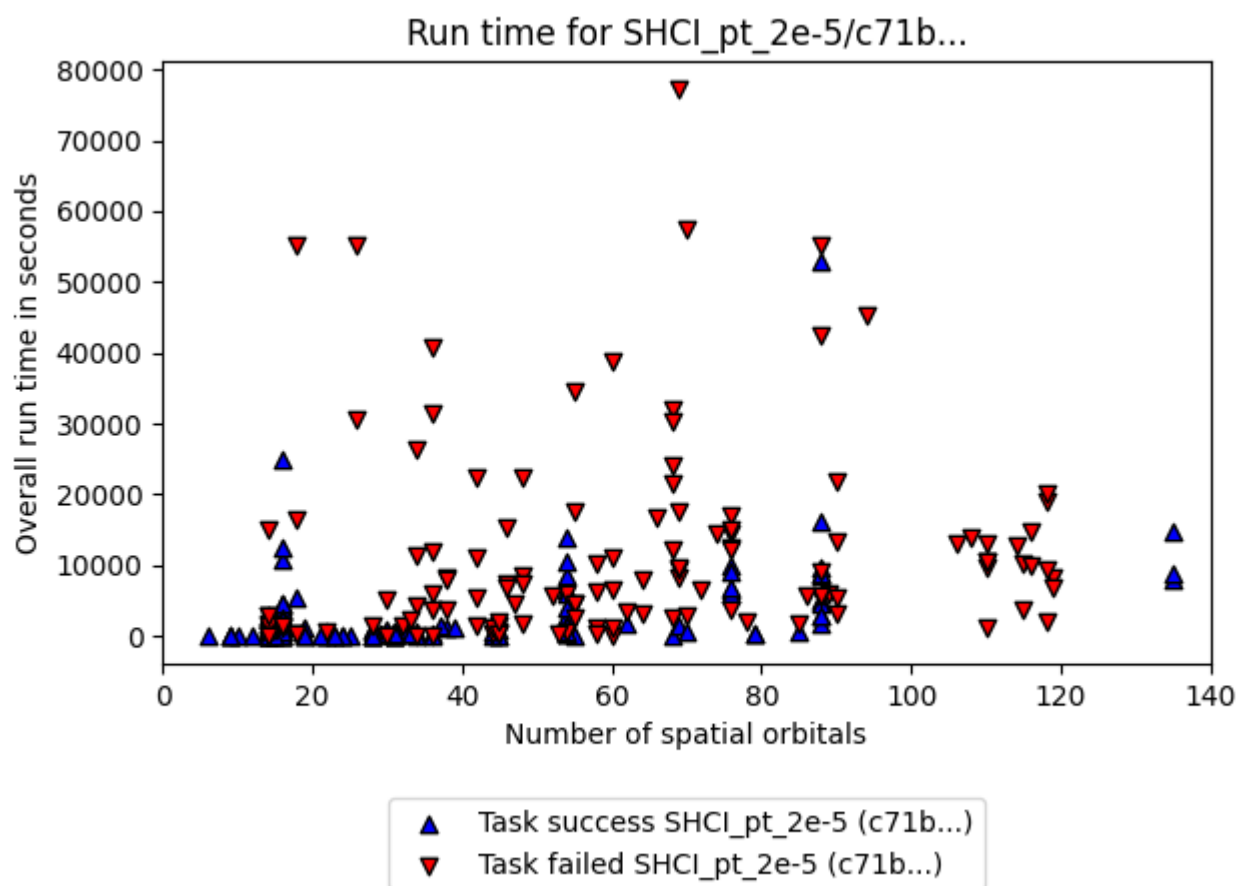
sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

solvability\_ratio: 0.8922

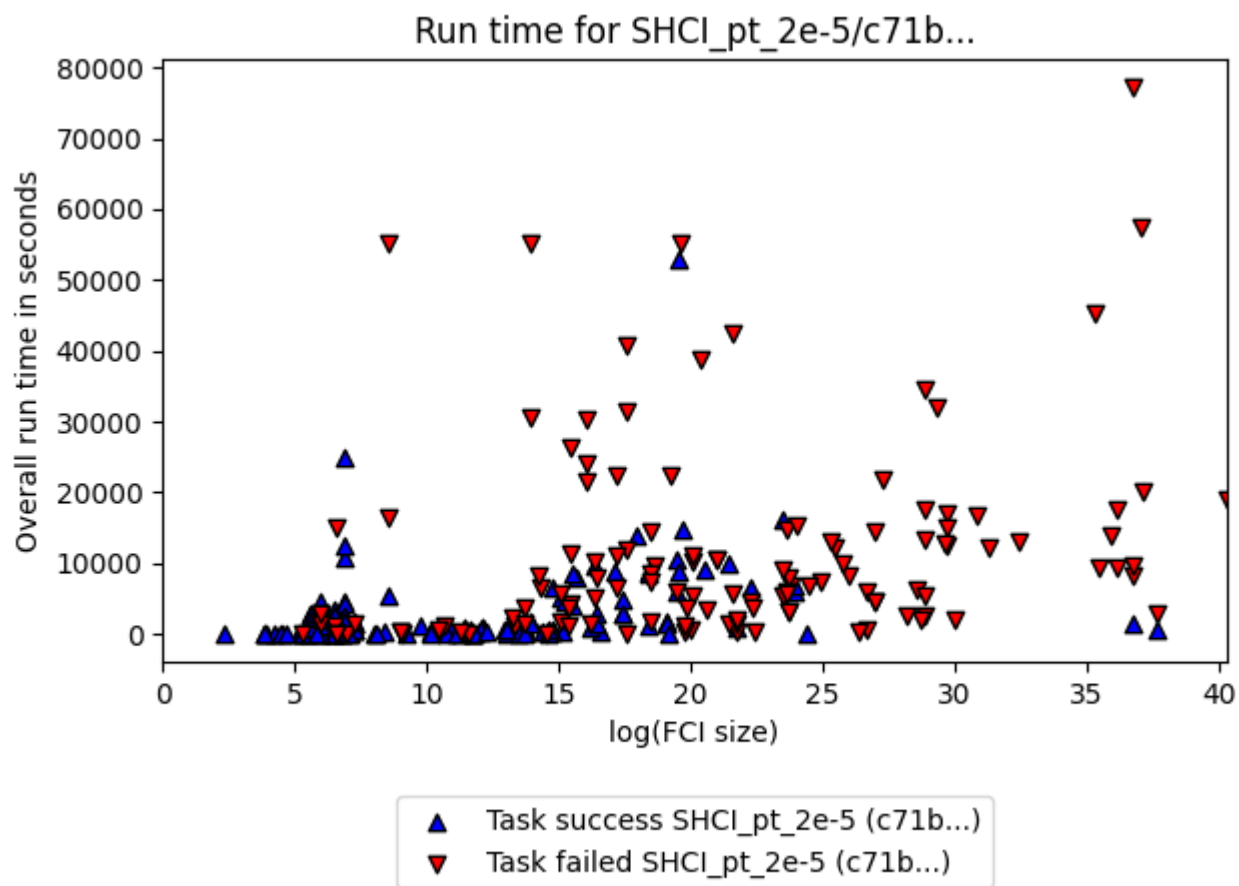
f1\_score: [1.0, 1.0]

ml\_metrics\_calculator\_version: 1





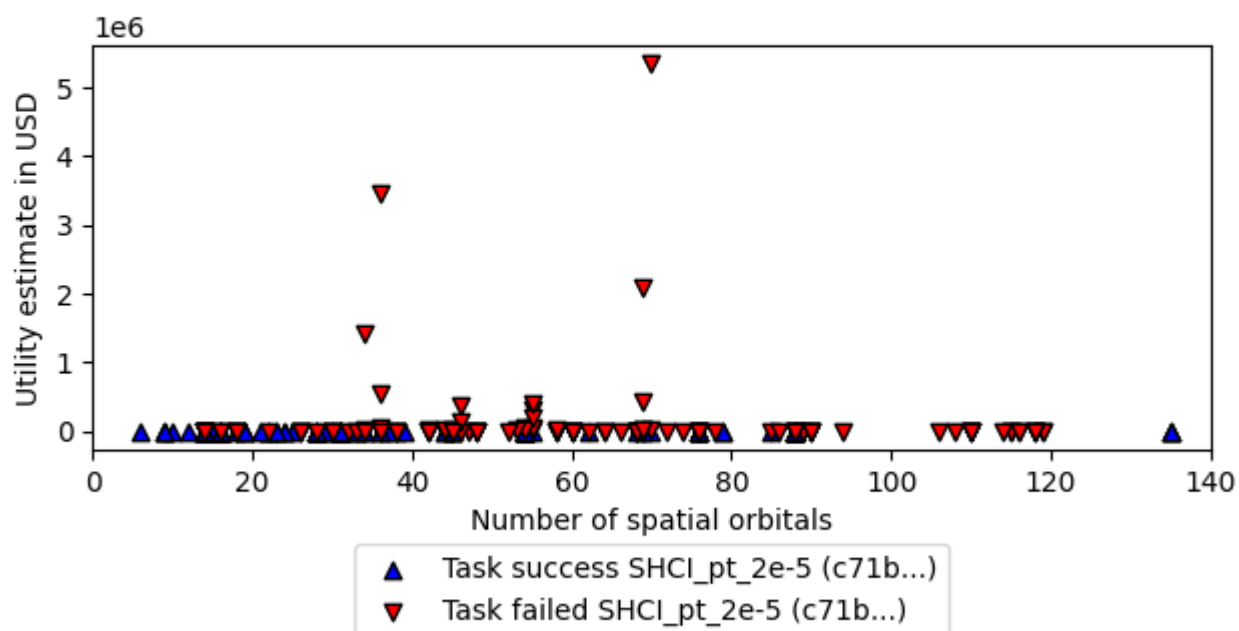
Note: plot only contains attempted tasks.

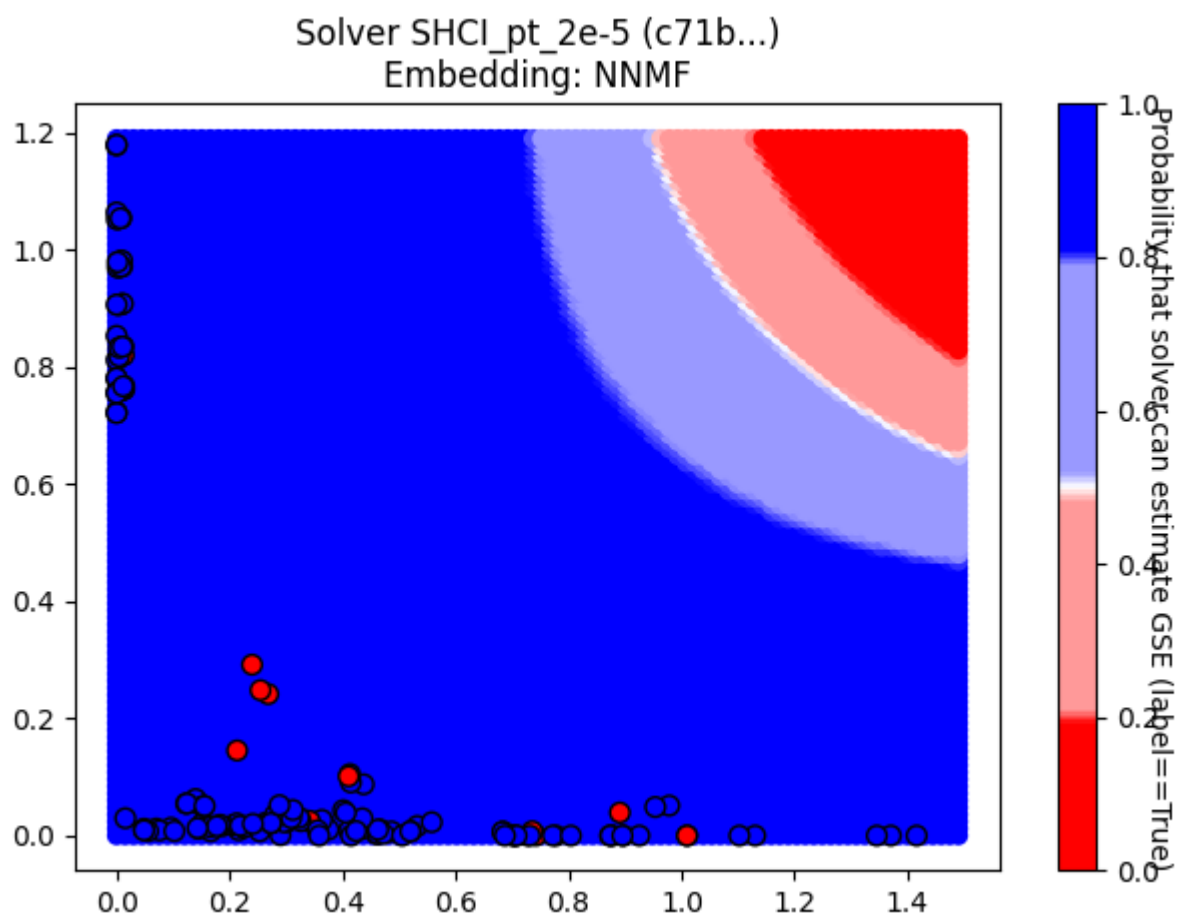


Note: plot only contains attempted tasks.

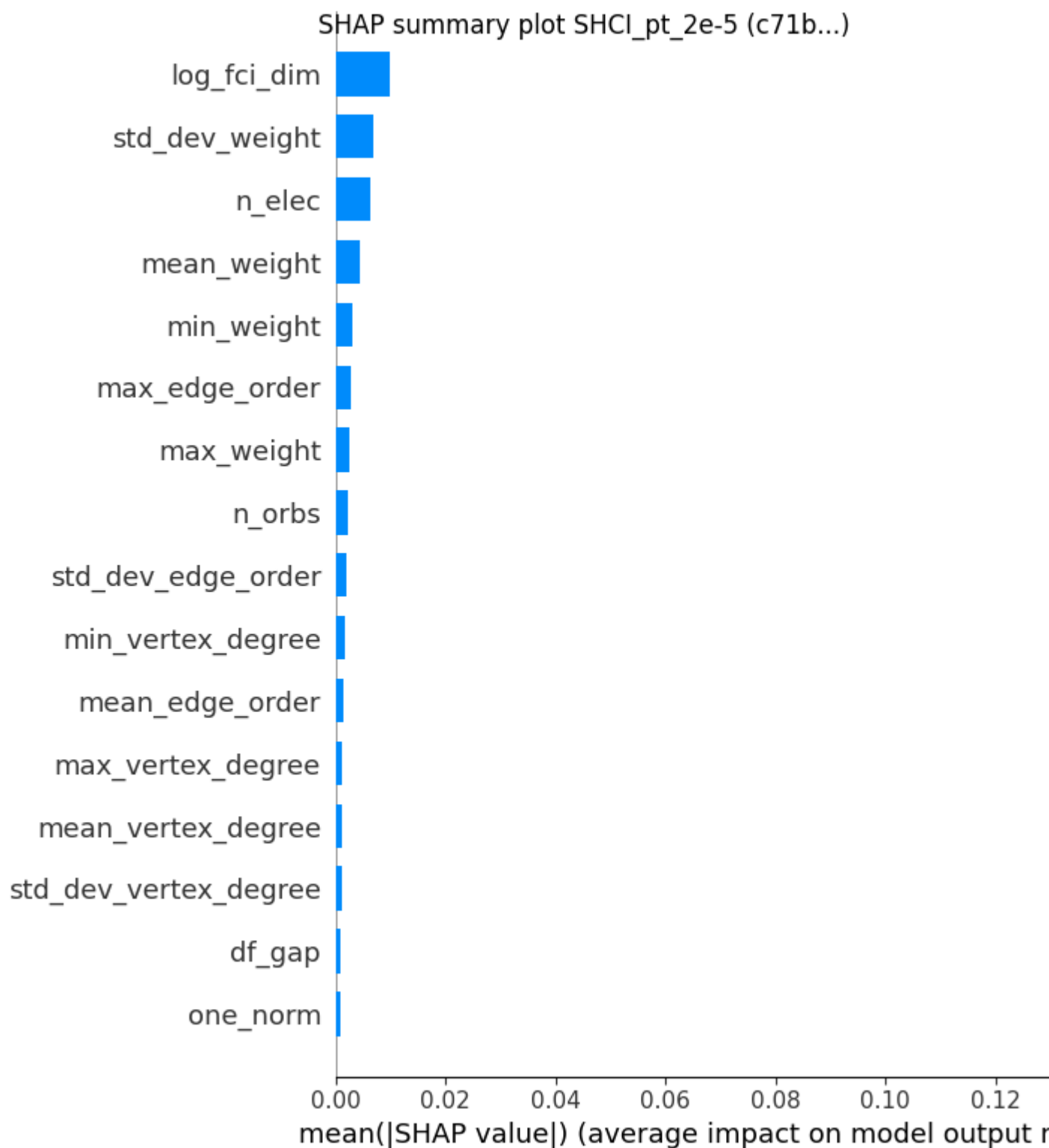
# Utility capture from SHCI\_pt\_2e-5/c71b...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: 7f93c734-4257-4fde-a274-92d36efd5e8e

creation\_timestamp: 2025-01-27T16:43:41.107794+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

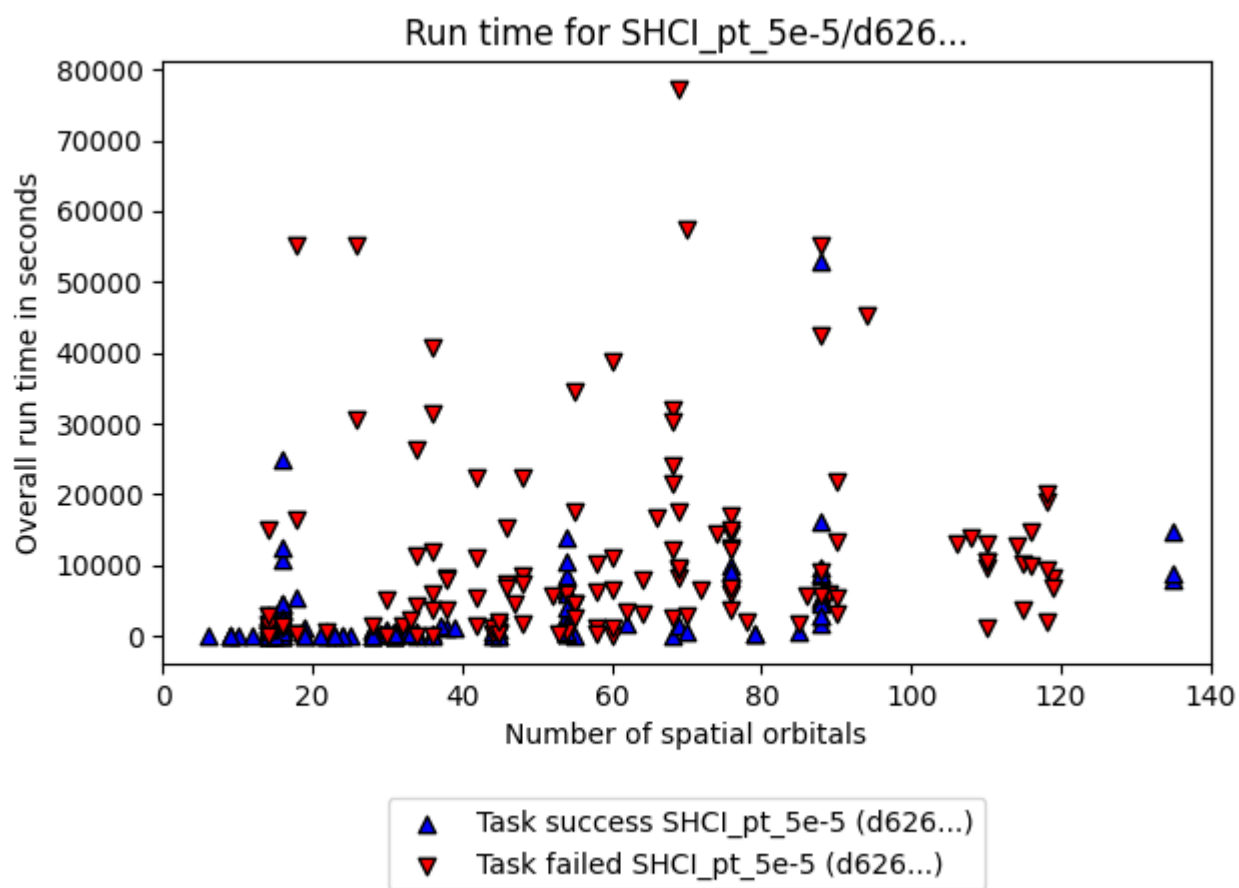
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

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

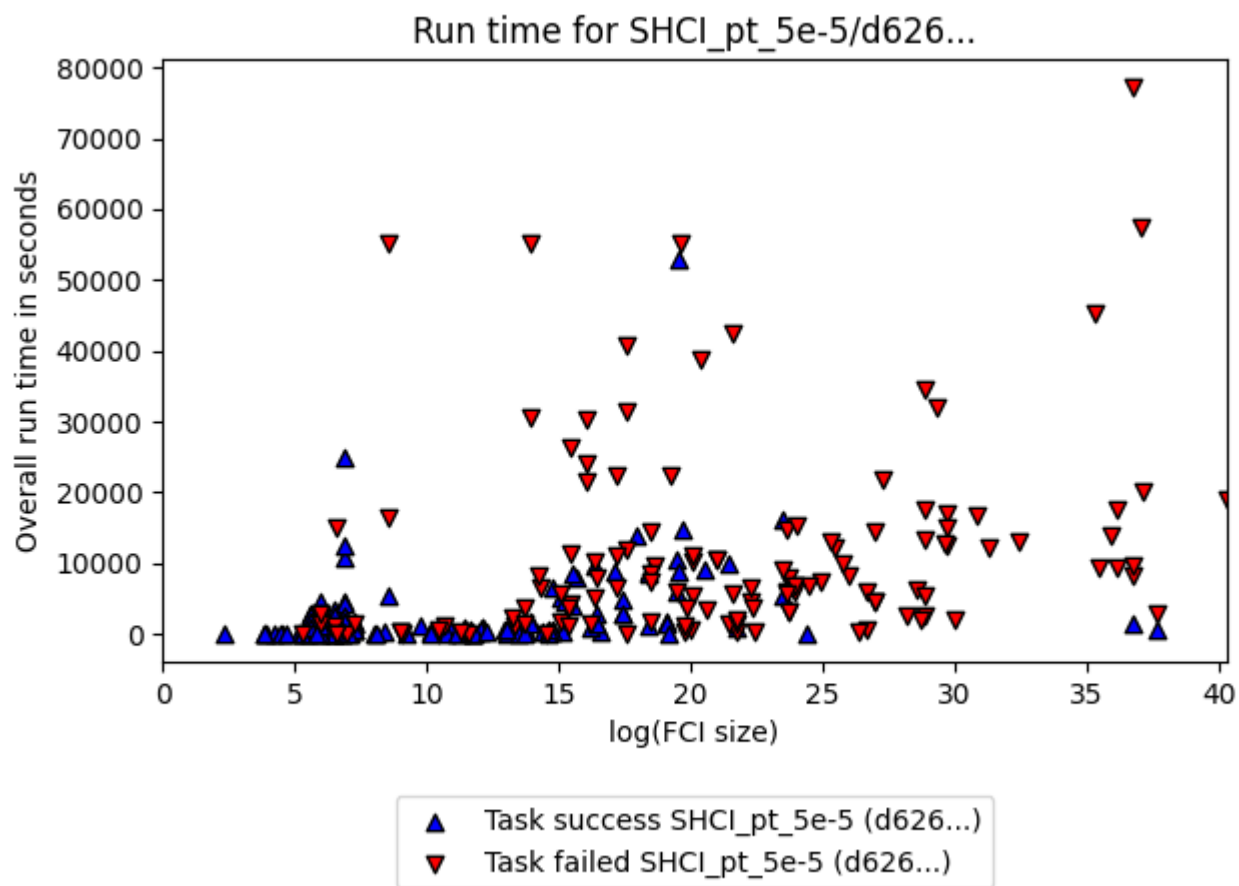
solvability\_ratio: 0.482

f1\_score: [0.75, 0.971830985915493]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

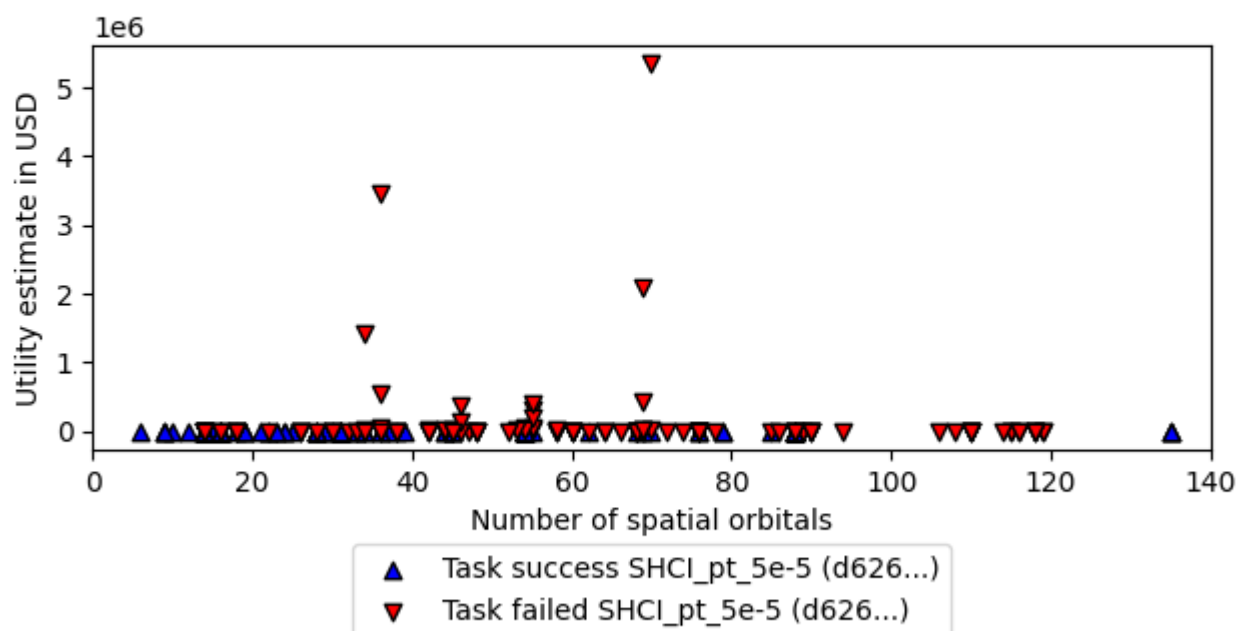


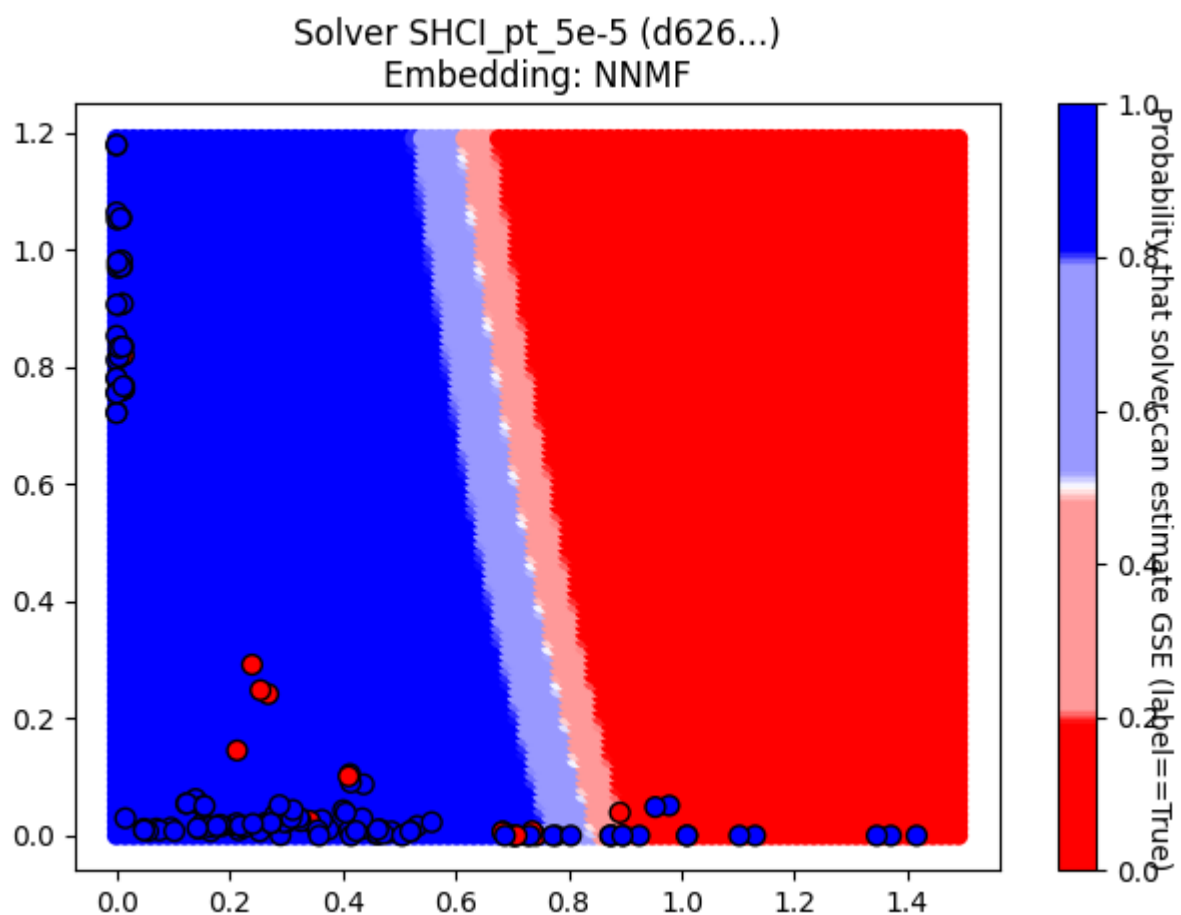
Note: plot only contains attempted tasks.



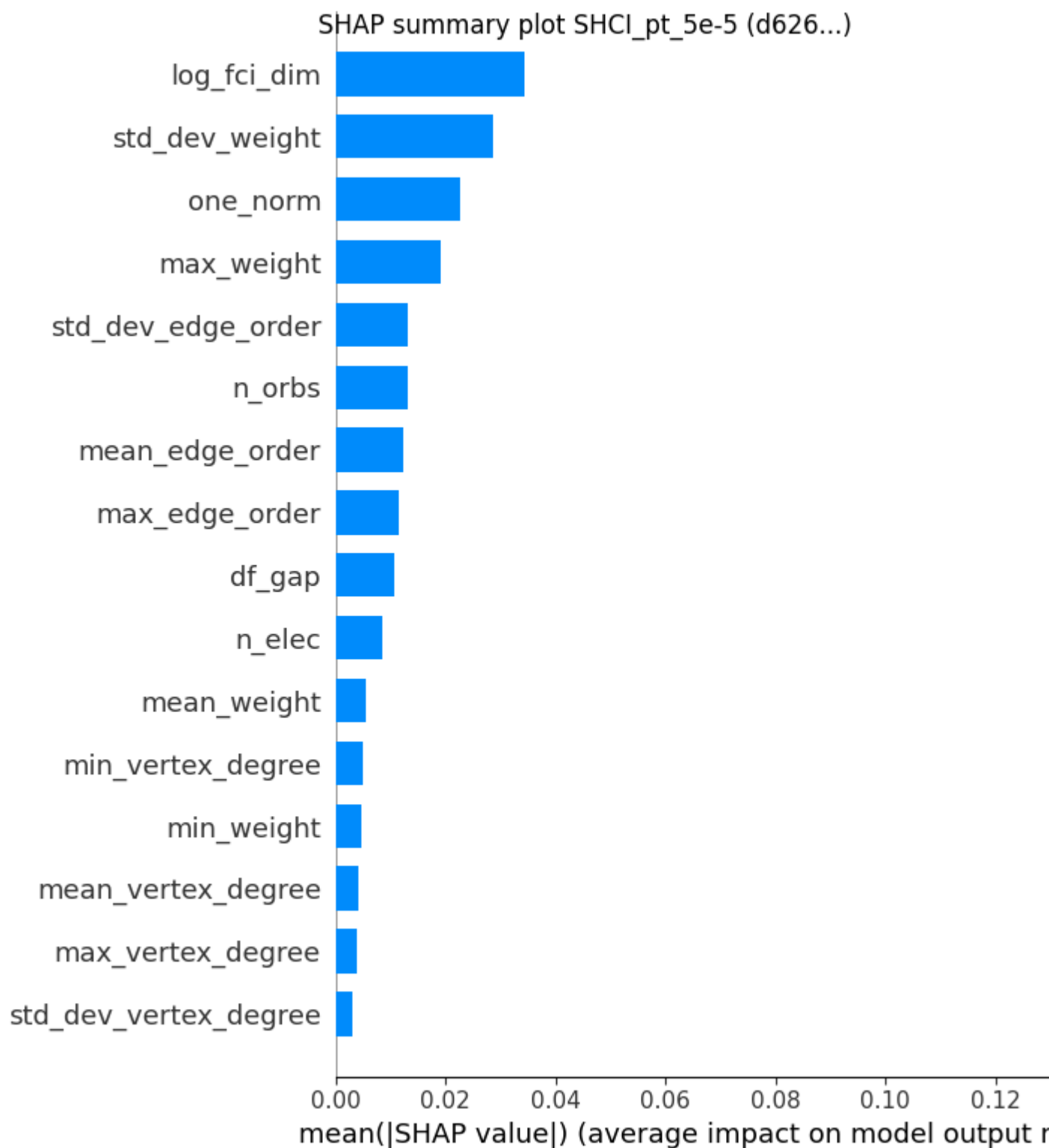
### Utility capture from SHCI\_pt\_5e-5/d626...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: 66ac8f5a-2694-4bbd-ab96-4cfdbe809b85

creation\_timestamp: 2025-01-27T16:43:41.107794+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

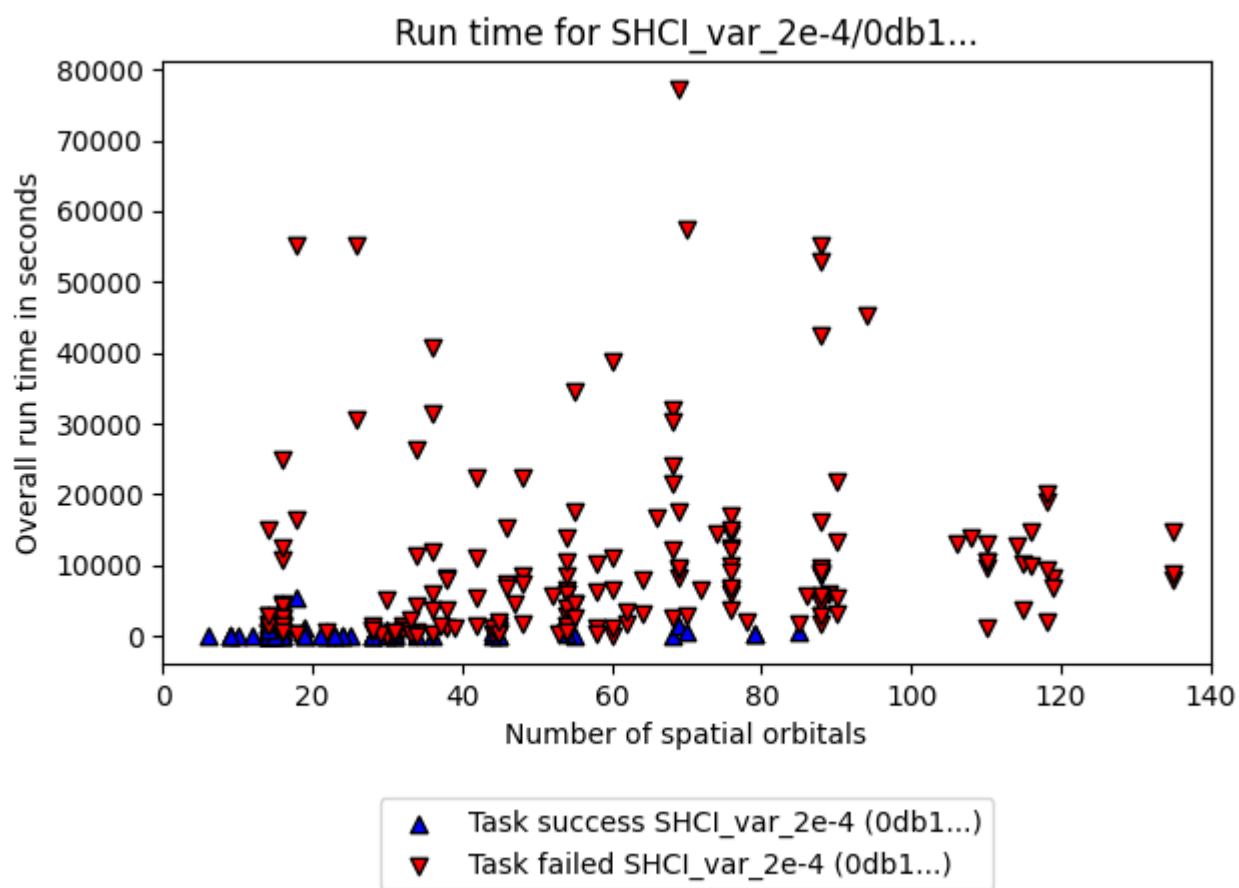
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

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

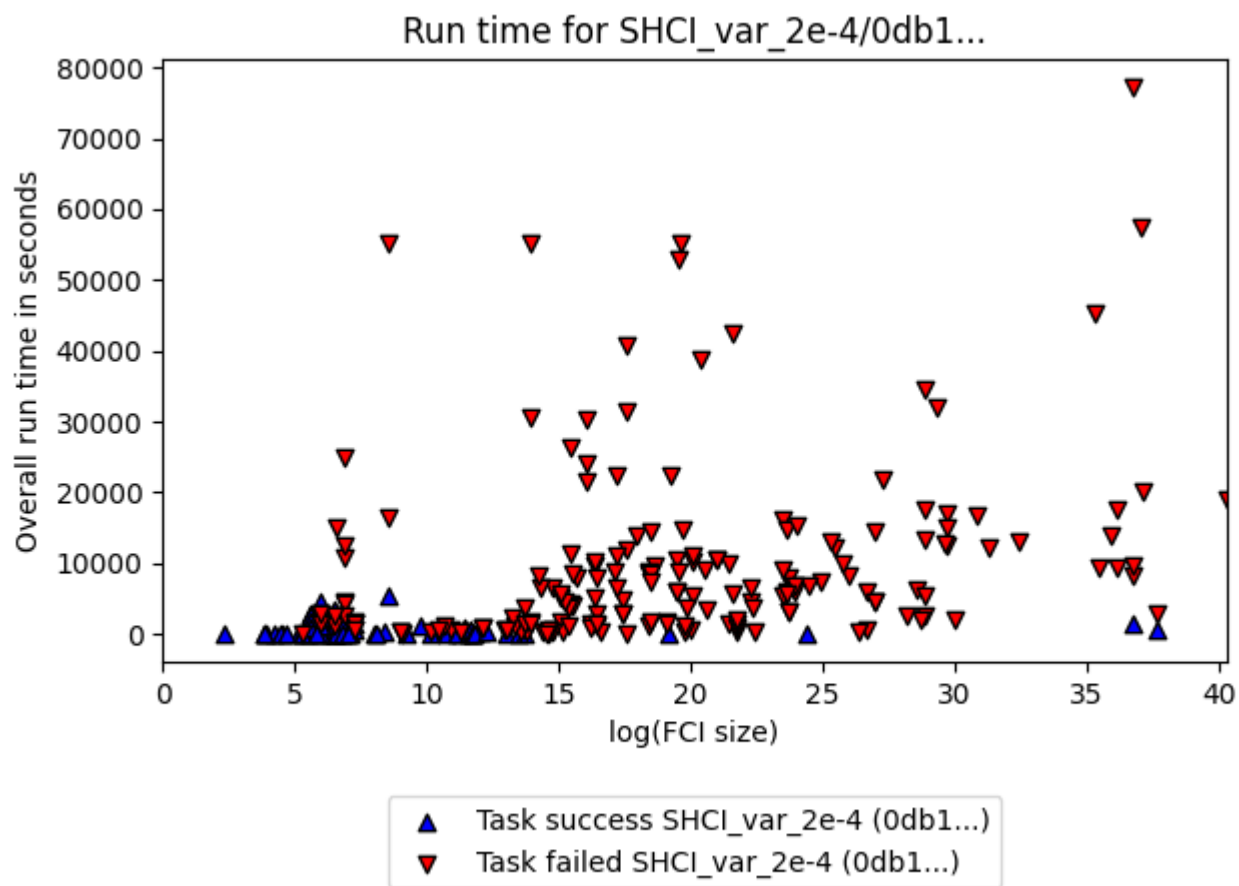
solvability\_ratio: 0.3462

f1\_score: [0.9864864864864865, 0.9880952380952381]

ml\_metrics\_calculator\_version: 1



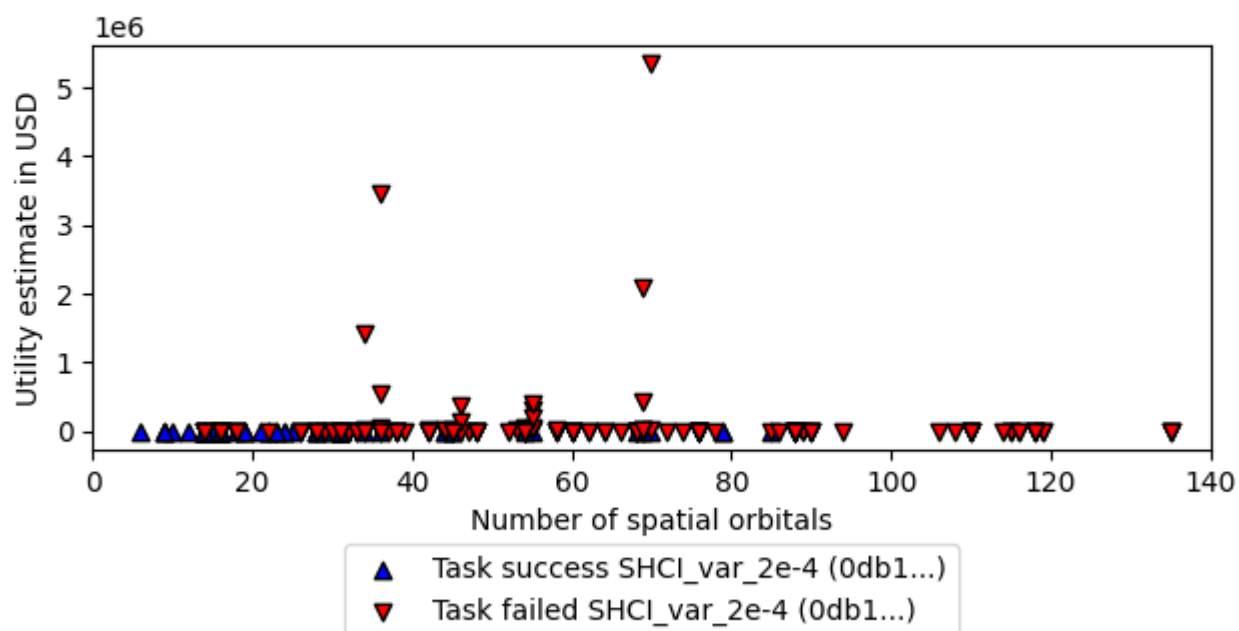
Note: plot only contains attempted tasks.

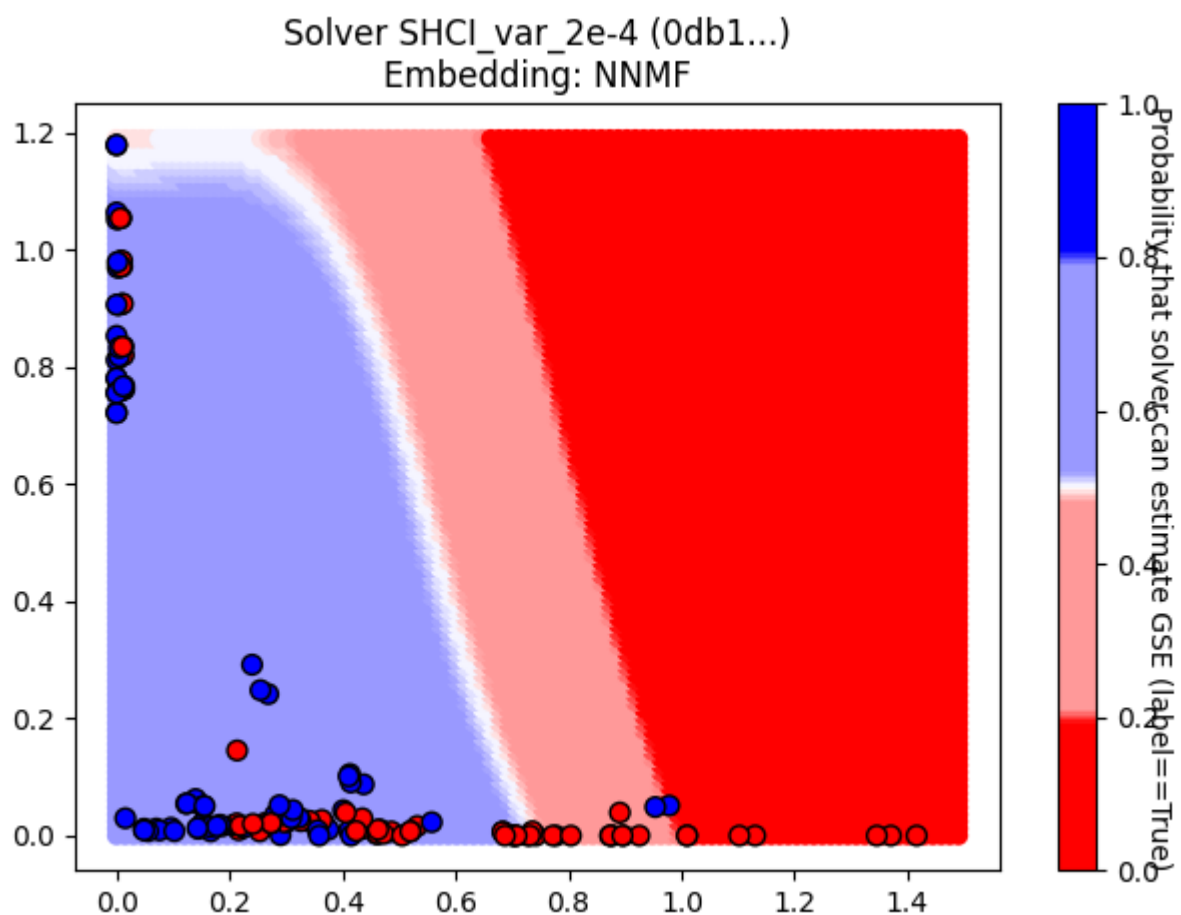


Note: plot only contains attempted tasks.

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

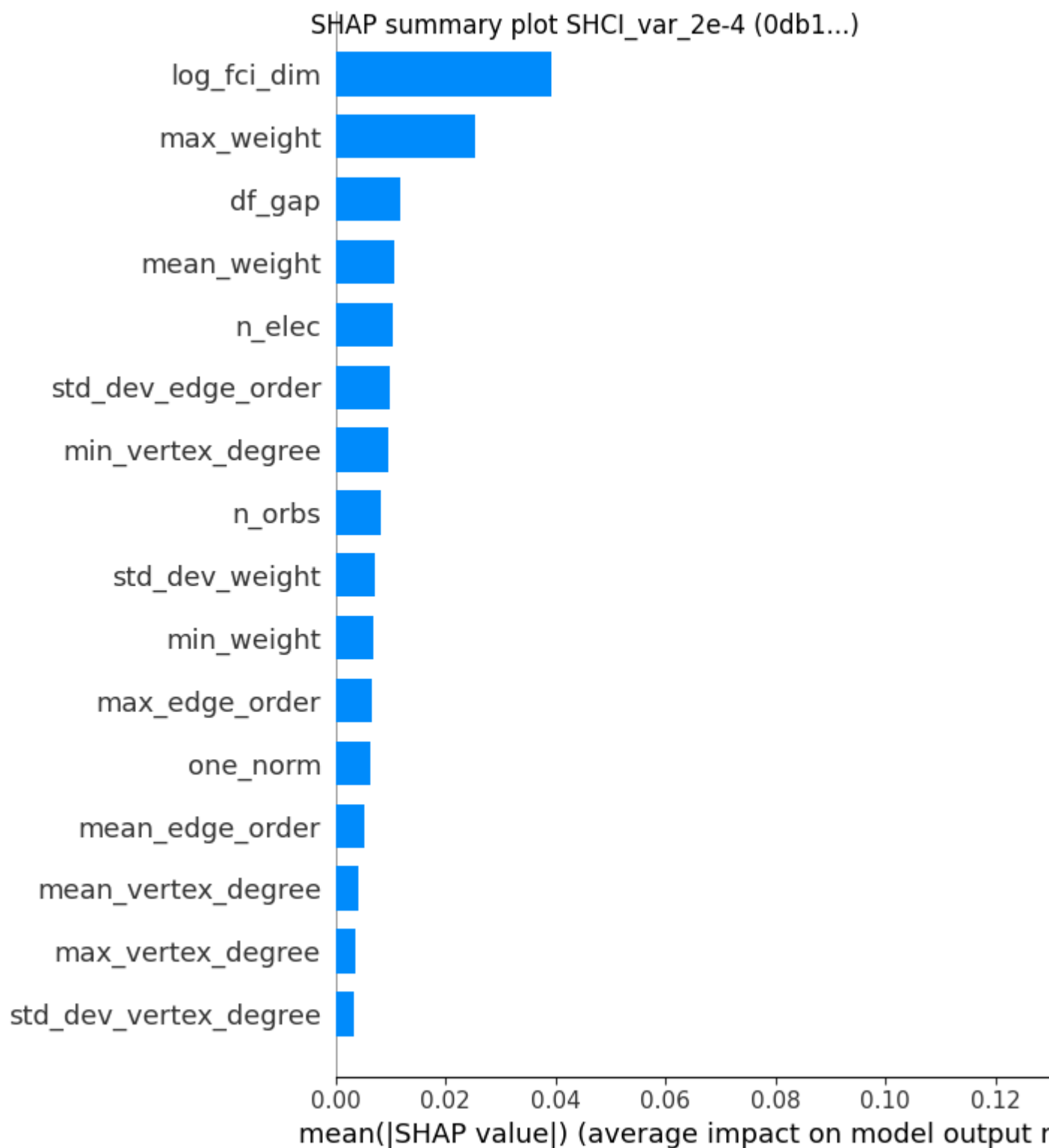
(captured:  $\$8.6\text{e}+01/1.5\text{e}+07$ , approximately  $5.8\text{e}-04\%$ )





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)





**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: ff59b049-307e-48e7-a451-b7b1710d23b2

creation\_timestamp: 2025-01-27T16:43:41.107794+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

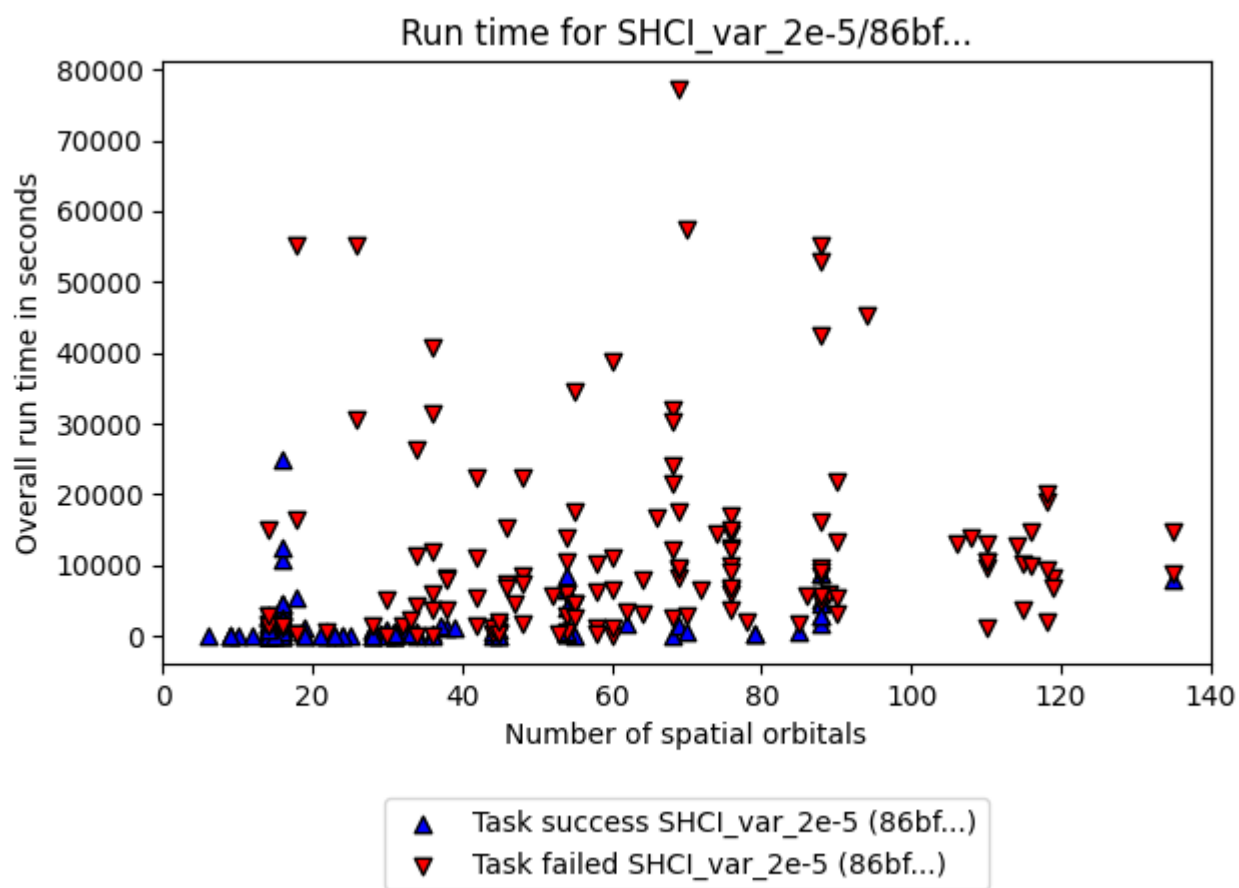
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002

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

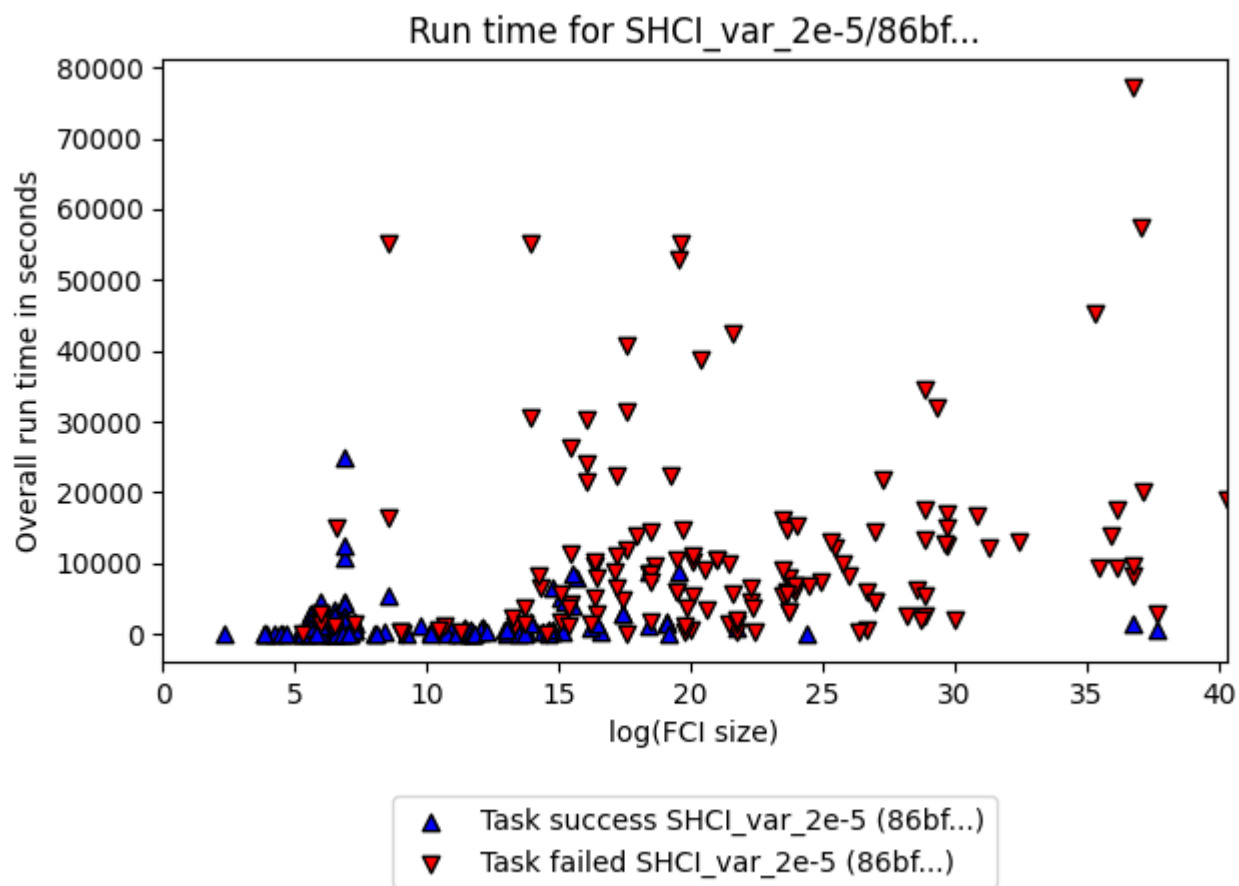
solvability\_ratio: 0.592

f1\_score: [0.8846153846153846, 0.9772727272727273]

ml\_metrics\_calculator\_version: 1



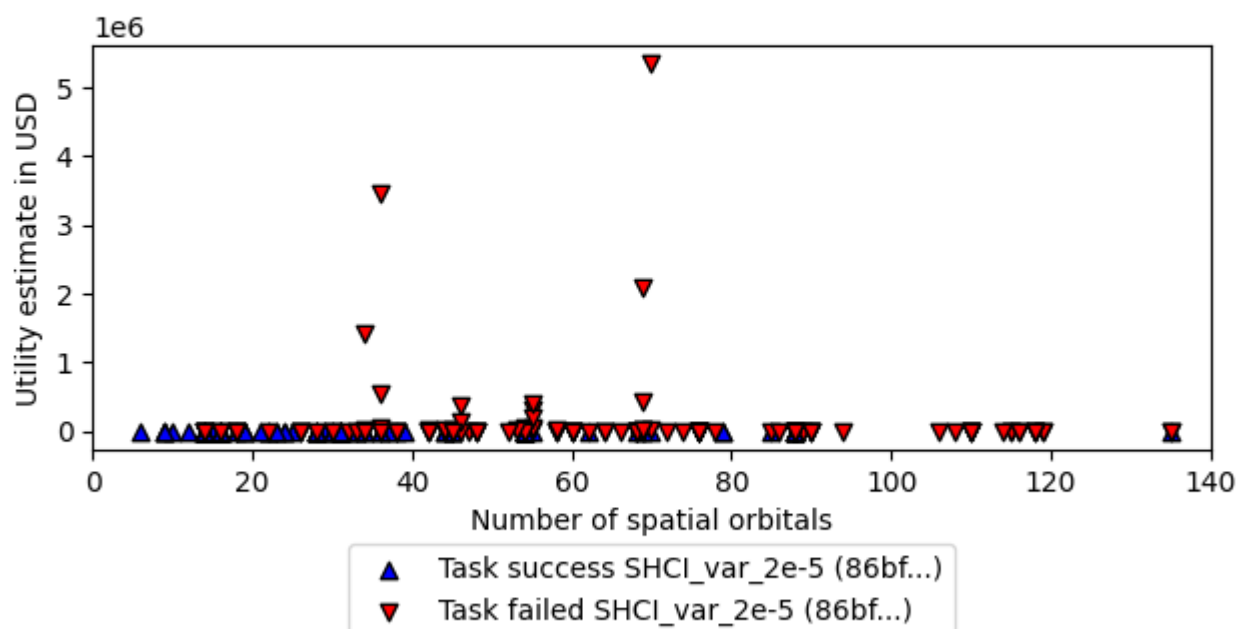
Note: plot only contains attempted tasks.

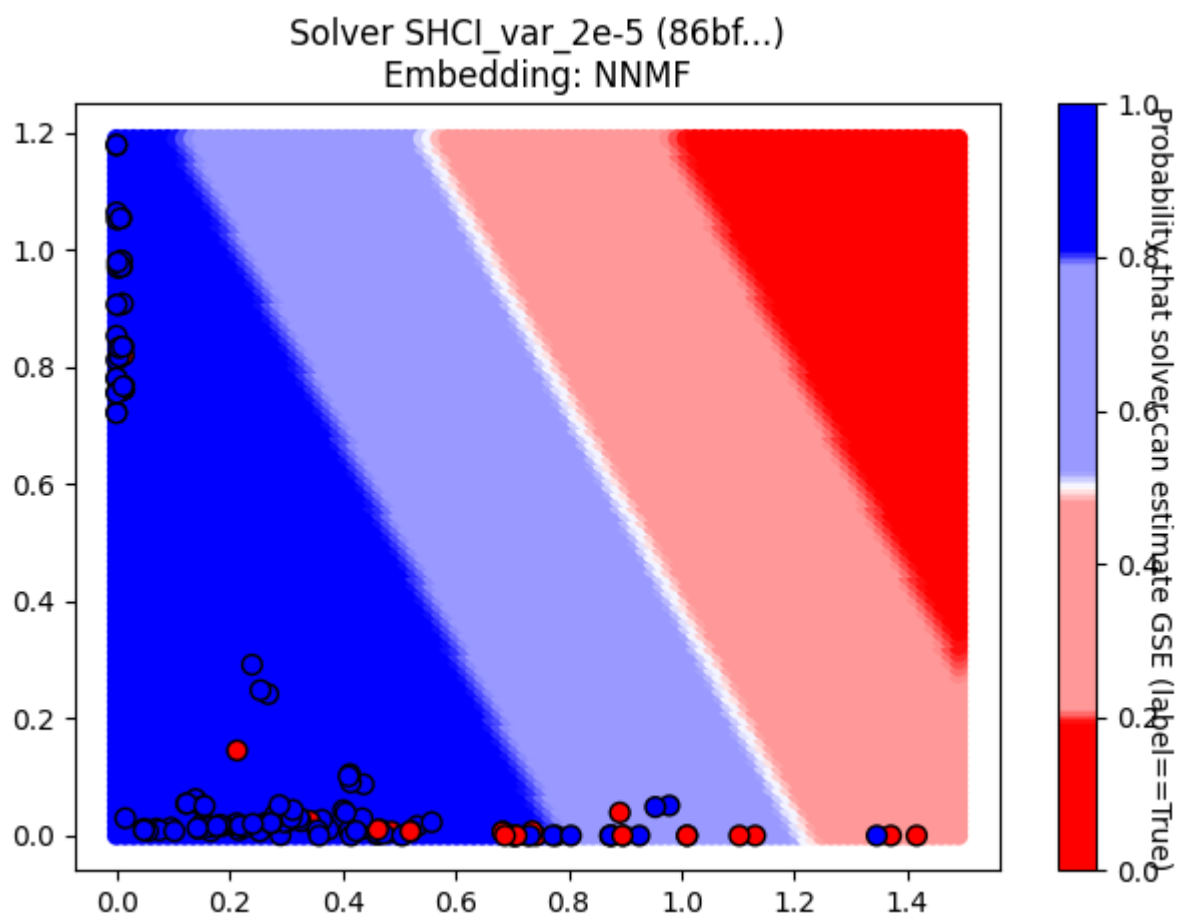


Note: plot only contains attempted tasks.

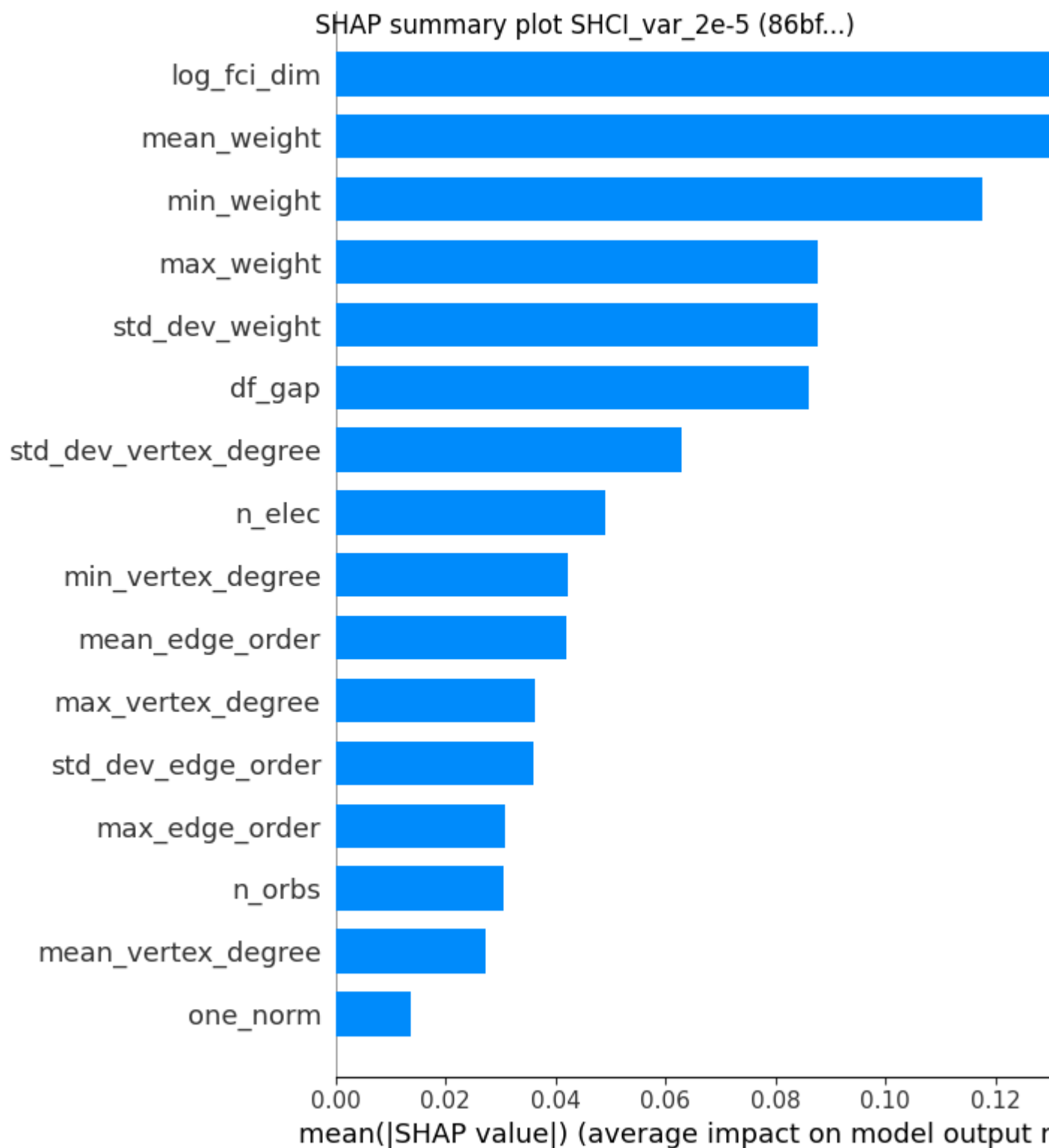
# Utility capture from SHCI\_var\_2e-5/86bf...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: e2a26353-84ed-4ce9-9510-ea5a65336239

creation\_timestamp: 2025-01-27T16:43:41.107794+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

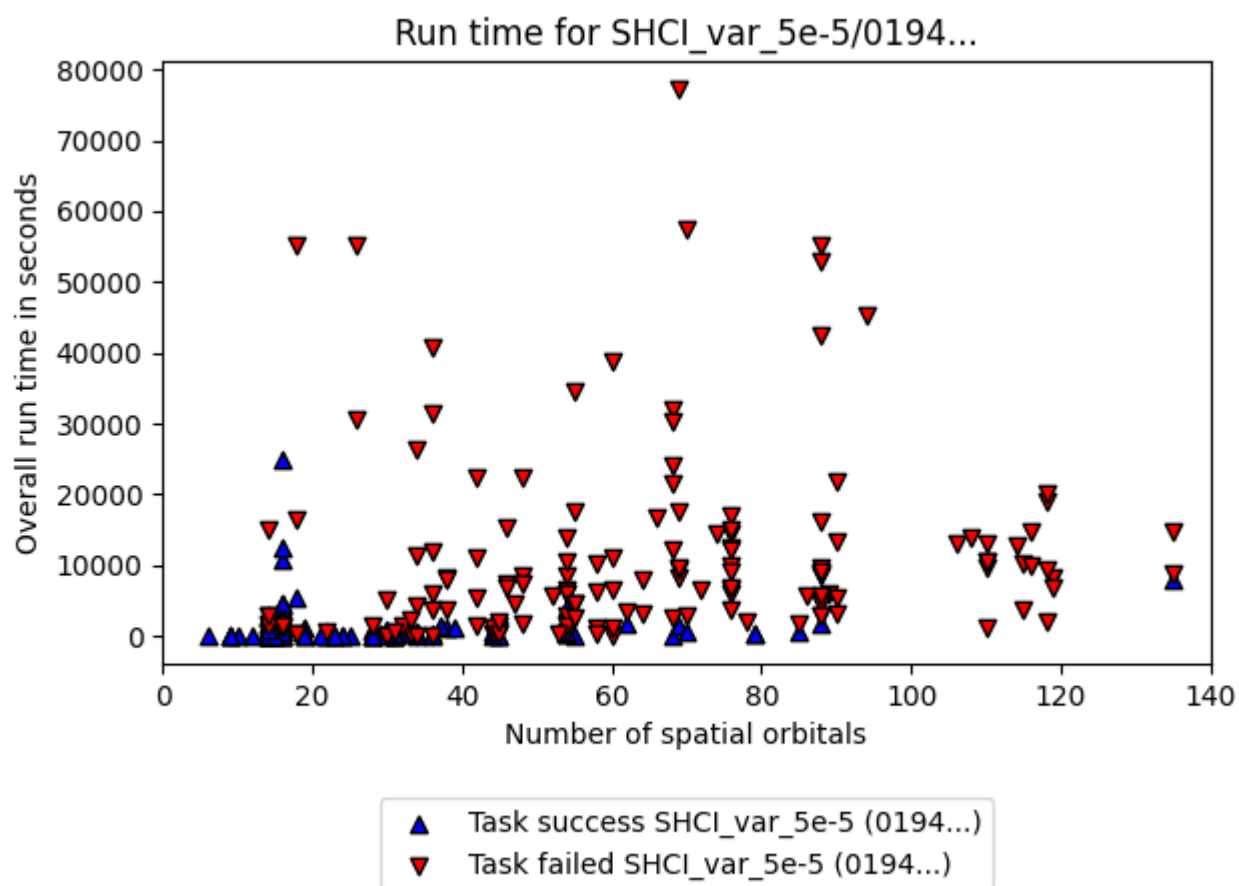
sum\_of\_run\_time\_of\_attempted\_tasks: 1863349.6330000001

solvability\_ratio: 0.3443

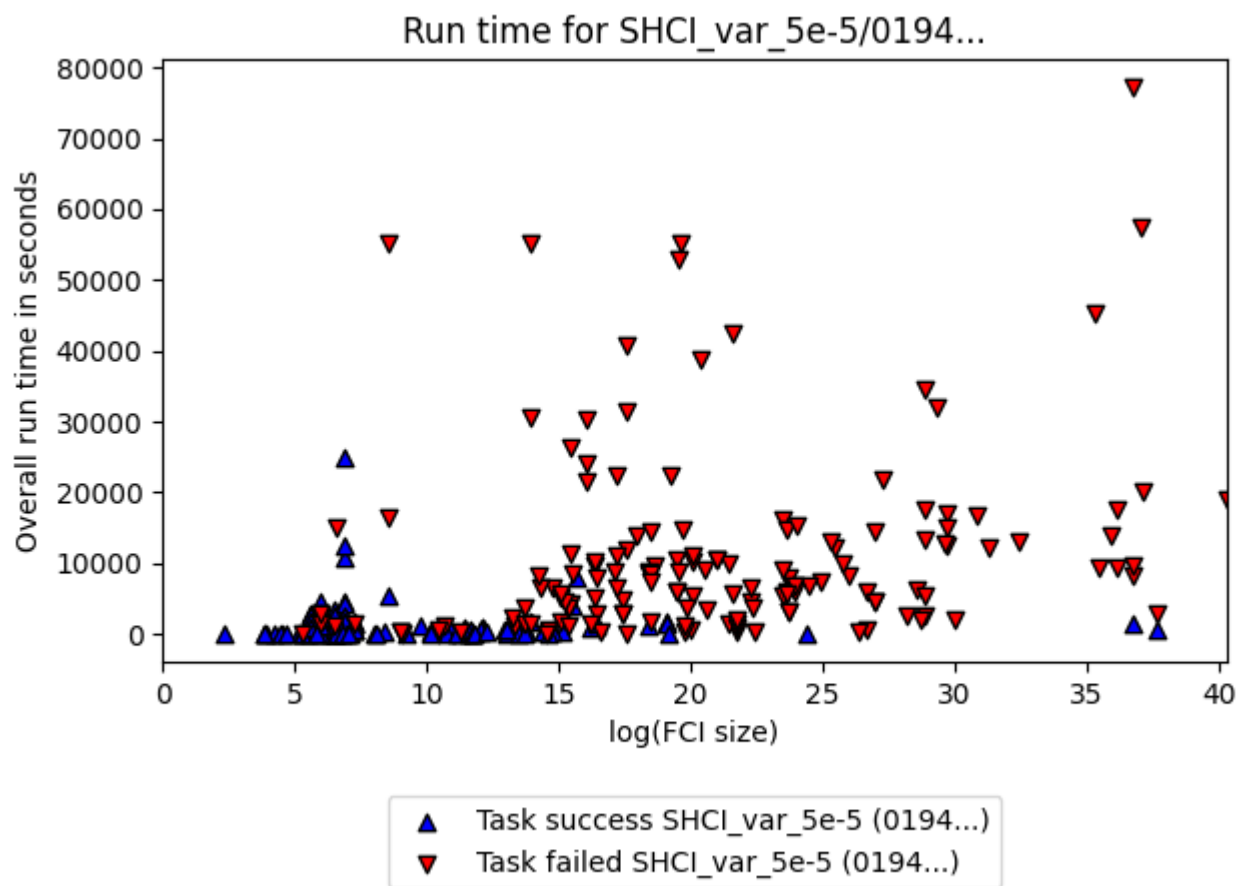
f1\_score: [0.85, 0.9491525423728814]

ml\_metrics\_calculator\_version: 1





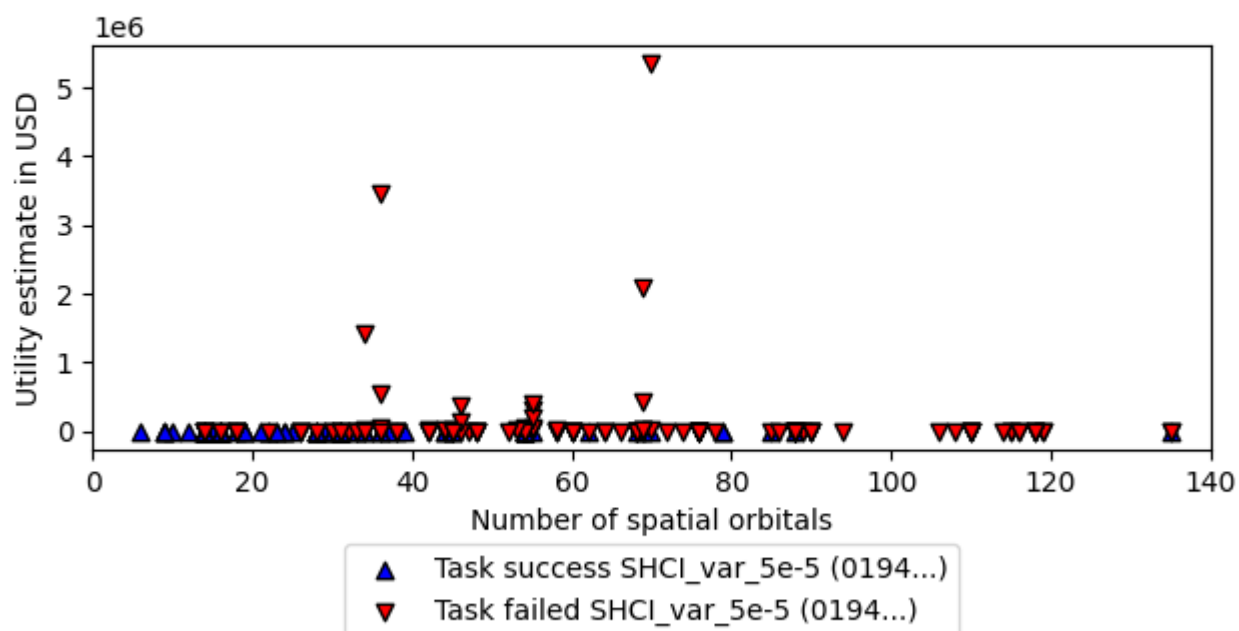
Note: plot only contains attempted tasks.

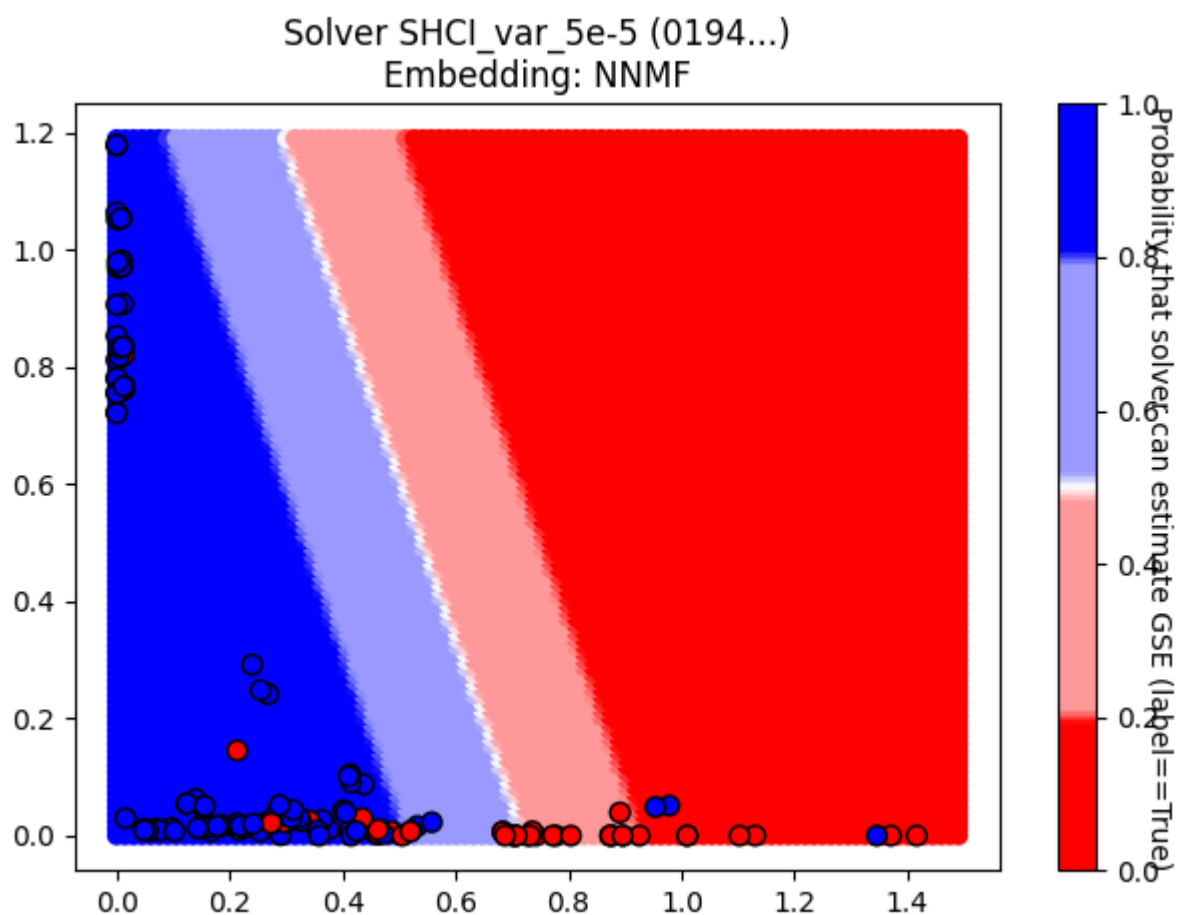


Note: plot only contains attempted tasks.

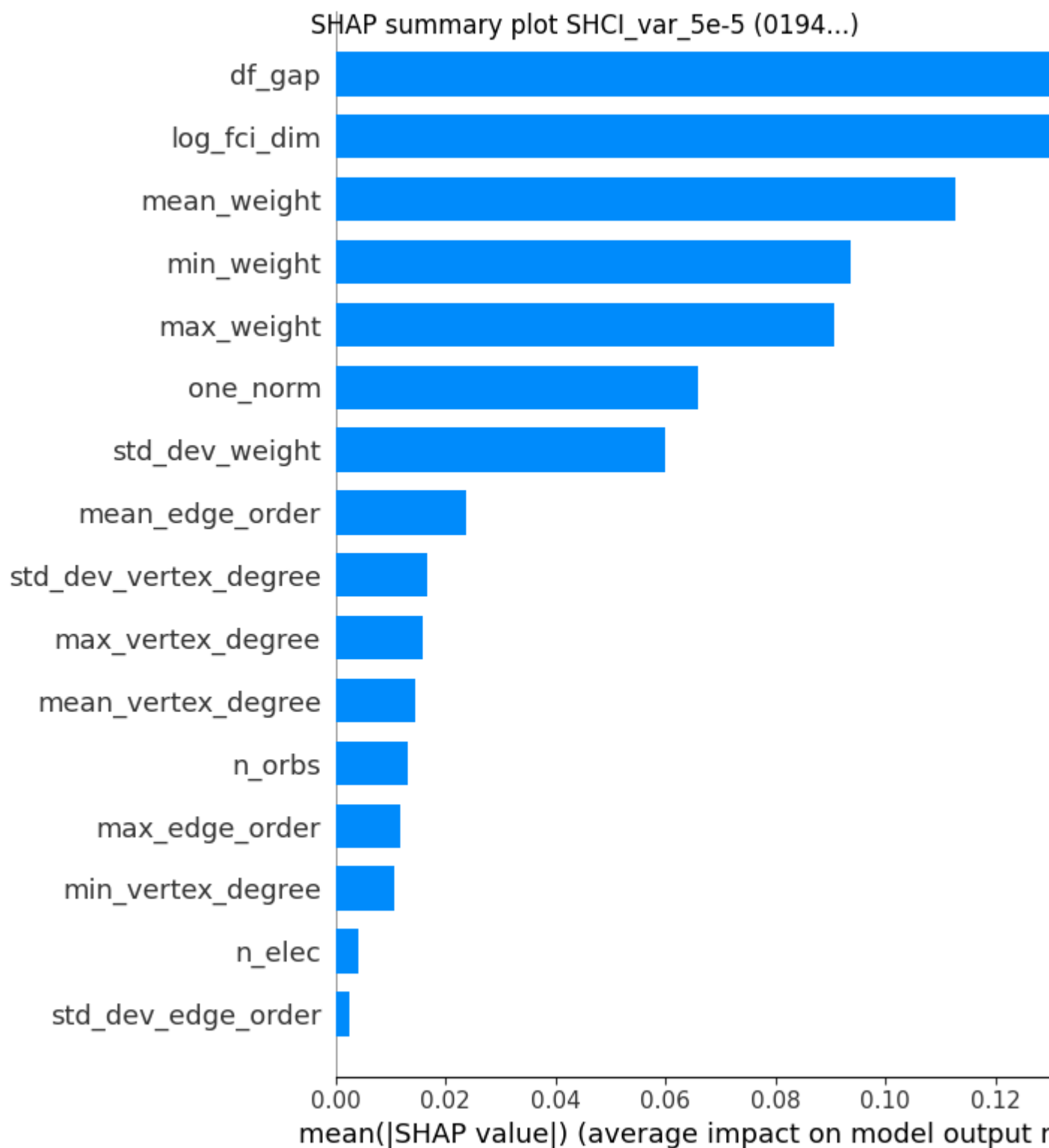
# Utility capture from SHCI\_var\_5e-5/0194...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: a8b4215c-28a2-4c78-ac6d-52a15ee10319

creation\_timestamp: 2025-01-27T16:43:41.107794+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

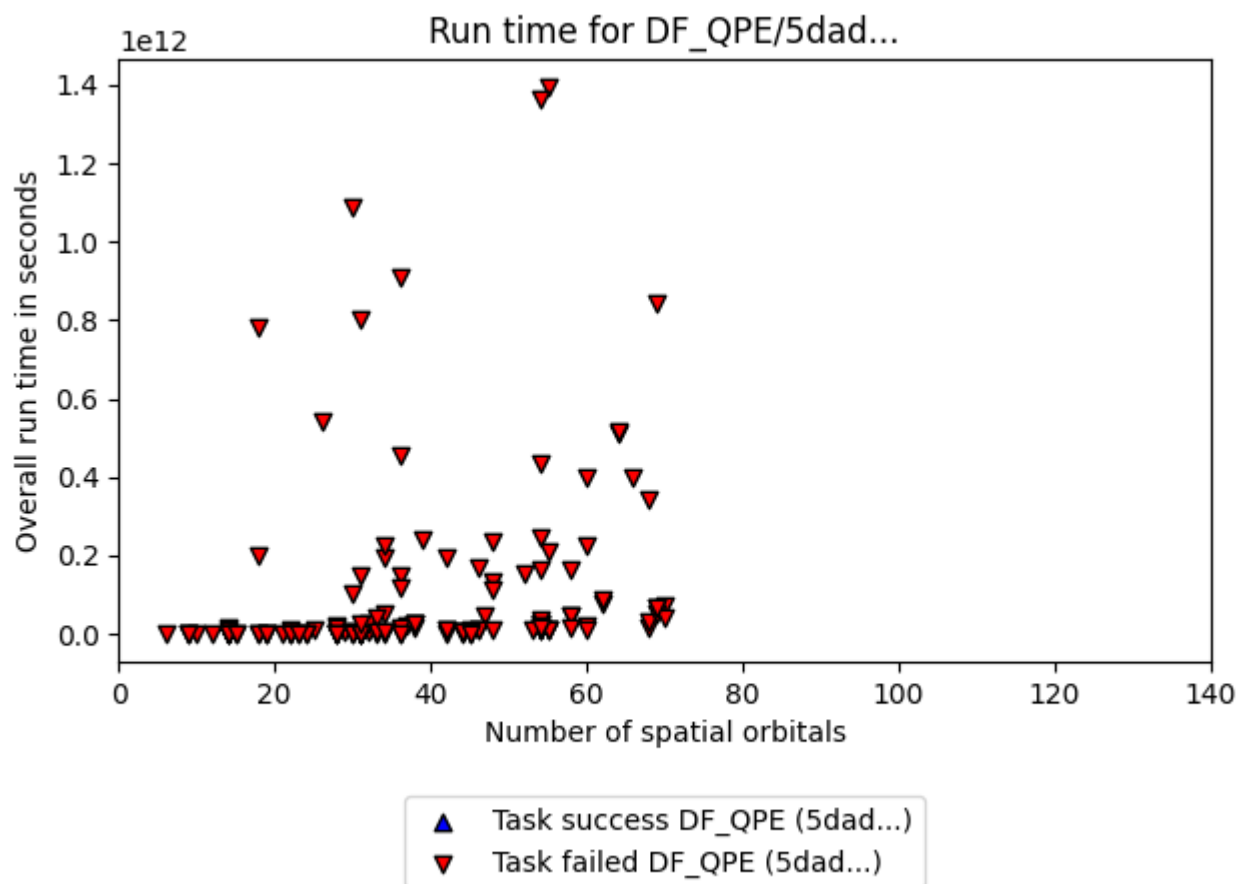
sum\_of\_run\_time\_of\_attempted\_tasks: 15652541022388.93

solvability\_ratio: None

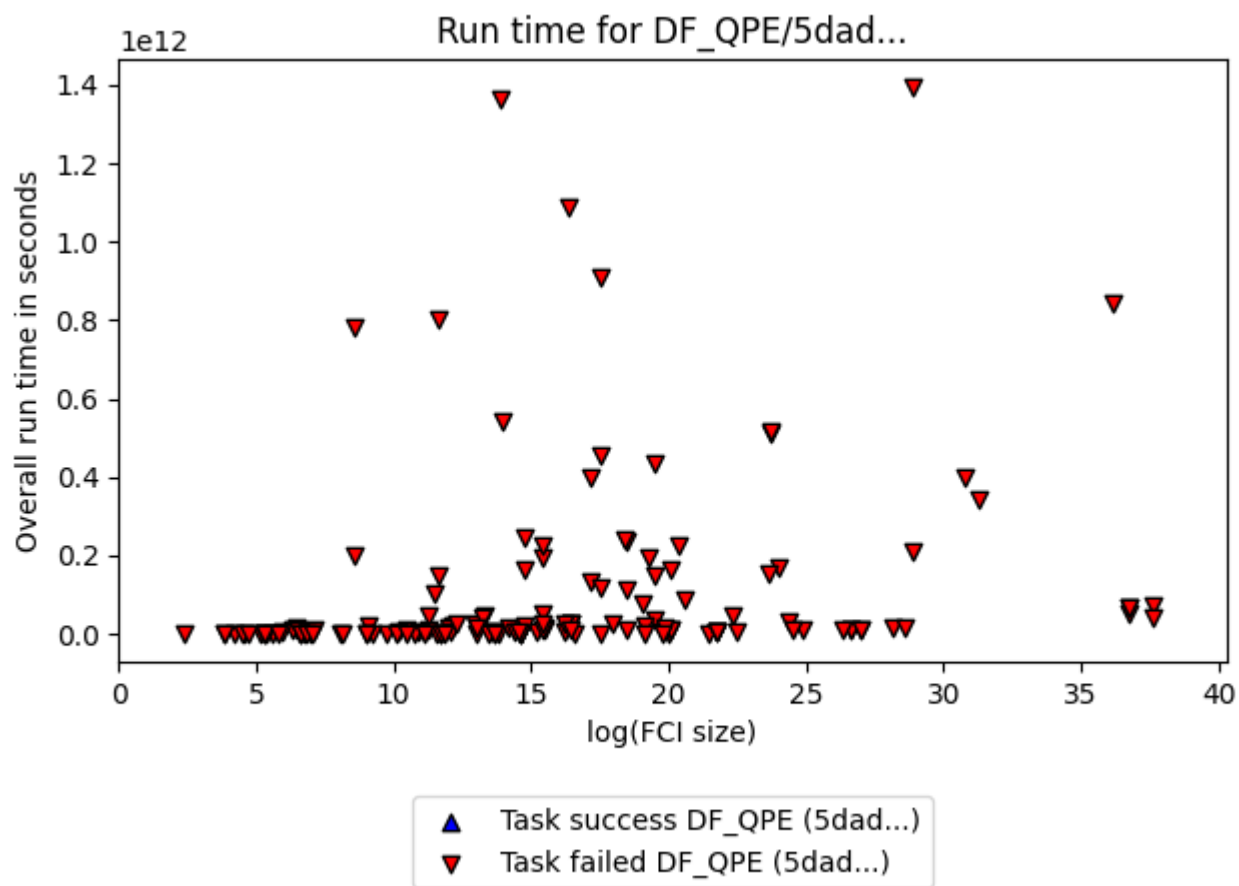
f1\_score: None

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.

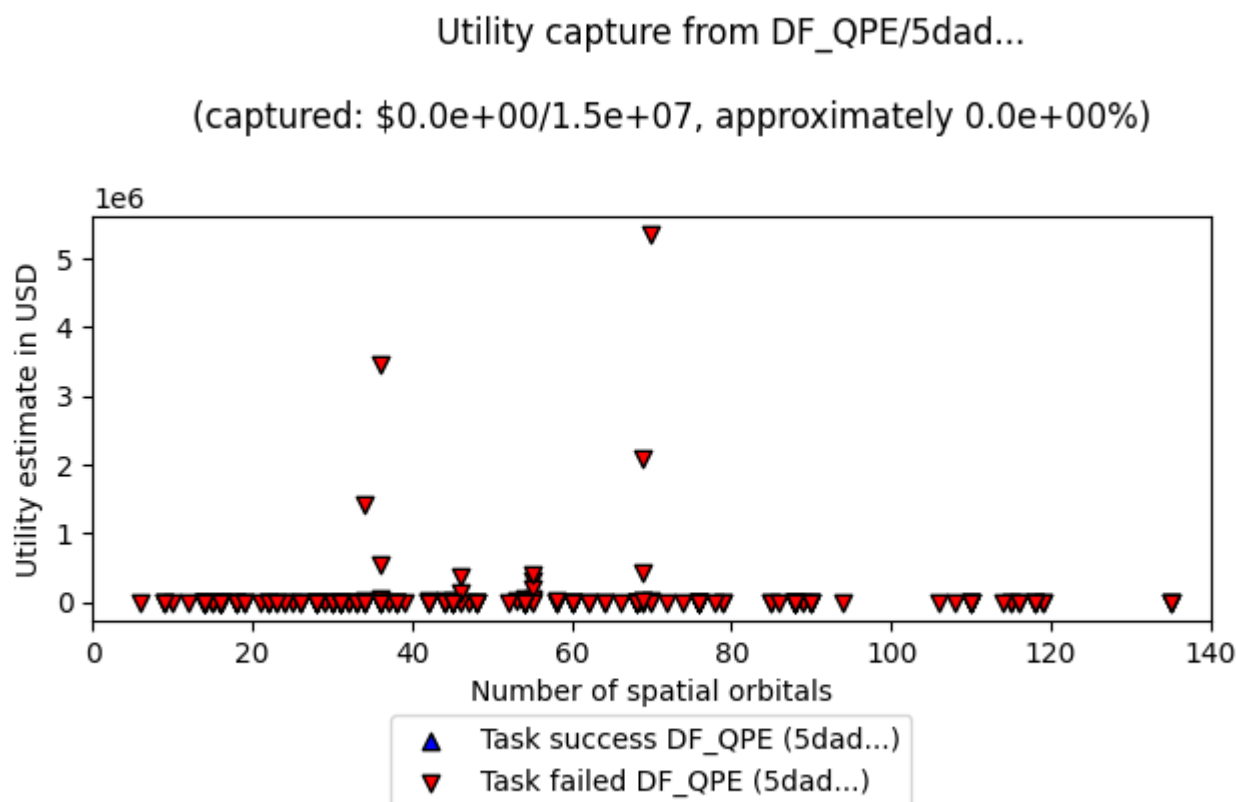


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.





Solver miniML plot

Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)

SHAP summary plot

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

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

solver\_short\_name:CISC

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:CISC

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

performance\_metrics\_uuid: 549cbae1-aff0-4b70-8808-18350977b8bf

creation timestamp: 2025-01-27T16:43:41.107794+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

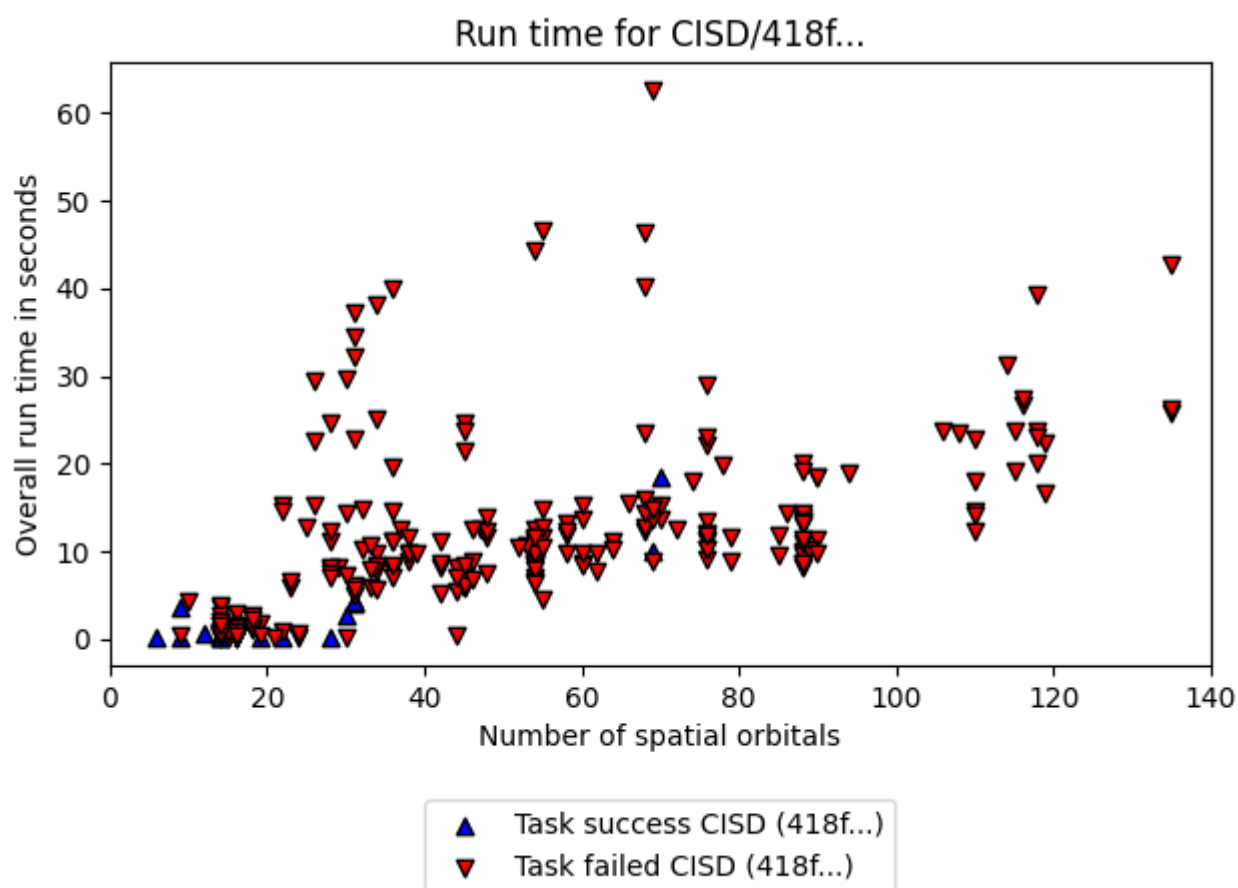
max run time of attempted tasks: 62.58296537399292

sum of run time of attempted tasks: 2929.870177745819

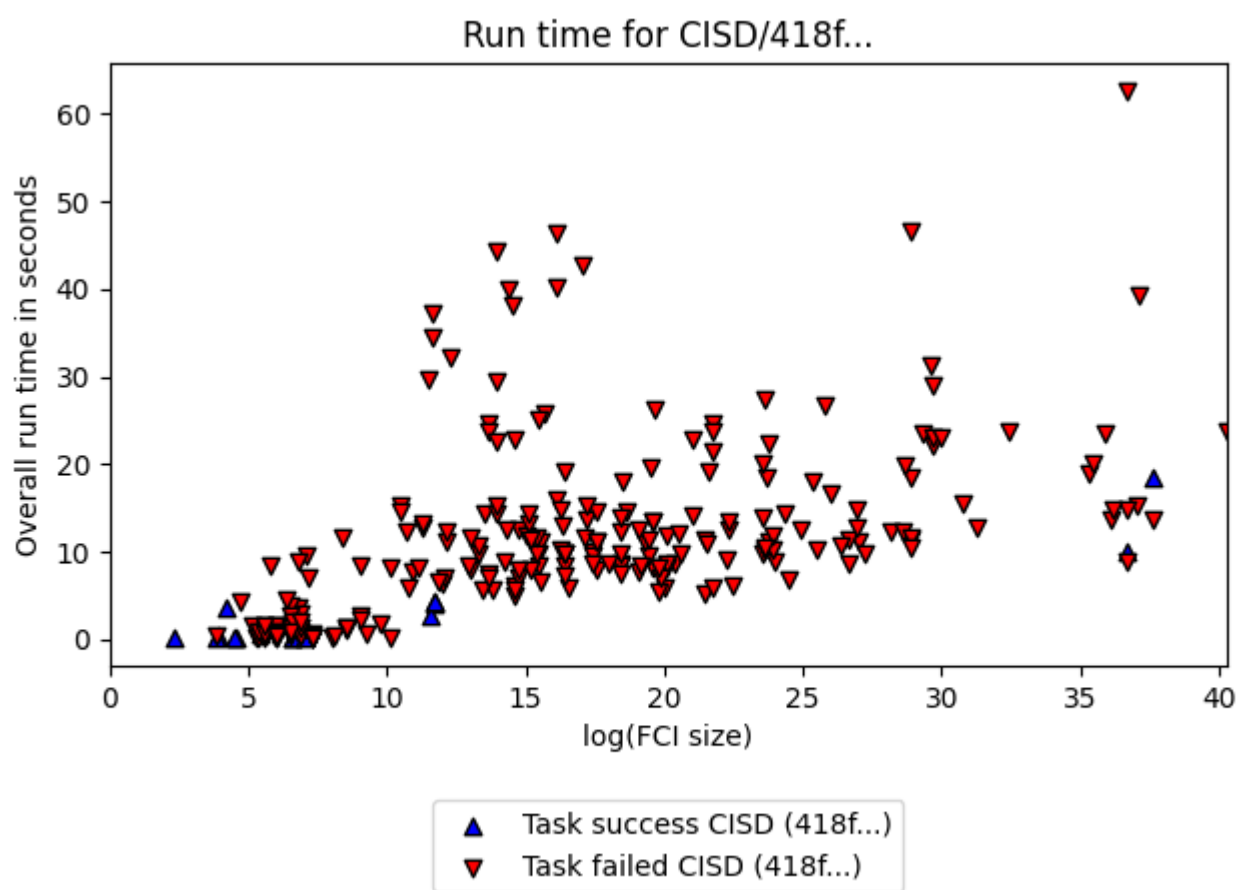
solvability ratio: 0.2773

f1 score: [0.9819494584837545, 0.8717948717948718]

ml metrics calculator version: 1



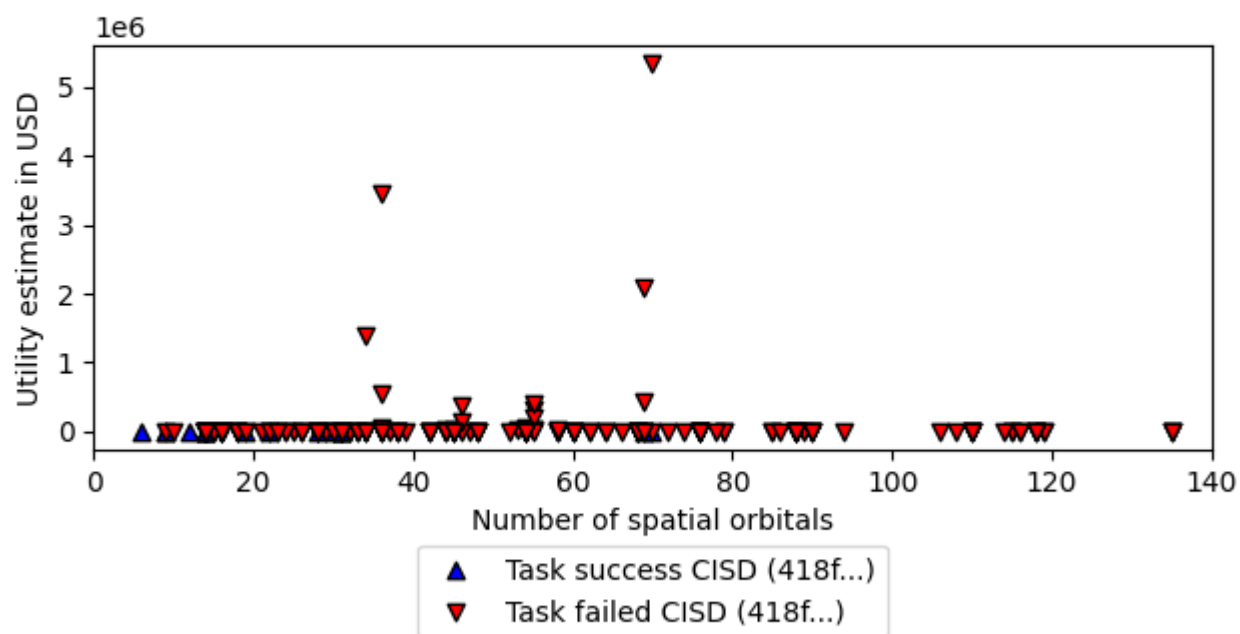
Note: plot only contains attempted tasks.

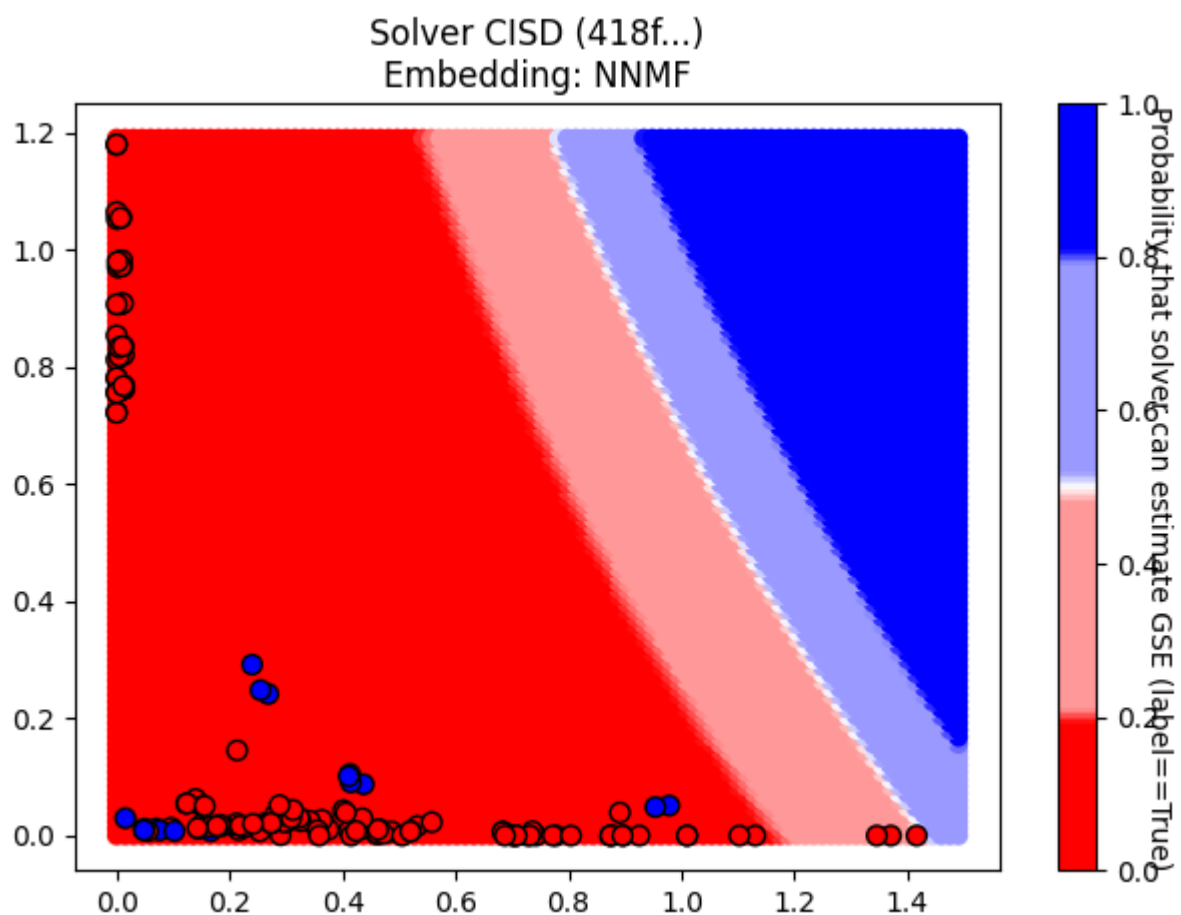


Note: plot only contains attempted tasks.

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

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: 9f1096ab-5993-4b40-9f98-ed62038d63e

creation\_timestamp: 2025-01-27T16:43:41.107794+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

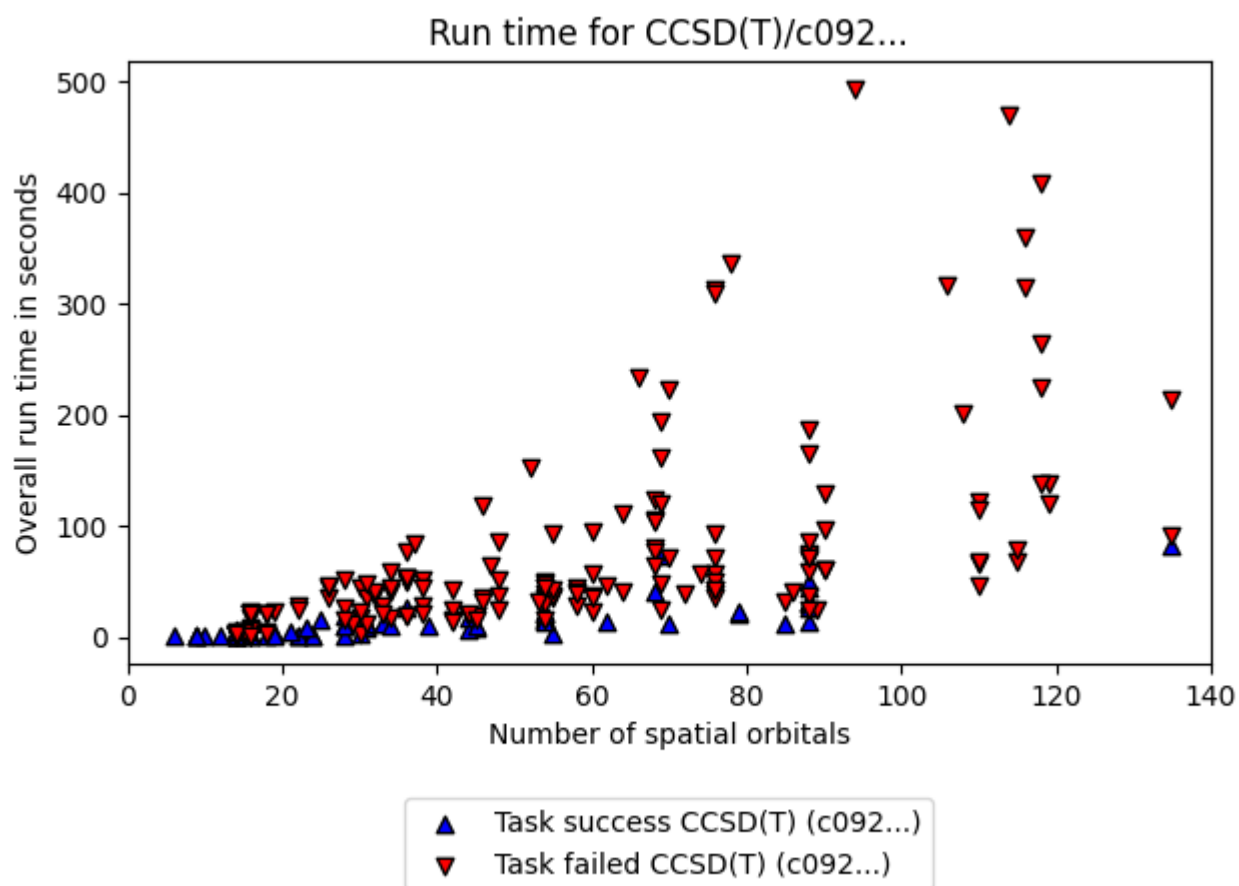
max\_run\_time\_of\_attempted\_tasks: 493.4080808162689

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

solvability\_ratio: 0.8567

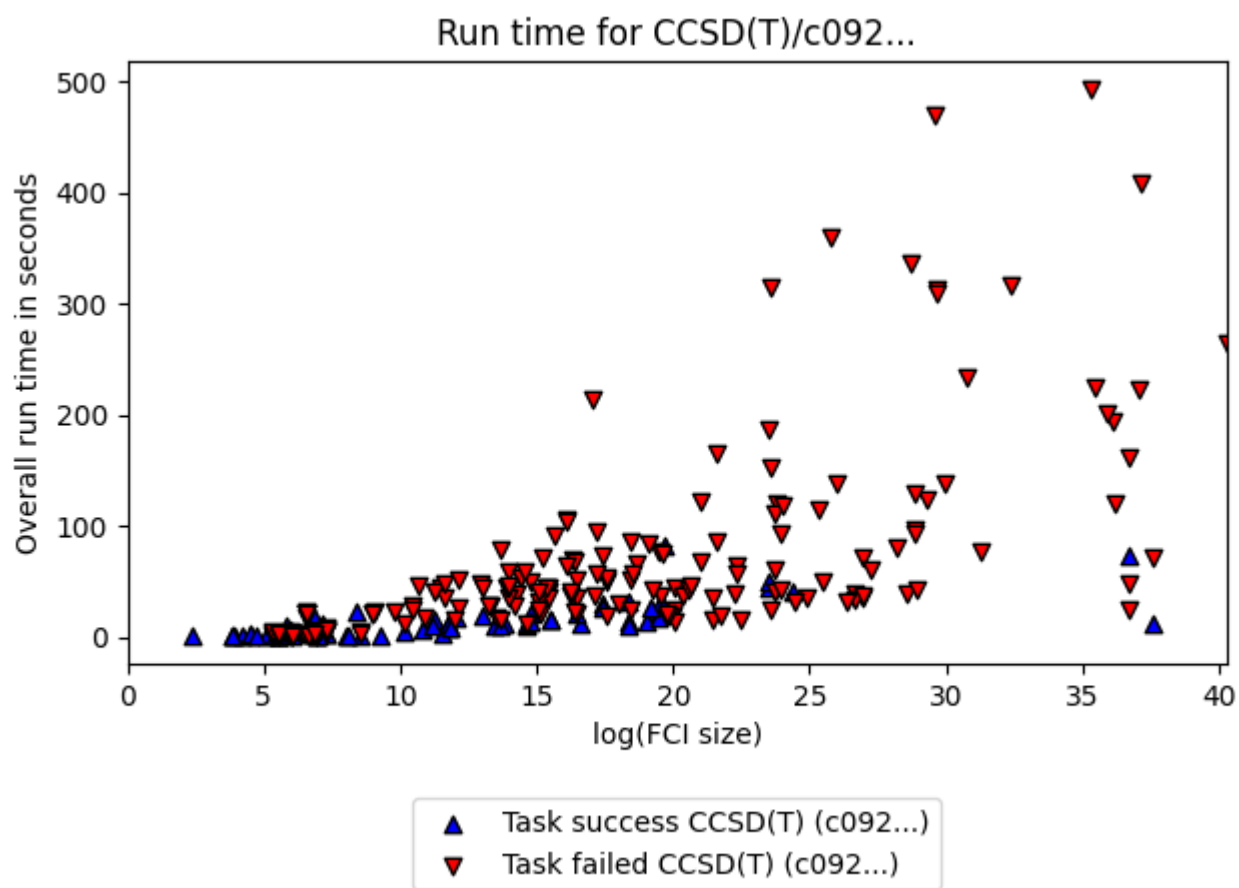
f1\_score: [0.8795180722891566, 0.8666666666666667]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

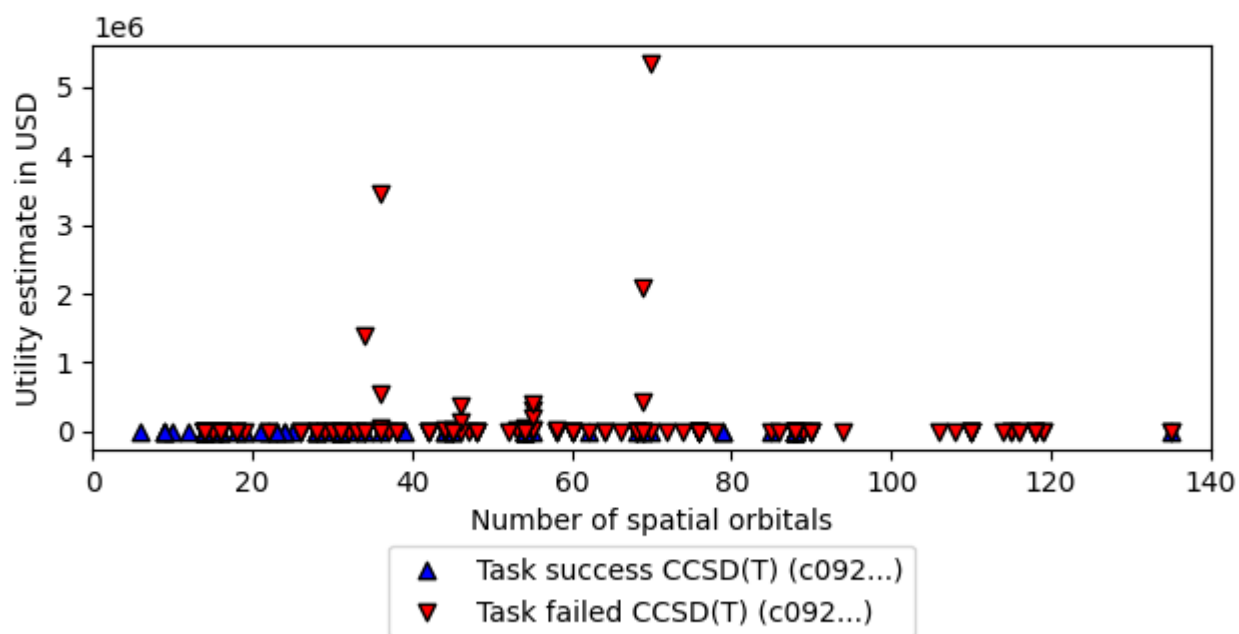


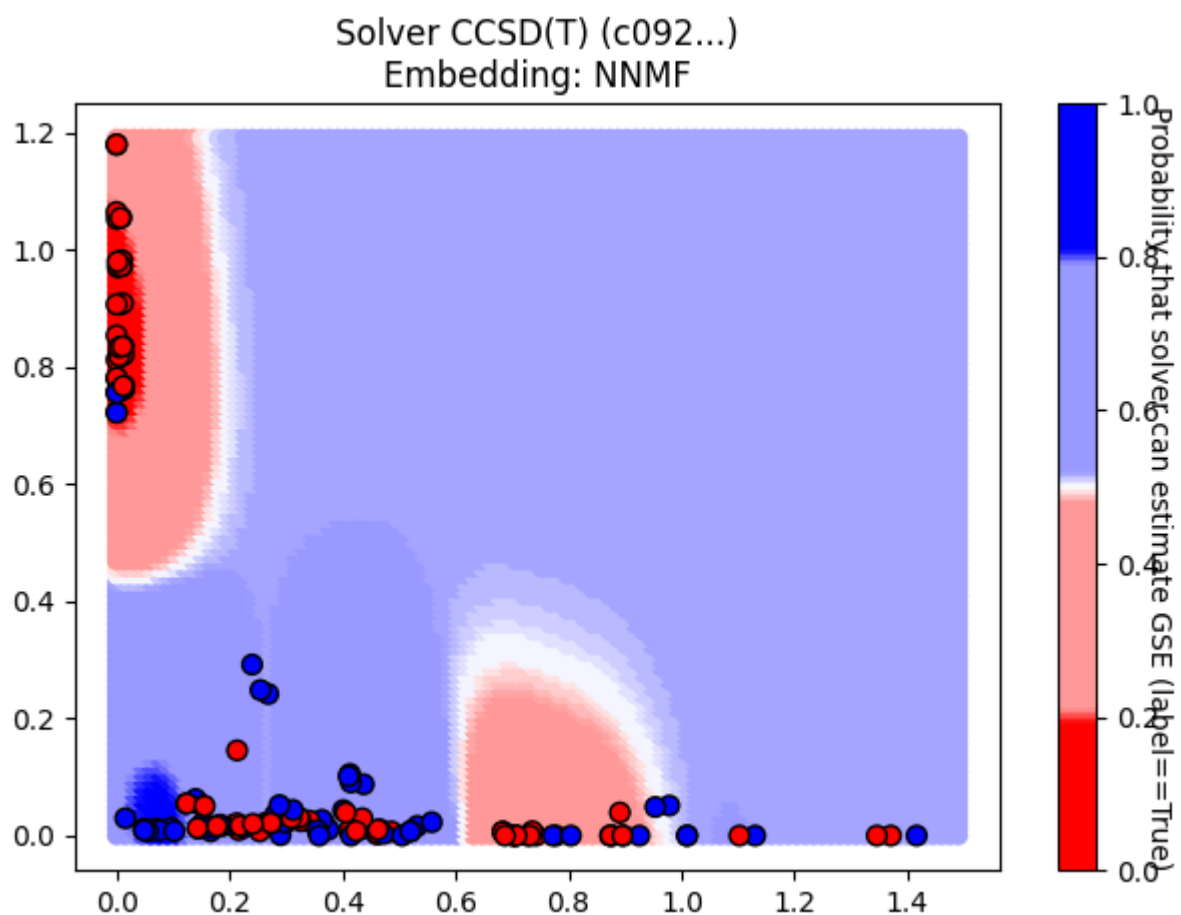


Note: plot only contains attempted tasks.

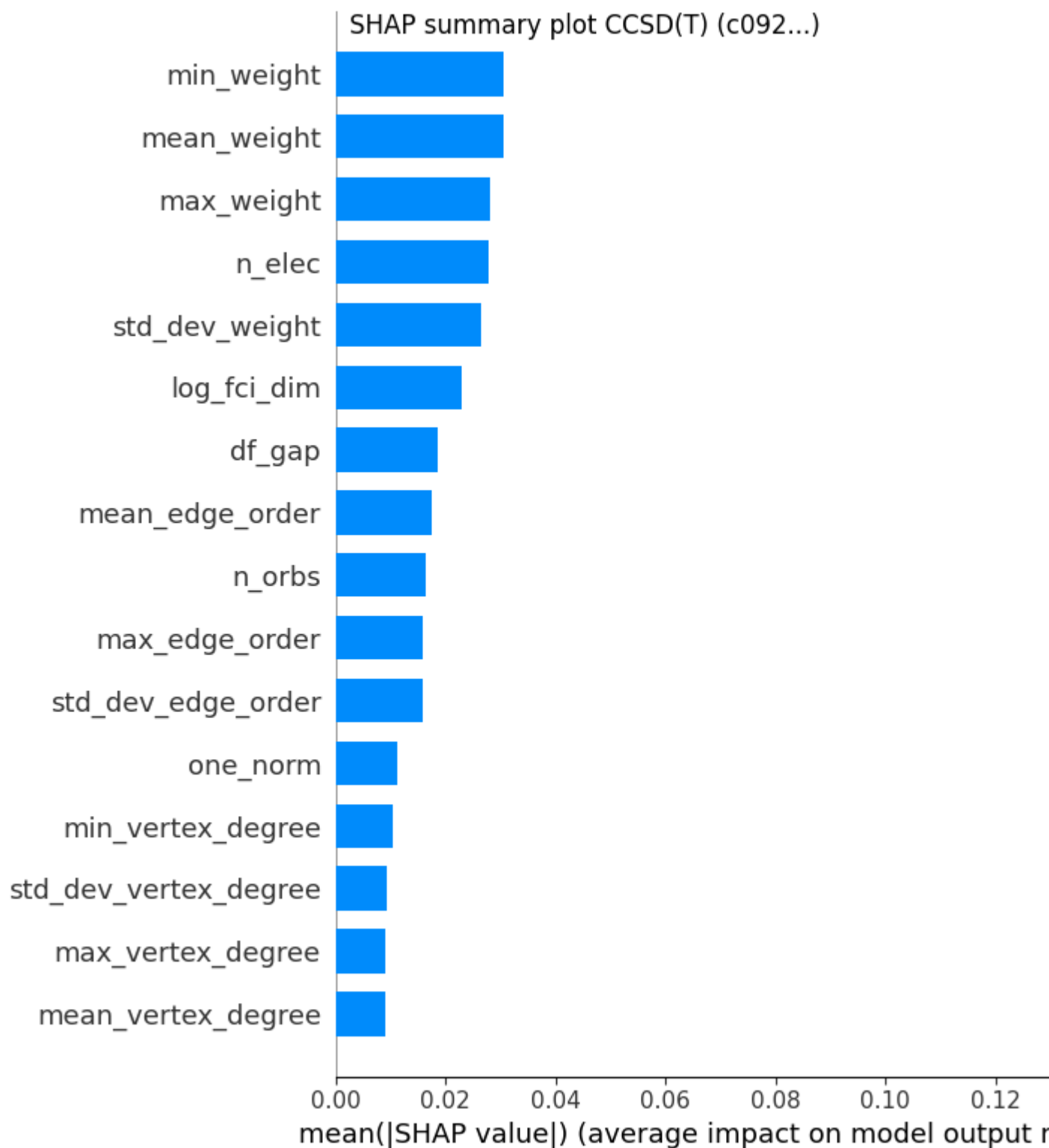
### Utility capture from CCSD(T)/c092...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: db60d1bb-2e53-4f87-985b-92edc7a2626c

creation\_timestamp: 2025-01-27T16:43:41.107794+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

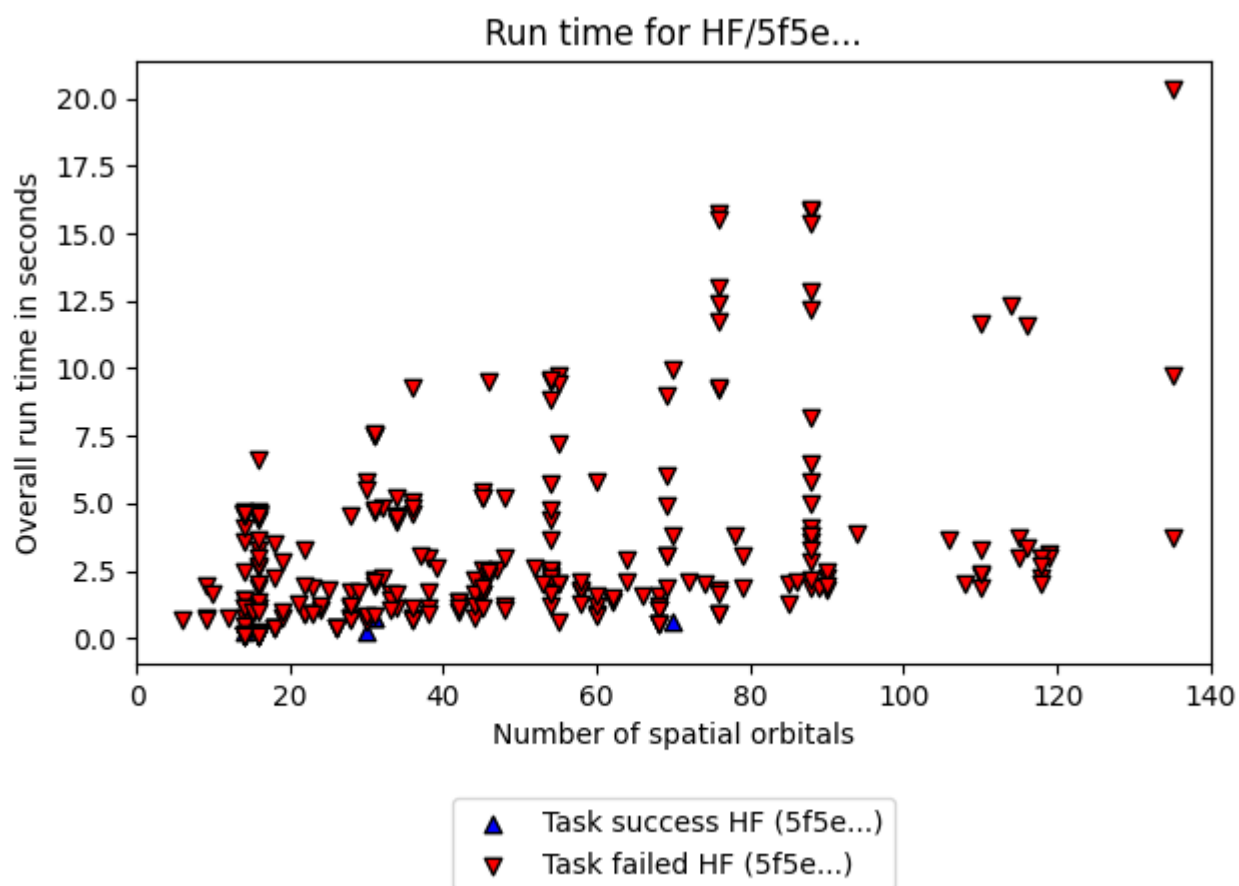
max\_run\_time\_of\_attempted\_tasks: 20.338801622390747

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

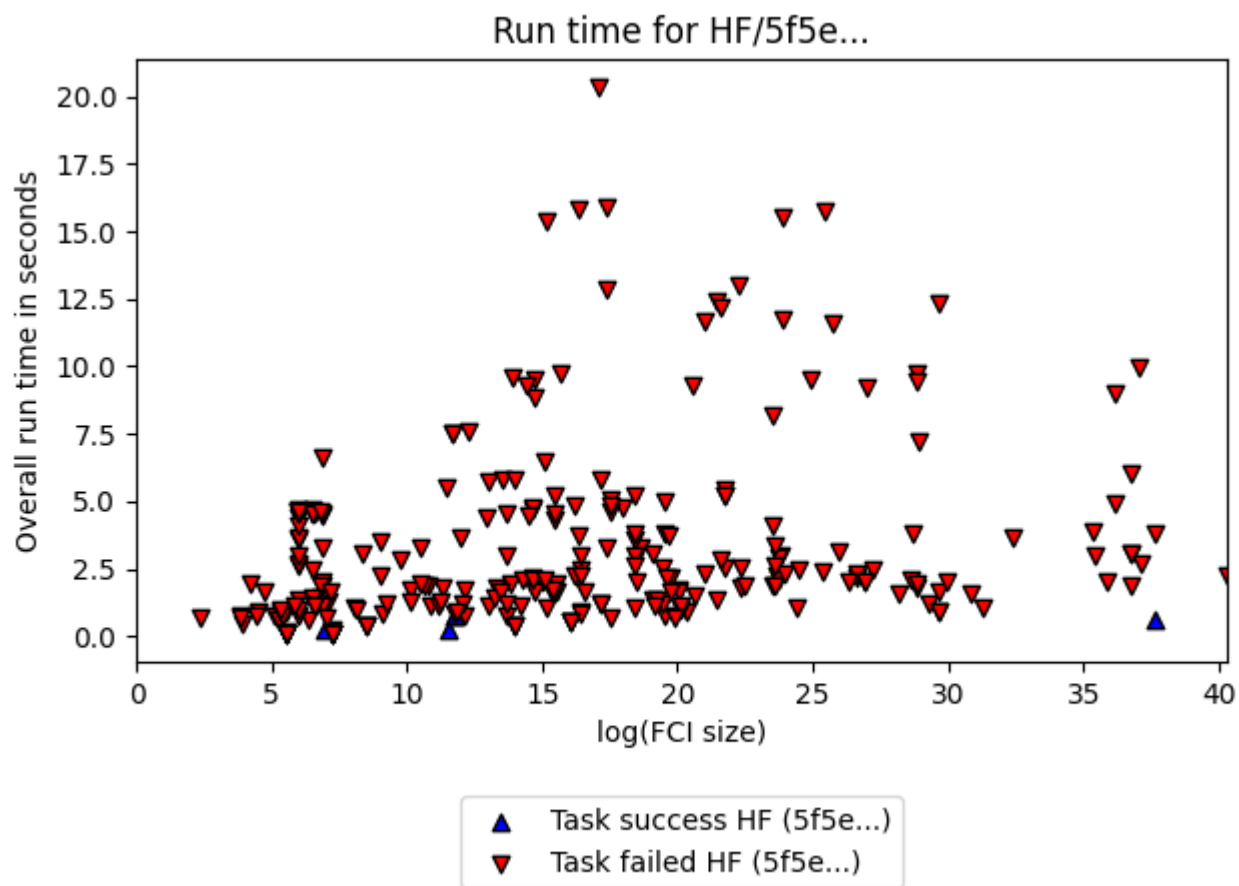
solvability\_ratio: 0.0

f1\_score: [0.9867549668874173, 0.7142857142857143]

ml\_metrics\_calculator\_version: 1



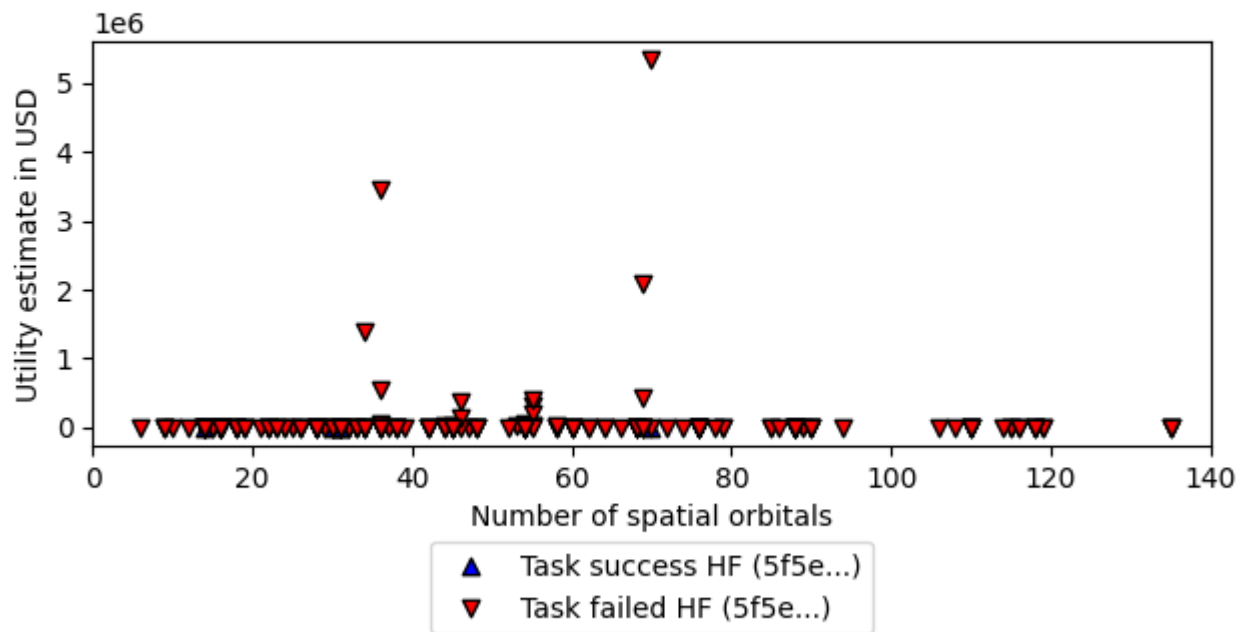
Note: plot only contains attempted tasks.



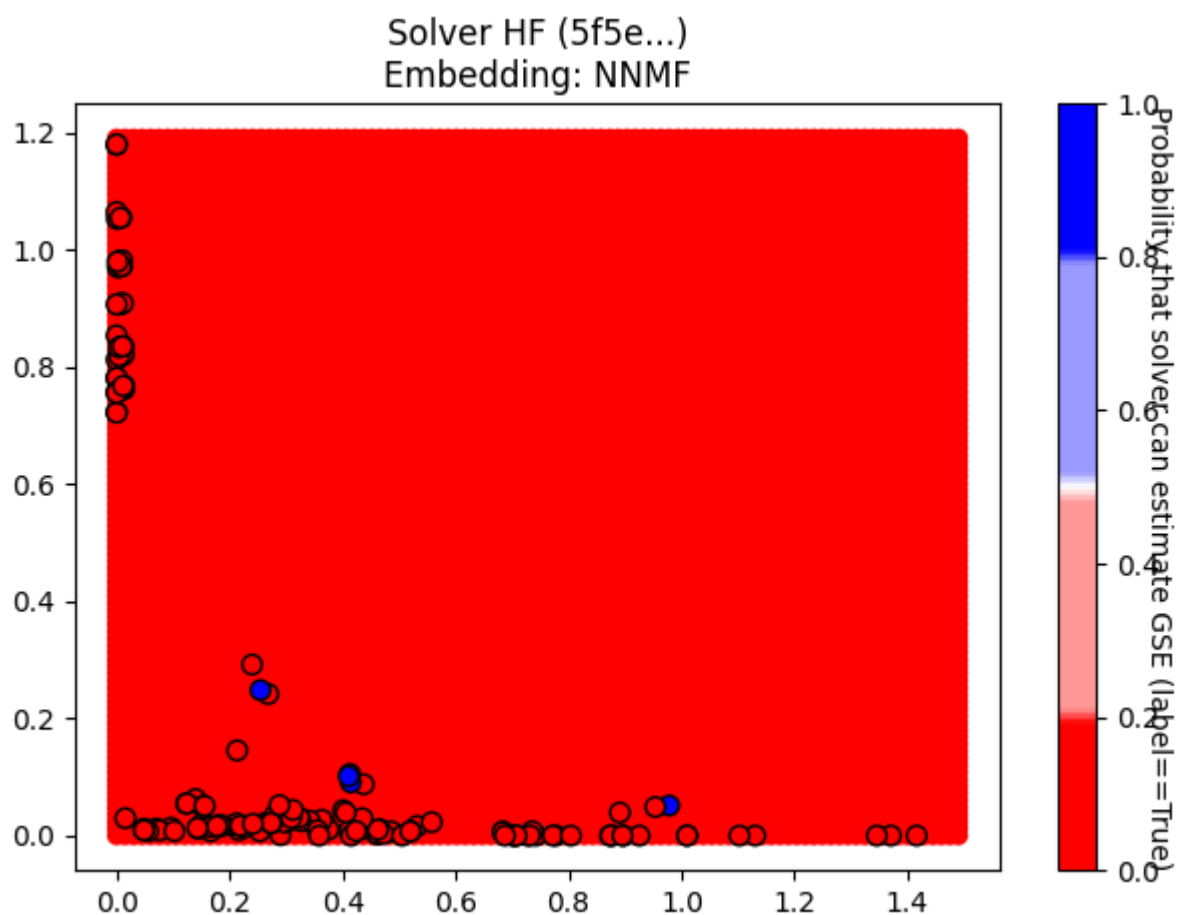
Note: plot only contains attempted tasks.

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

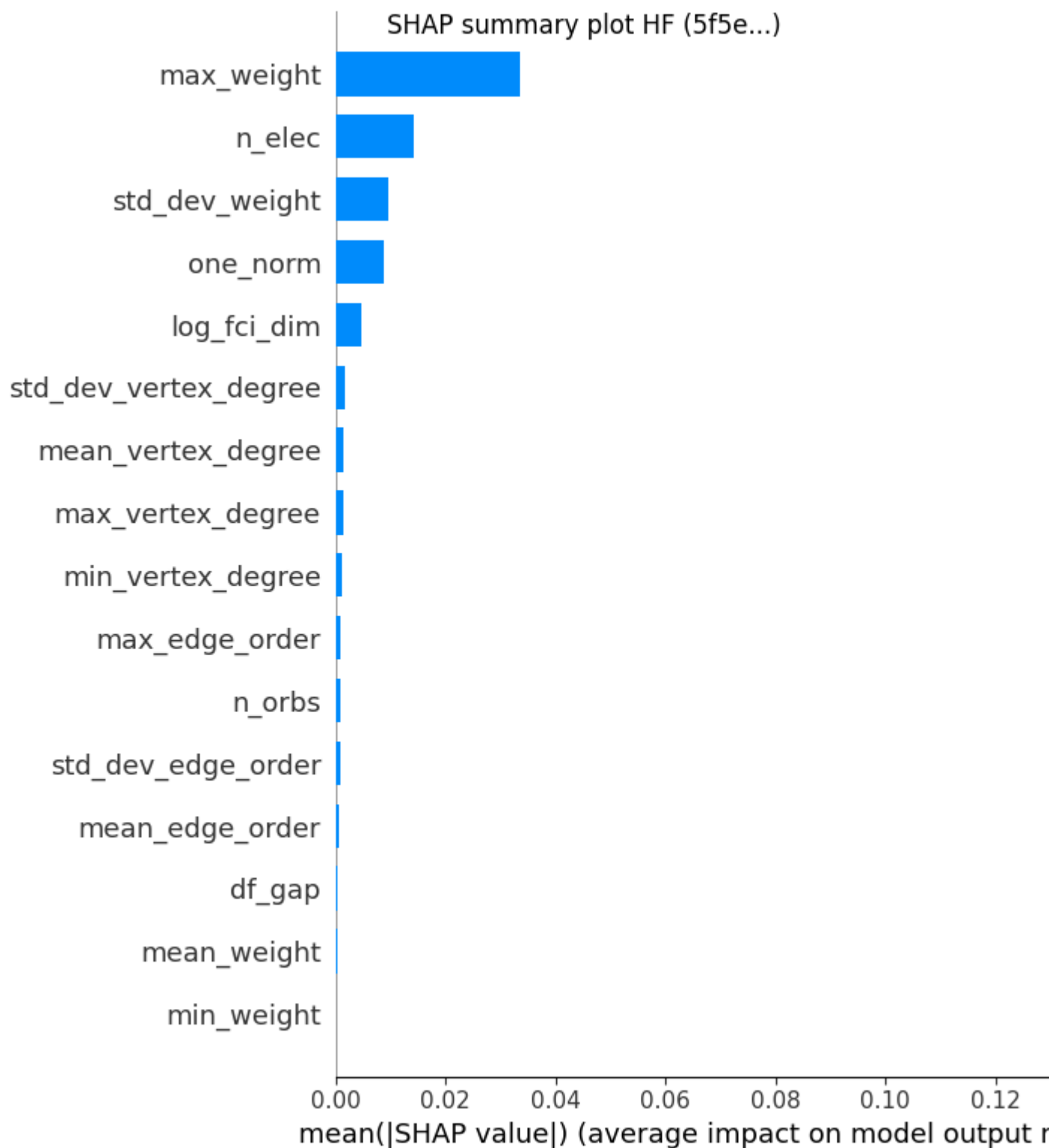
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)







Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: 4f63aecd-749b-42f3-9038-55bb58c83b82

creation\_timestamp: 2025-01-27T16:43:41.107794+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

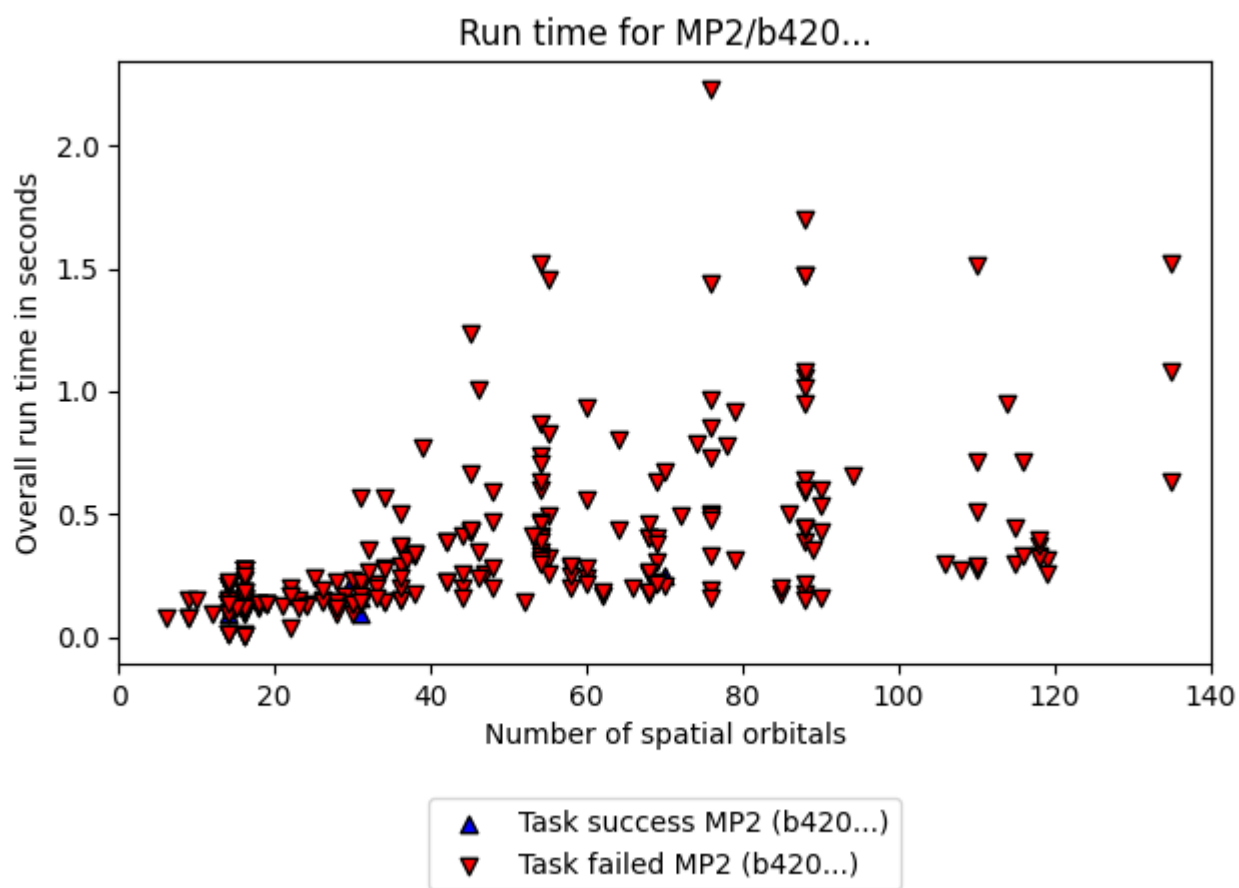
max\_run\_time\_of\_attempted\_tasks: 2.230440139770508

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

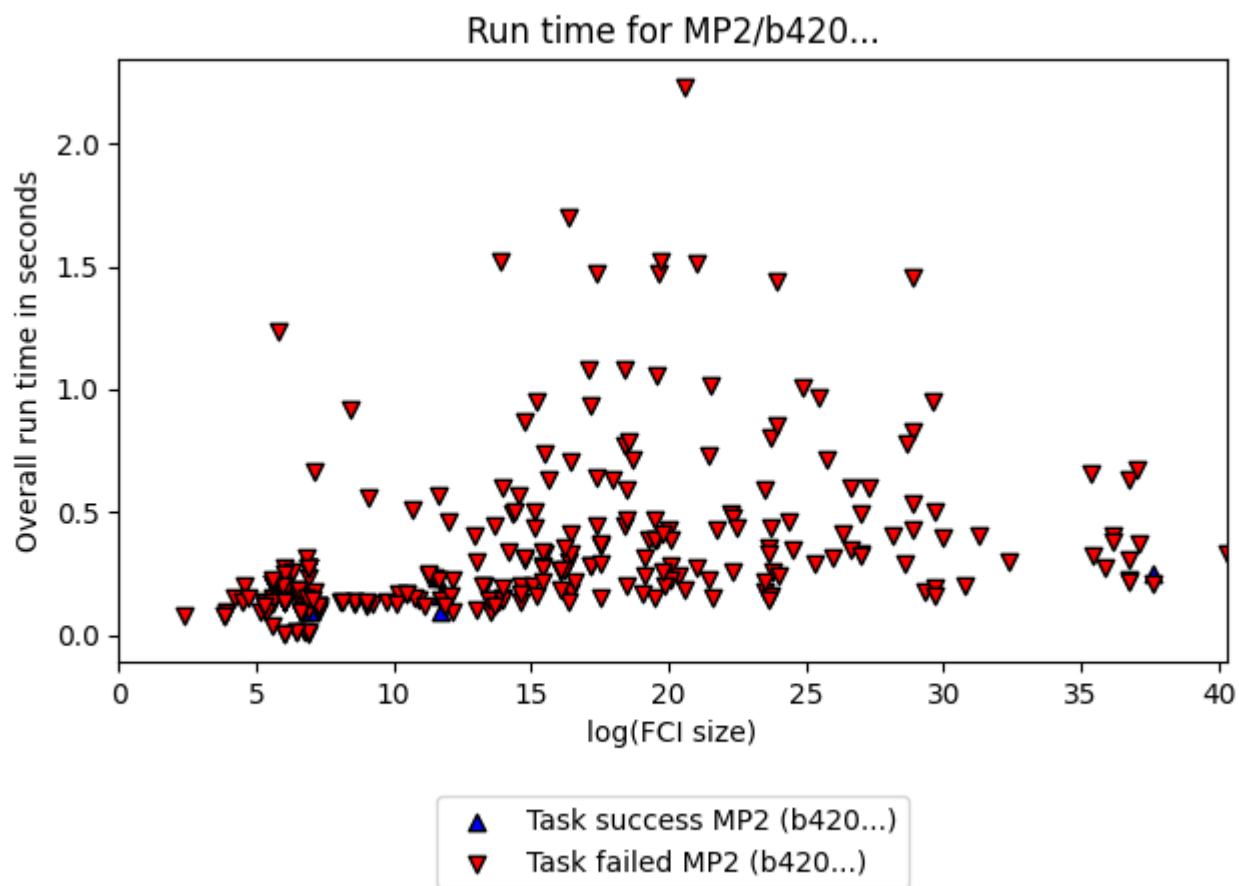
solvability\_ratio: 0.0

f1\_score: [0.9867549668874173, 0.7142857142857143]

ml\_metrics\_calculator\_version: 1



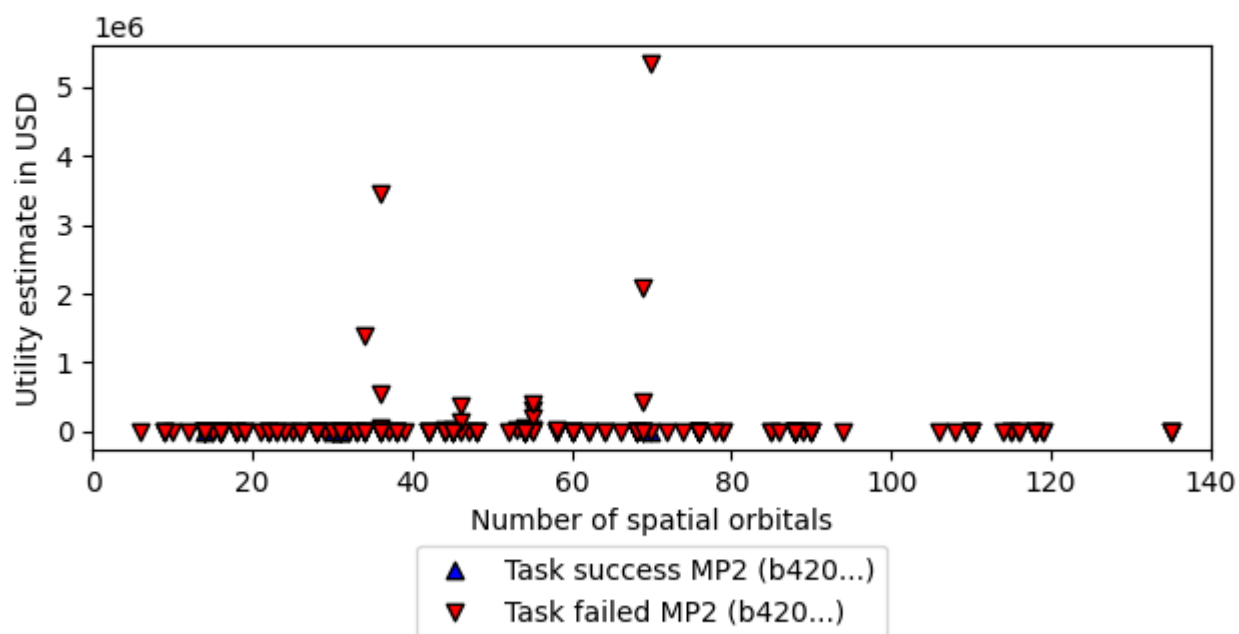
Note: plot only contains attempted tasks.

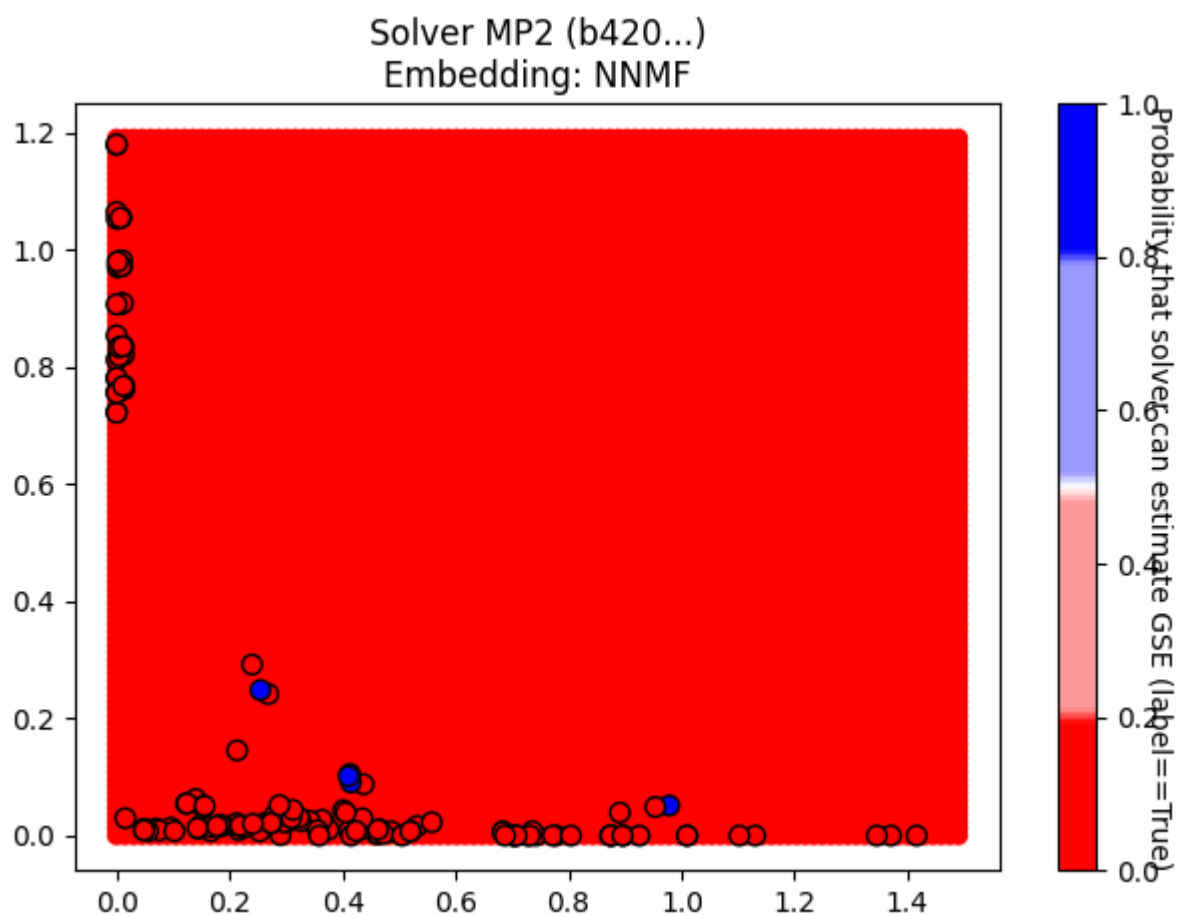


Note: plot only contains attempted tasks.

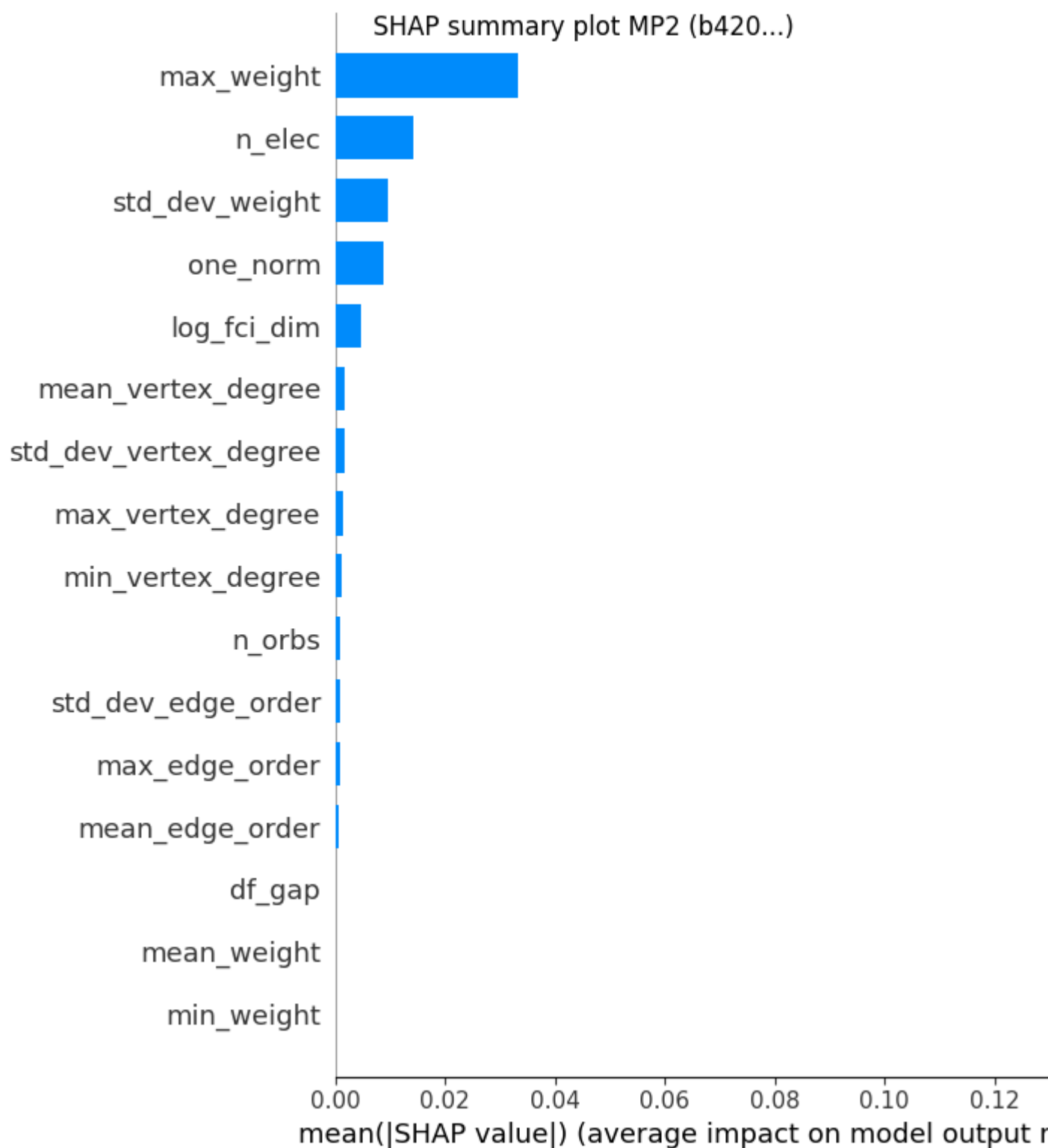
### Utility capture from MP2/b420...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: a835435f-cb20-4071-86e8-99a3f456c997

creation\_timestamp: 2025-01-27T16:43:41.107794+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

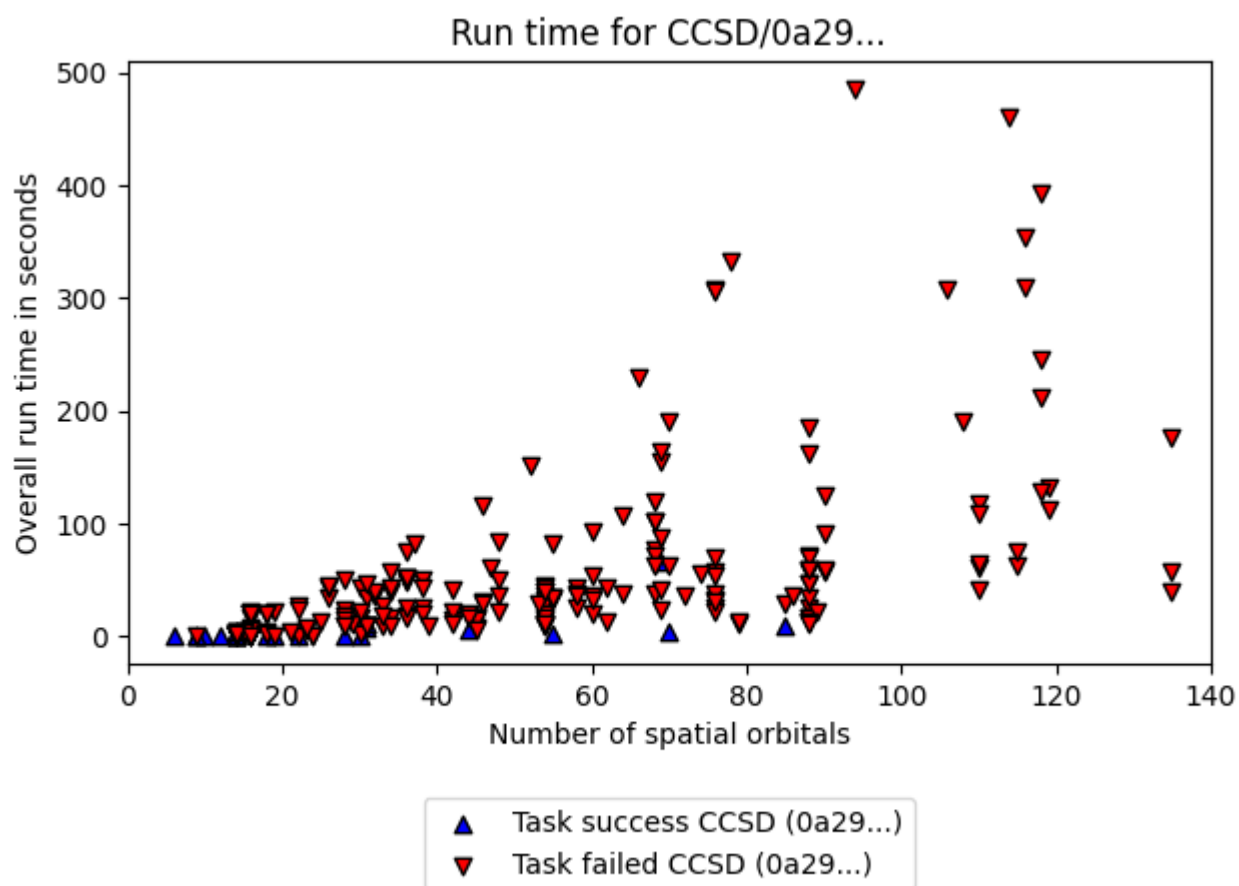
max\_run\_time\_of\_attempted\_tasks: 485.1982181072235

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

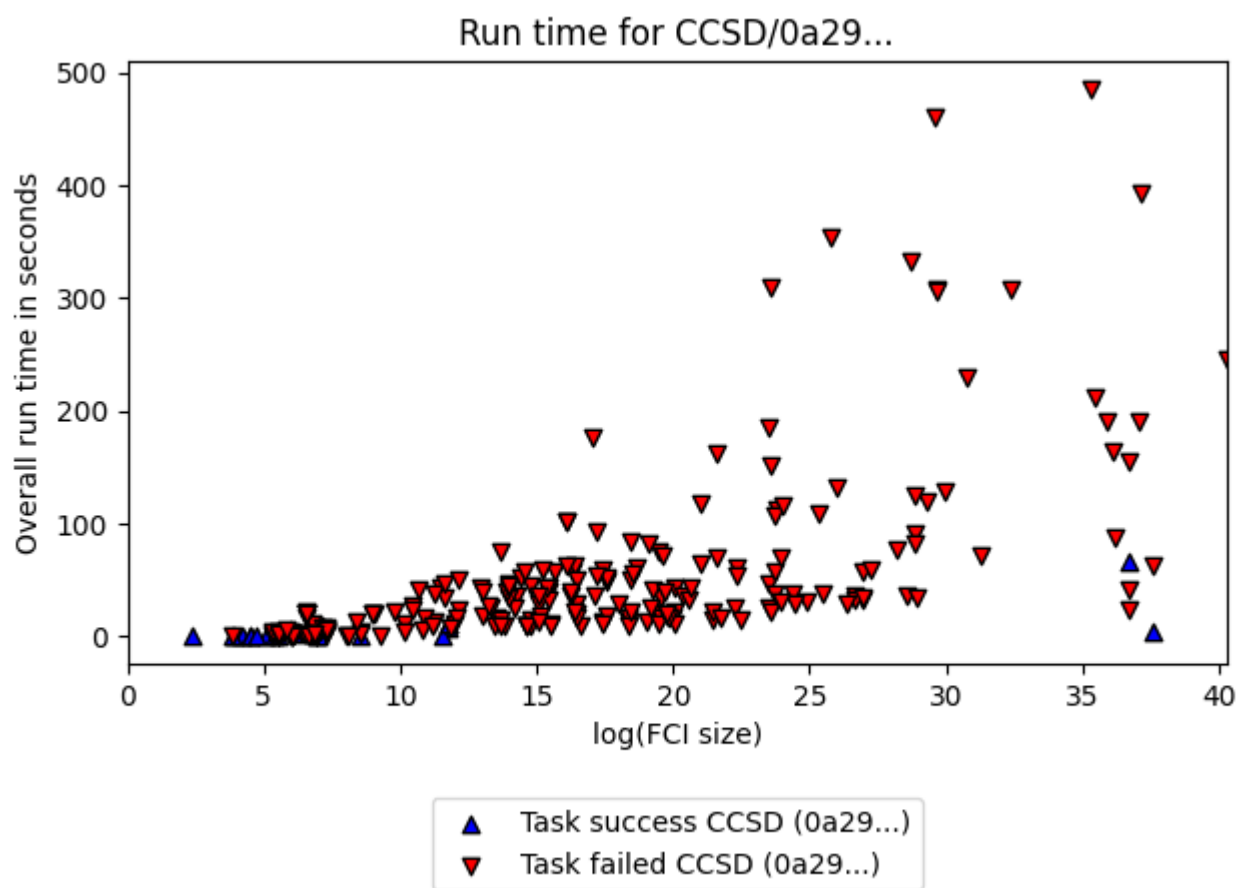
solvability\_ratio: 0.0154

f1\_score: [0.9777777777777777, 0.8695652173913043]

ml\_metrics\_calculator\_version: 1



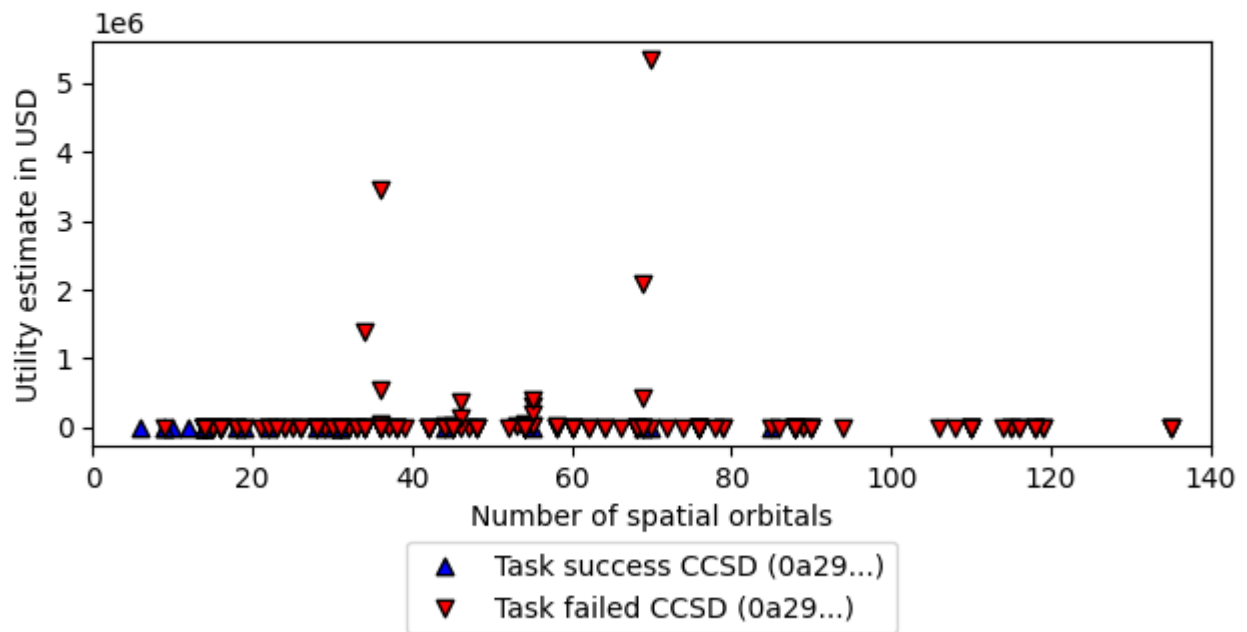
Note: plot only contains attempted tasks.

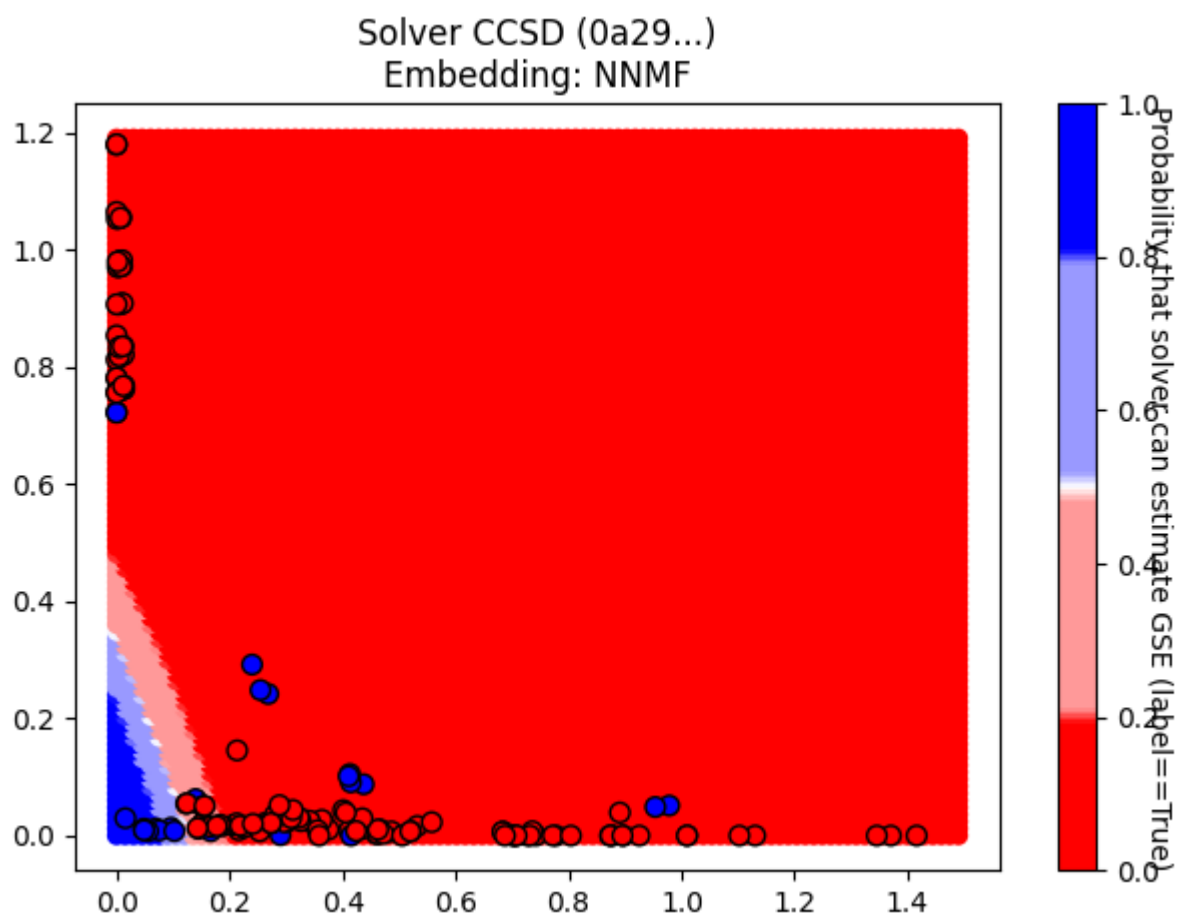


Note: plot only contains attempted tasks.

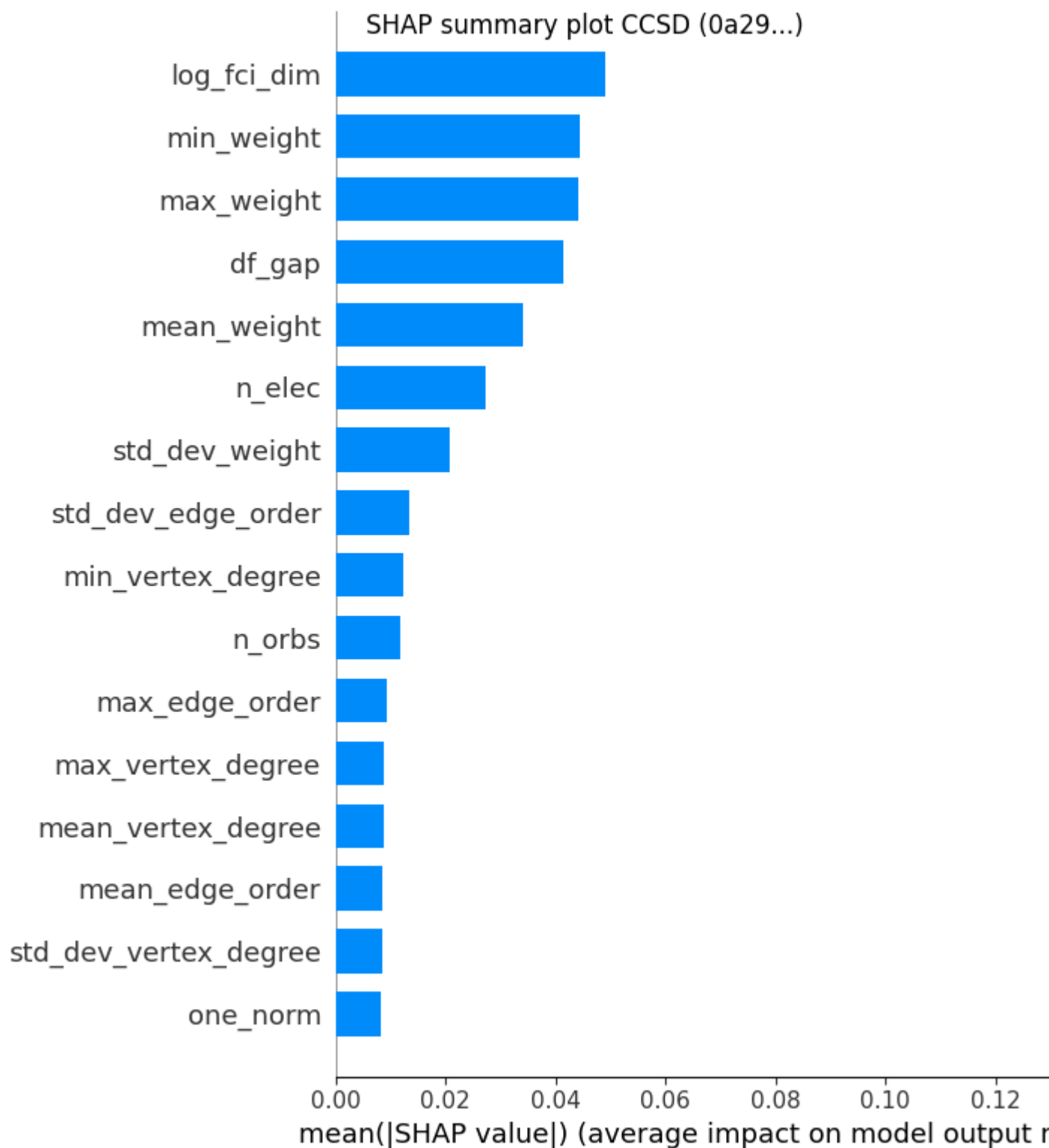
# Utility capture from CCSD/0a29...

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





Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



**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: cb5e8e7c-fe2c-4b83-84b1-b49f3c752896

creation\_timestamp: 2025-01-27T16:43:41.107794+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

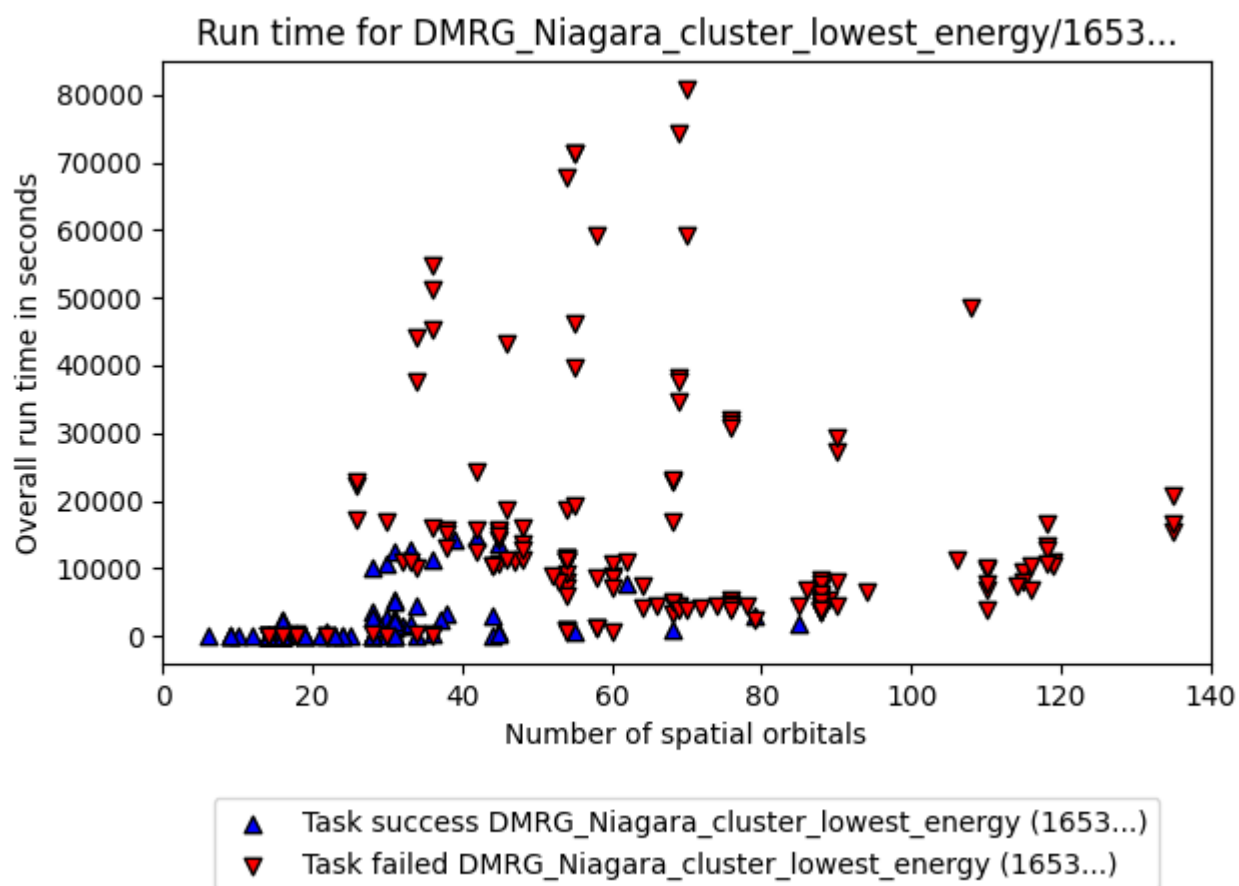
max\_run\_time\_of\_attempted\_tasks: 80820.729907066

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

solvability\_ratio: 0.3405

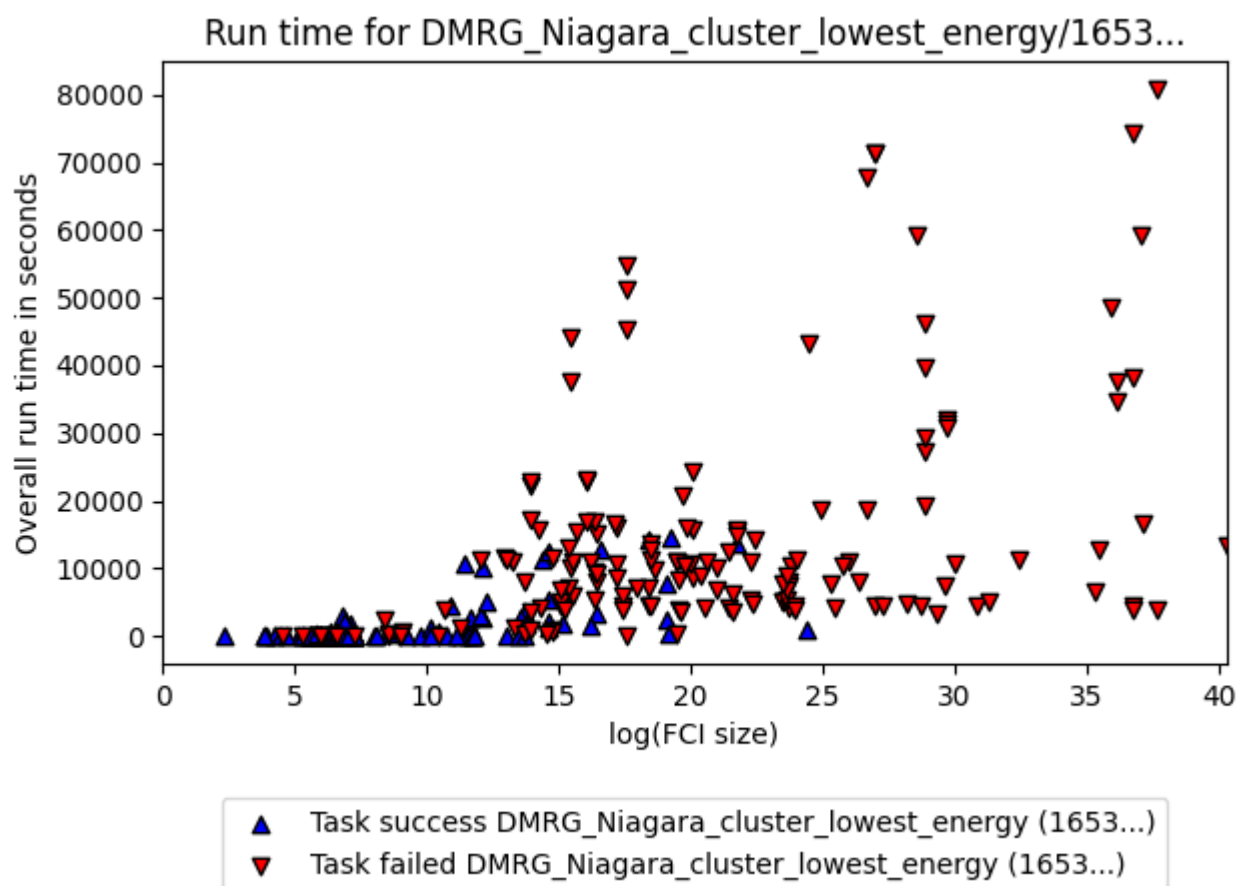
f1\_score: [0.9662921348314607, 0.986784140969163]

ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

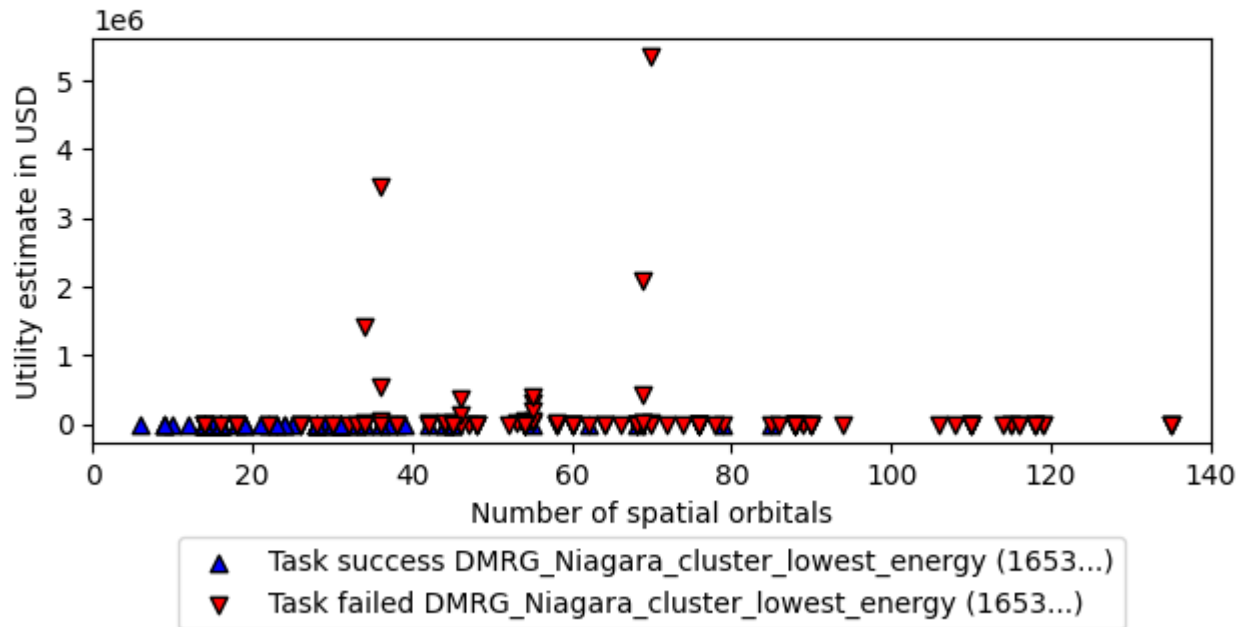


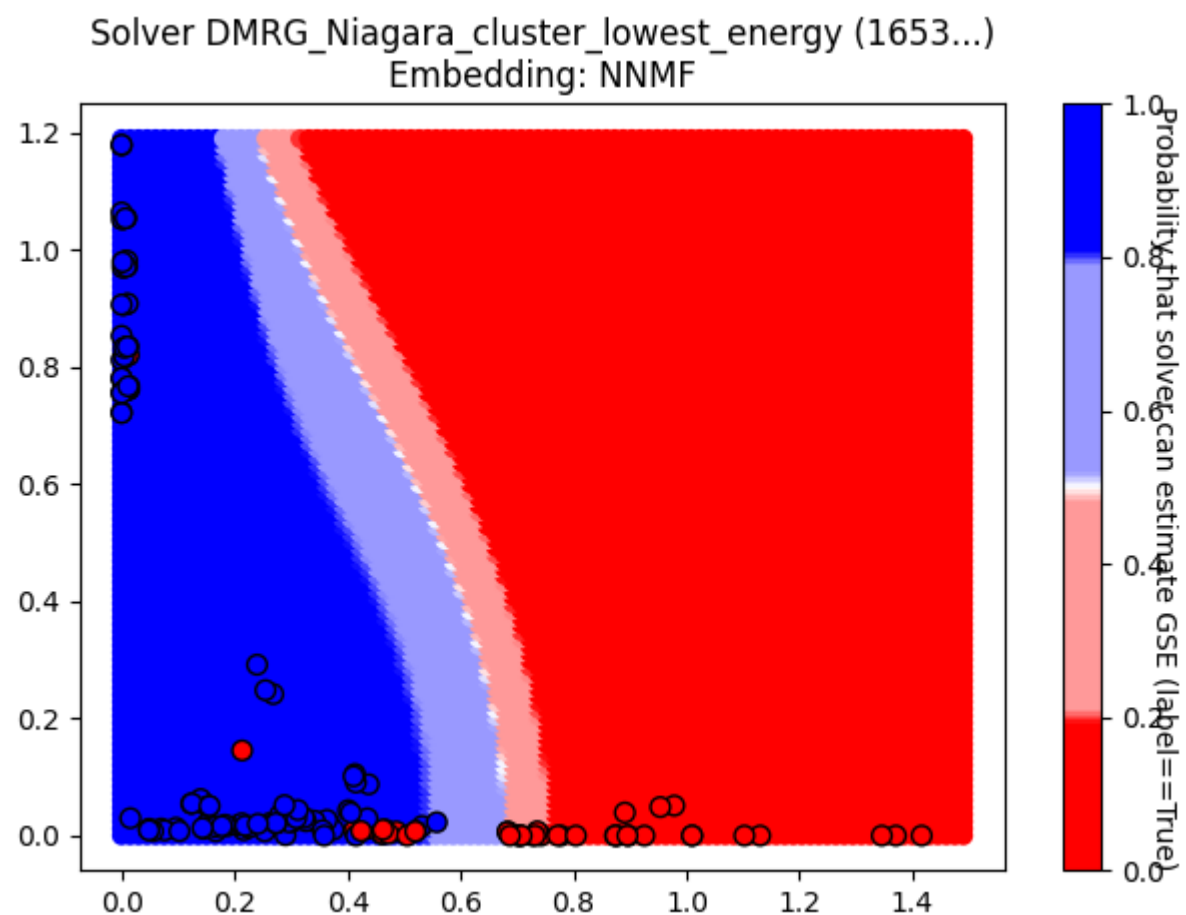


Note: plot only contains attempted tasks.

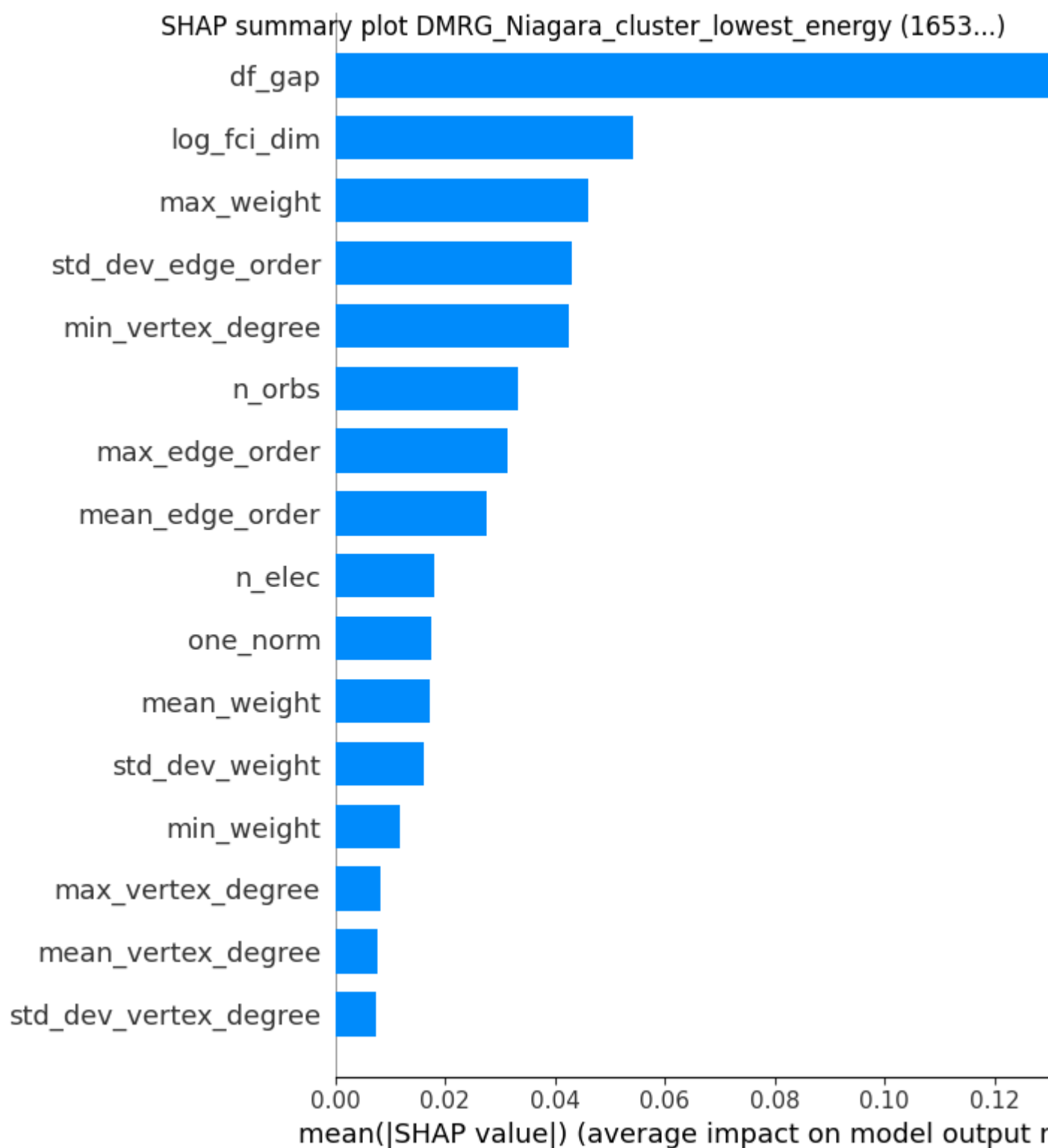
Utility capture from DMRG\_Niagara\_cluster\_lowest\_energy/1653..

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

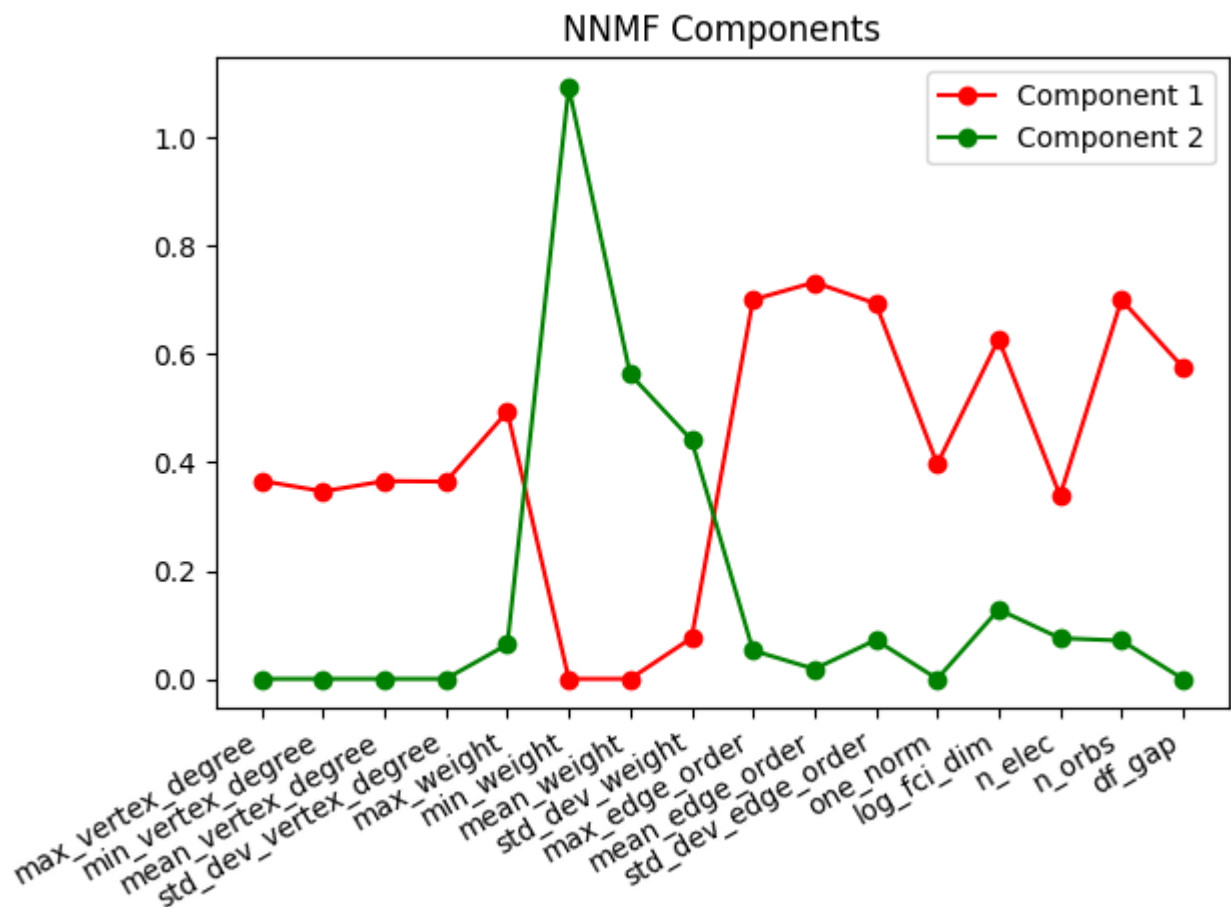




Note: ML surface plot is based on Hamiltonians where a reference\_energy was provided. (attempted may be True or False.)



# 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: [0.36604788 0.3465517 0.3656555 0.36466294 0.49391307  
0. 0. 0.07560829 0.70083452 0.73297542 0.69367903 0.39707278  
0.62804024 0.33874397 0.7006798 0.57585866]

Component 2: [0. 0. 0. 0. 0.06352889 1.09340886 0.56300493 0.44159773  
0.05242832 0.01821226 0.07191467 0. 0.12812831 0.07525071 0.07071245  
0. ]