

# GSEE Benchmark Standard Report

Report based on data from 2025-03-12T17:03:13.578128+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Mon Mar 10 07:44:57 2025

Input data: GSEE-  
`HC_utility_estimates_all_instances_task_uuids_v2.csv`, last modified  
Mon Jan 27 08:10:10 2025

Latest creation time for a `problem_instance.json` file: Mon Mar 10 07:44:57 2025

Latest creation time for a `solution.json` file: Wed Mar 12 11:27:42 2025

## Problem Instance Summary Statistics

number of `problem_instances`: 68.

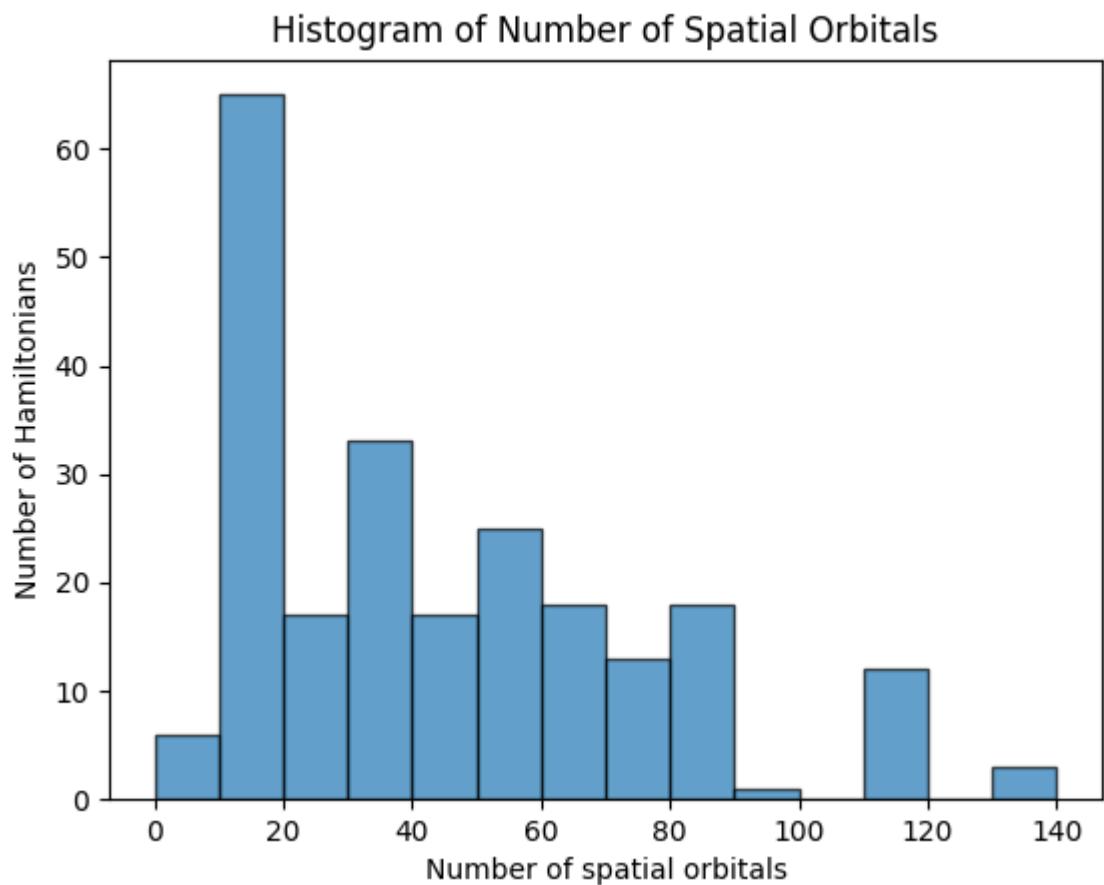
`problem_instance.json` with the most tasks: 30 (`hubbard_square/614c4444-a31a-4348-b24d-01040208651c`)

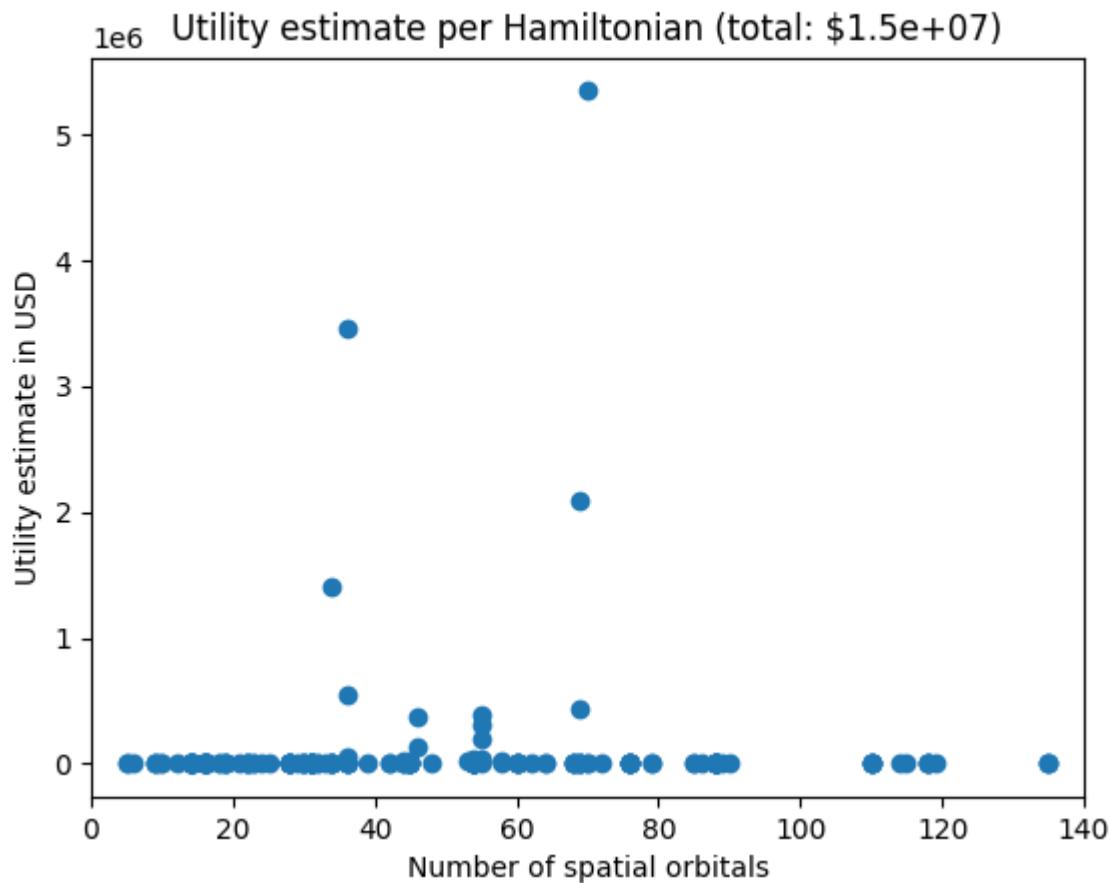
number of Hamiltonians (i.e., tasks) we have features calculated for: 228

minimum number of orbitals: 5

median number of orbitals: 36.0

maximum number of orbitals: 135





## Solver Summary Statistics

number of unique participating solvers: 21

Solver: SHCI\_opt/2dde727e-a881-44fa-aabf-bba6248e4baf, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.85714286 0.98947368]

Solver: DF\_QPE/f6b36bde-be4a-4eee-975b-2c5f7e553f5f, ML Solvability Ratio: {'PCA': 0.013, 'NNMF': 0.0006}, F1 Score: [0.99319728 0.83333333]

Solver: SHCI\_pt\_1e-4/4ed500f1-0650-41e3-af00-e4d0359394b4, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.70588235 0.96323529]

Solver: SHCI\_var\_1e-4/7e730dfb-57ee-480b-a8a1-4b73f5f07c54, ML Solvability Ratio: {'PCA': 0.6661, 'NNMF': 0.7848}, F1 Score: [0.98484848 0.98850575]

Solver: SHCI\_pt\_2e-4/ad964781-302e-4728-a26d-39918e0a6cdb, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.64864865 0.95167286]

Solver: SHCI\_pt\_2e-5/c71b90bd-3250-4c0c-b4e7-fc9878f141f6, ML  
Solvability Ratio: {'PCA': 1.0, 'NNMF': 0.8735}, F1 Score: [0.74285714  
0.96678967]

Solver: SHCI\_pt\_5e-5/d626506c-7aae-4ad6-802a-b29af5f2bb93, ML  
Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.8 0.97416974]

Solver: SHCI\_var\_2e-4/0db183e3-a86d-491b-9125-599556e37c7a, ML  
Solvability Ratio: {'PCA': 0.7146, 'NNMF': 0.7963}, F1 Score: [0.98630137  
0.9875 ]

Solver: SHCI\_var\_2e-5/86bfe50c-9342-4d54-bb68-abc8abd95688, ML  
Solvability Ratio: {'PCA': 0.5598, 'NNMF': 0.5682}, F1 Score: [0.81967213  
0.95510204]

Solver: SHCI\_var\_5e-5/01949b95-c427-4693-9134-01f47f688c09, ML  
Solvability Ratio: {'PCA': 0.9462, 'NNMF': 0.7526}, F1 Score: [0.95454545  
0.98165138]

Solver: DF\_QPE/4b07b89f-c66f-4e72-8c24-df3e4222cb41, ML Solvability  
Ratio: {'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [1. 1.]

Solver: DF\_QPE/5dad4064-cd11-412f-85cb-d722afe3b3de, ML Solvability  
Ratio: {'PCA': 0.0394, 'NNMF': 0.0199}, F1 Score: [1. 1.]

Solver: CISD/418f060e-496b-4024-8d2d-9b1f8791e76d, ML Solvability  
Ratio: {'PCA': 0.0, 'NNMF': 0.0139}, F1 Score: [0.97744361 0.85 ]

Solver: HF/5f5e617a-19c2-4d82-bebc-b2d6b3dcb012, ML Solvability Ratio:  
'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98630137 0.71428571]

Solver: MP2/b420358b-5def-41e6-8c5d-b9d93b6aecd2, ML Solvability Ratio:  
'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98630137 0.71428571]

Solver: CCSD/0a29e54f-bef9-4d19-bafa-d94b1c4b37aa, ML Solvability Ratio:  
'PCA': 0.0, 'NNMF': 0.0232}, F1 Score: [0.97637795 0.88461538]

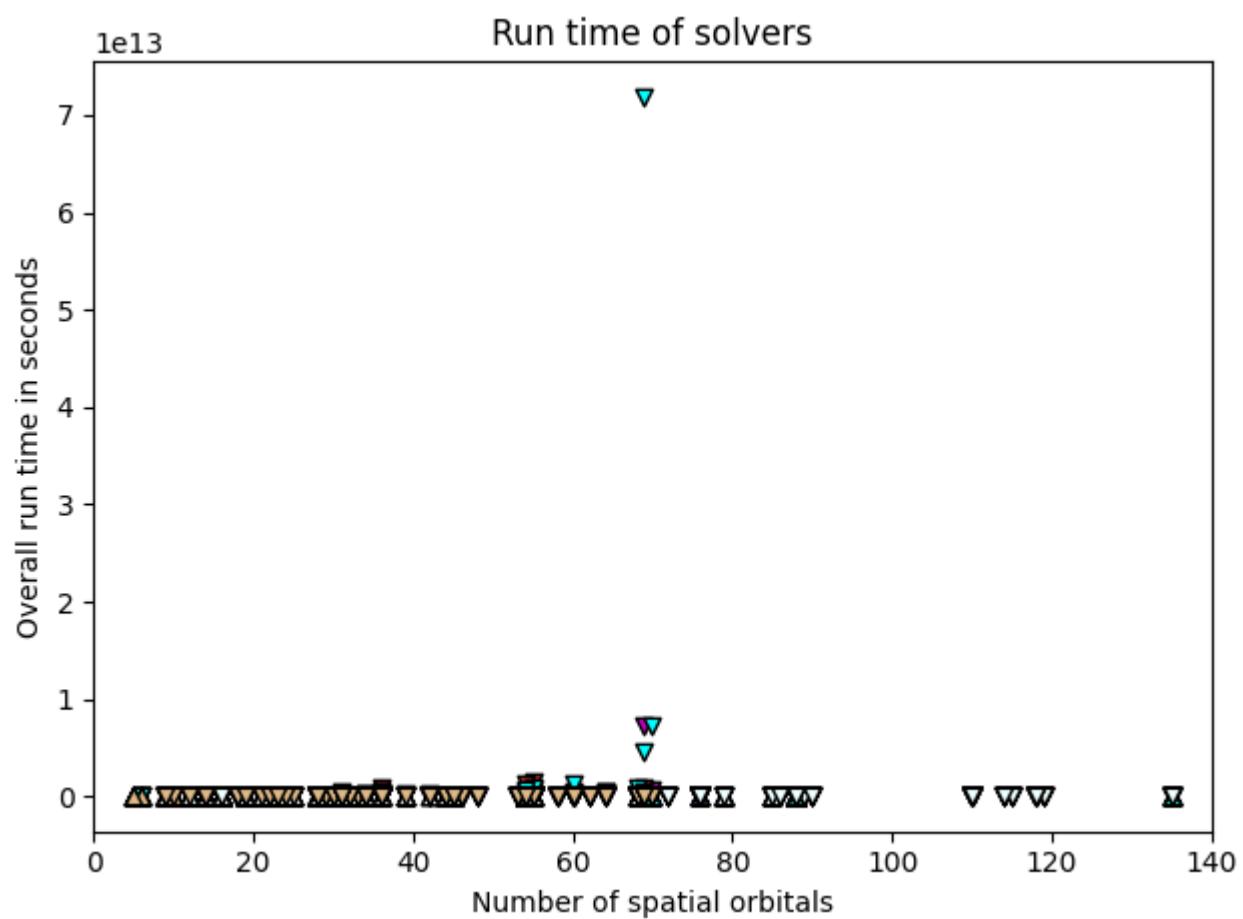
Solver: CCSD(T)/c09217e6-d0f7-4b0f-81c4-79210b7ac878, ML Solvability  
Ratio: {'PCA': 0.305, 'NNMF': 0.4969}, F1 Score: [0.95121951 0.94366197]

Solver: DF\_QPE/7c8ef984-4d3a-4468-8900-e0da3bd8b22d, ML Solvability  
Ratio: {'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.93706294 0.1 ]

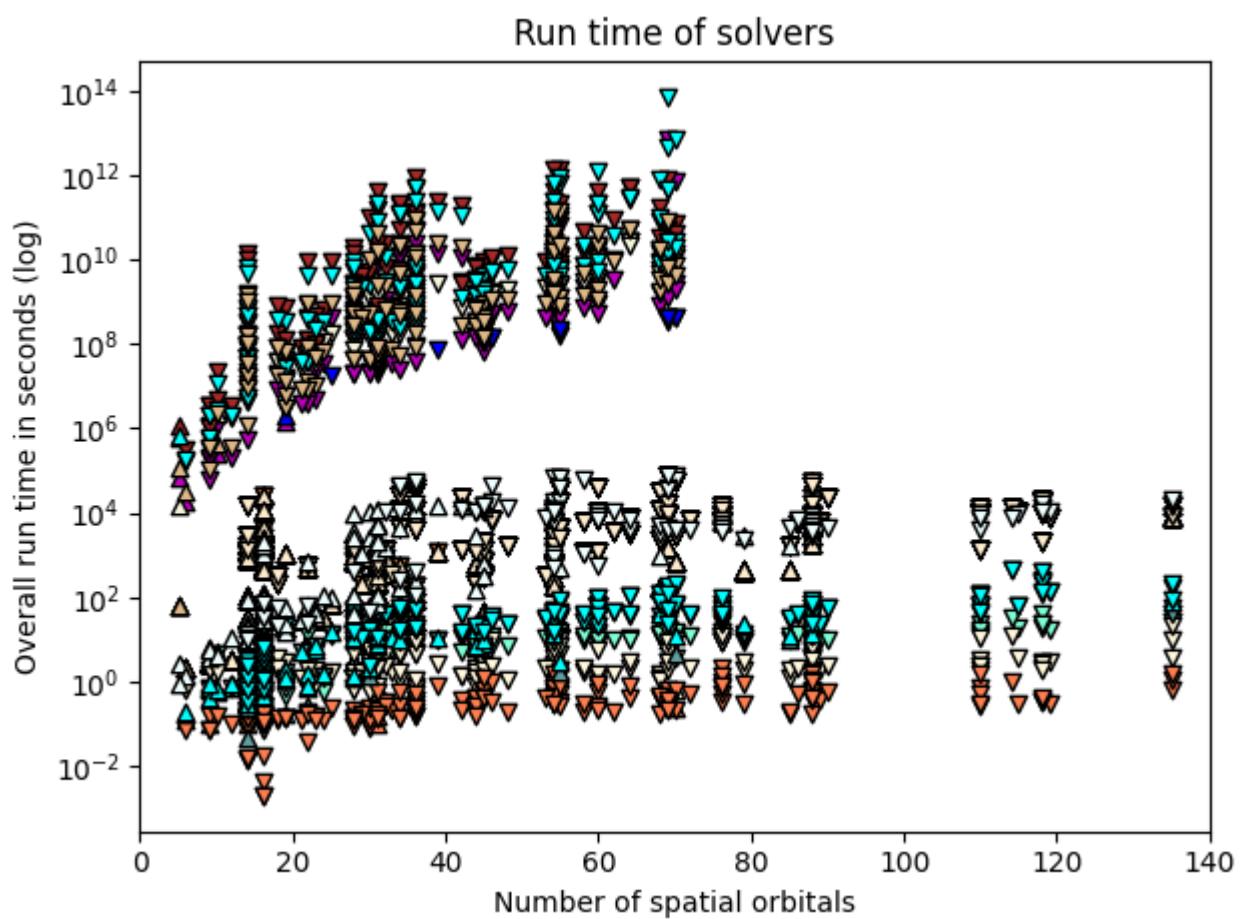
Solver: DF\_QPE/5d768520-b3d0-4292-bbb4-9776fa128107, ML Solvability  
Ratio: {'PCA': 0.0394, 'NNMF': 0.0199}, F1 Score: [1. 1.]

Solver: DMRG\_Niagara\_cluster\_lowest\_energy/16537433-9f4c-4eae-  
a65d-787dc3b35b59, ML Solvability Ratio: {'PCA': 0.4126, 'NNMF':  
0.3022}, F1 Score: [0.91304348 0.96261682]

Solver: DF\_QPE/2610d8de-bd3a-469e-9a80-473e8988755f, ML Solvability  
Ratio: {'PCA': 0.0716, 'NNMF': 0.0}, F1 Score: [1. 1.]

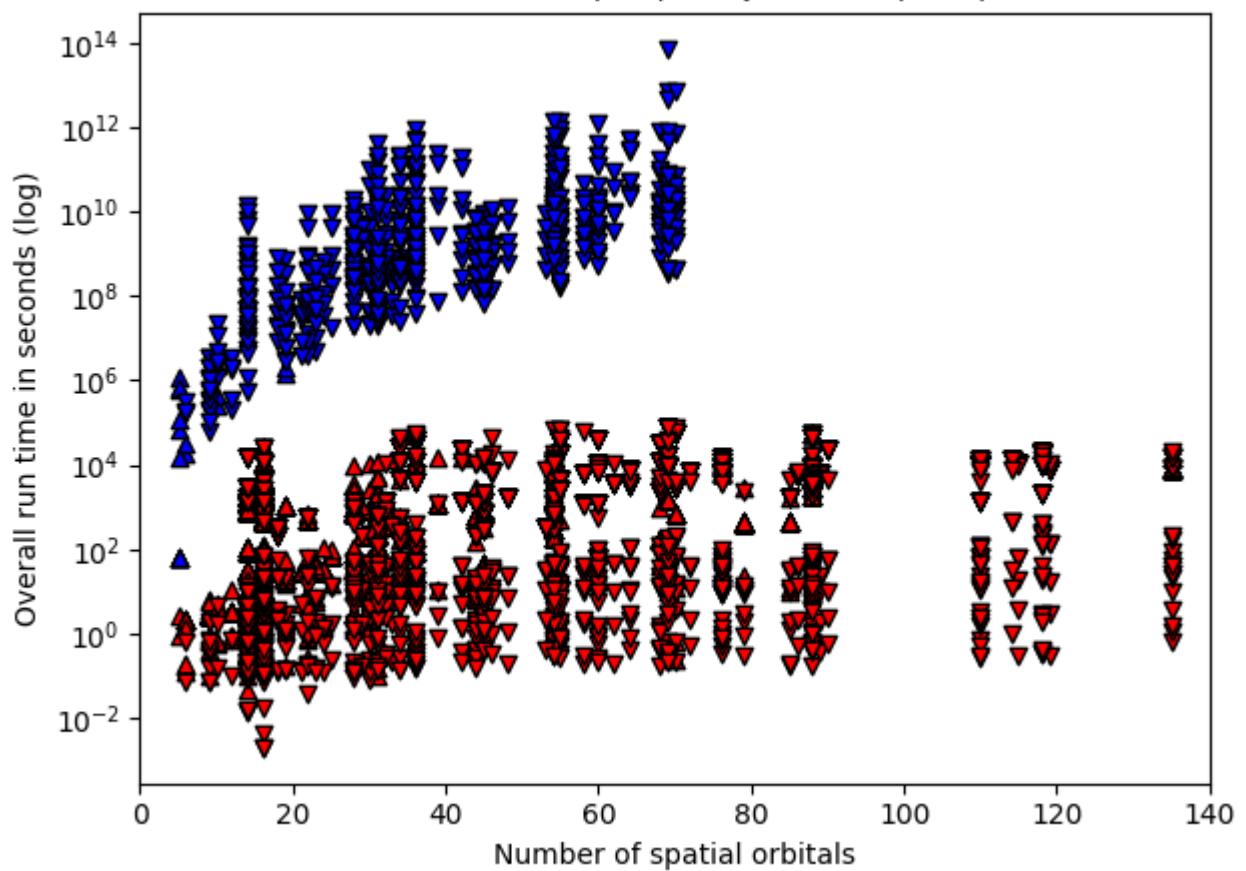


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

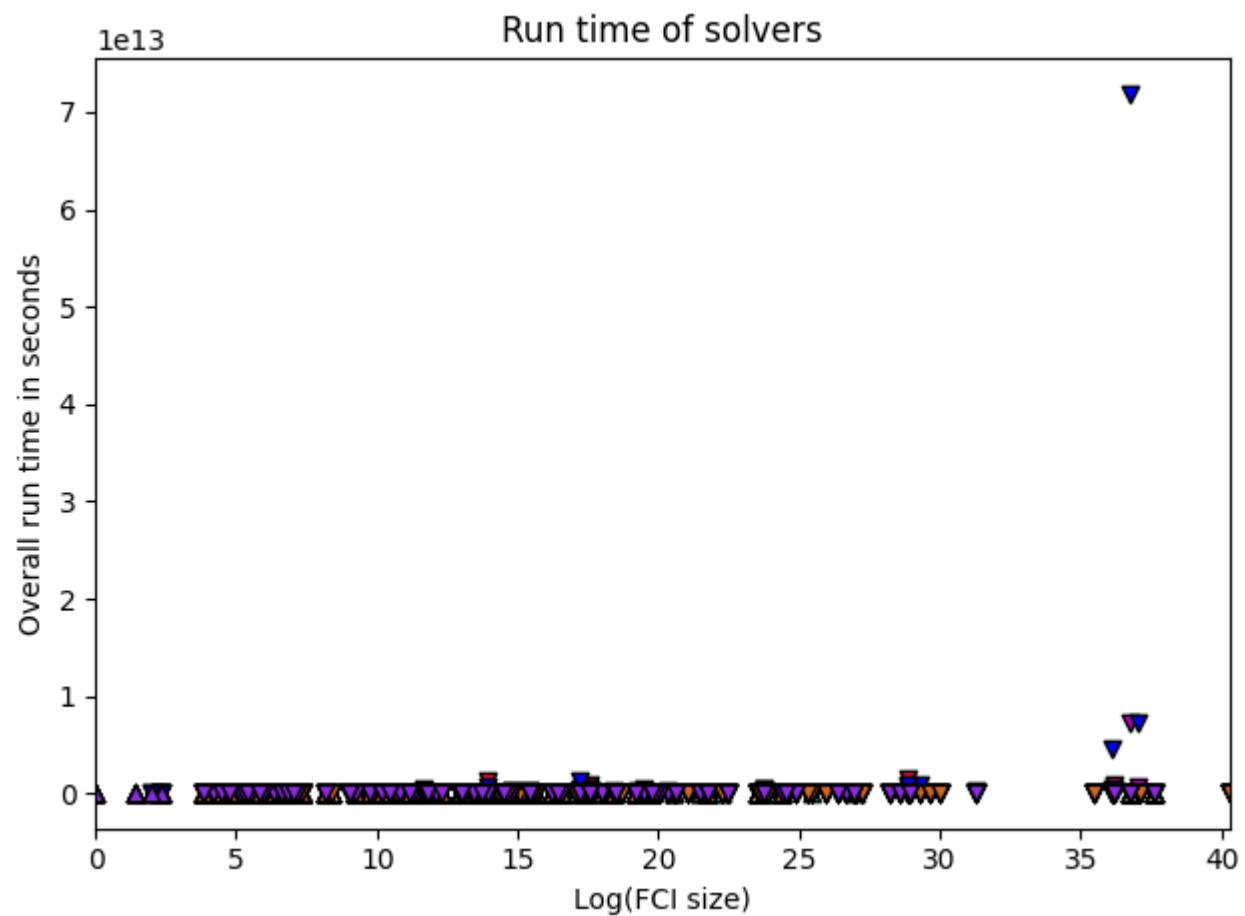


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

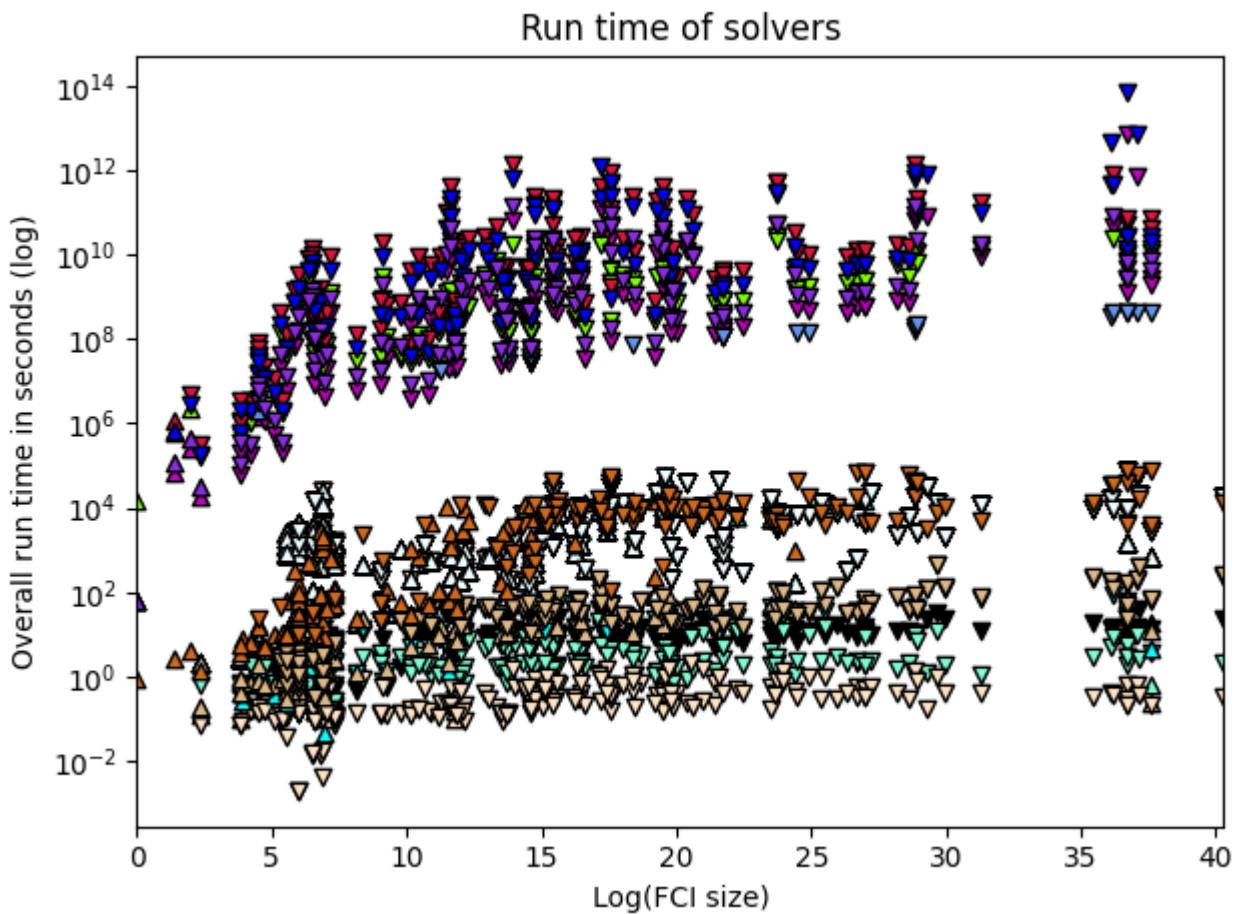
Run time of Classical (red) vs Quantum (blue) solvers



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

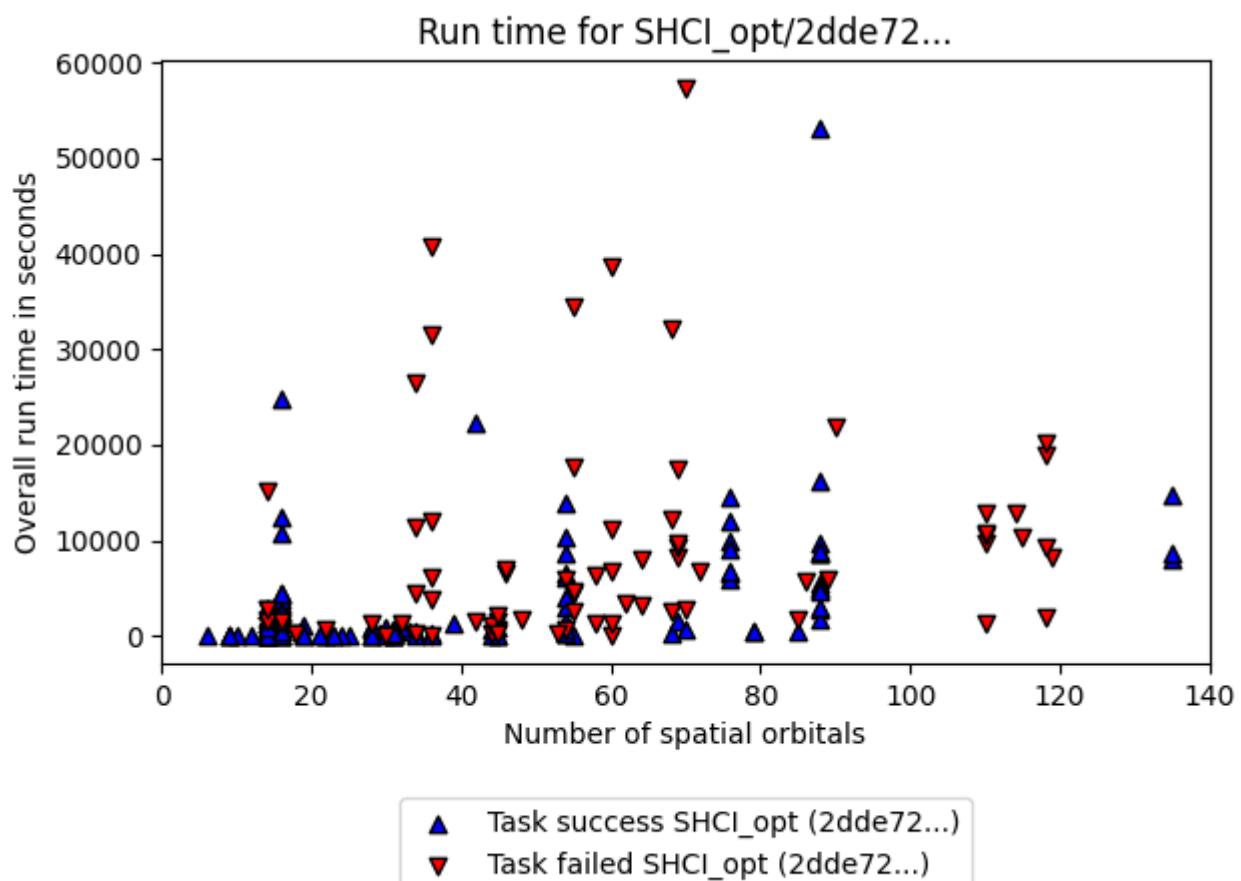
software\_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance\_metrics\_uuid: 0f5b2258-8d3d-4239-b4cb-2bbf91fa0391

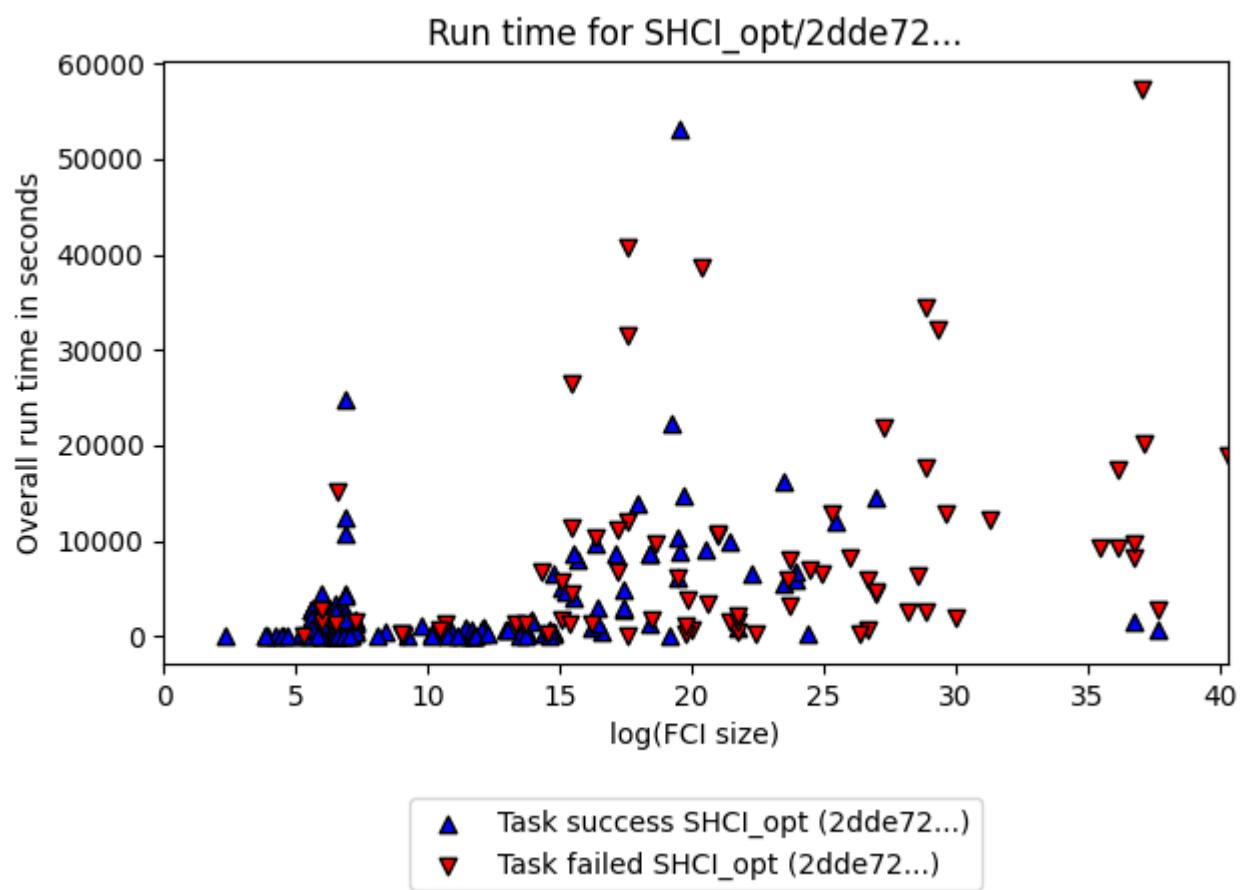
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 62  
number\_of\_problem\_instances\_solved: 33  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 222  
number\_of\_tasks\_solved: 144  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 222  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 144  
max\_run\_time\_of\_attempted\_tasks: 57334.2  
sum\_of\_run\_time\_of\_attempted\_tasks: 1100315.9169999997  
solvability\_ratio: 1.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.8571428571428571, 0.9894736842105263]  
ml\_metrics\_calculator\_version: 1



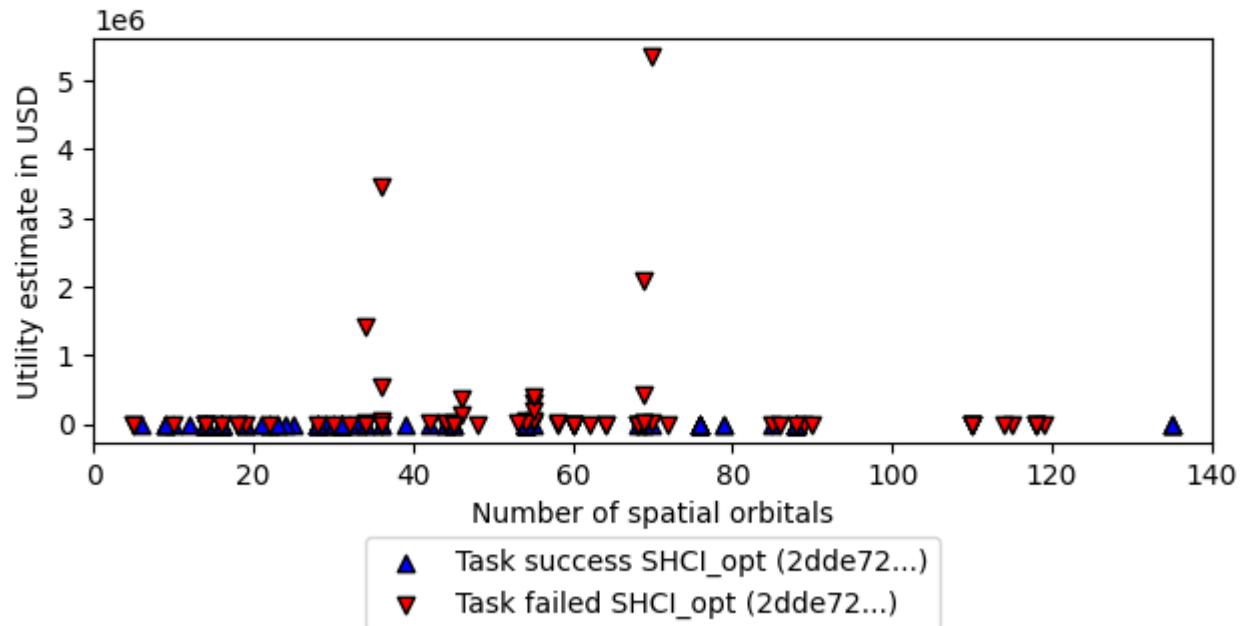
Note: plot only contains attempted tasks.



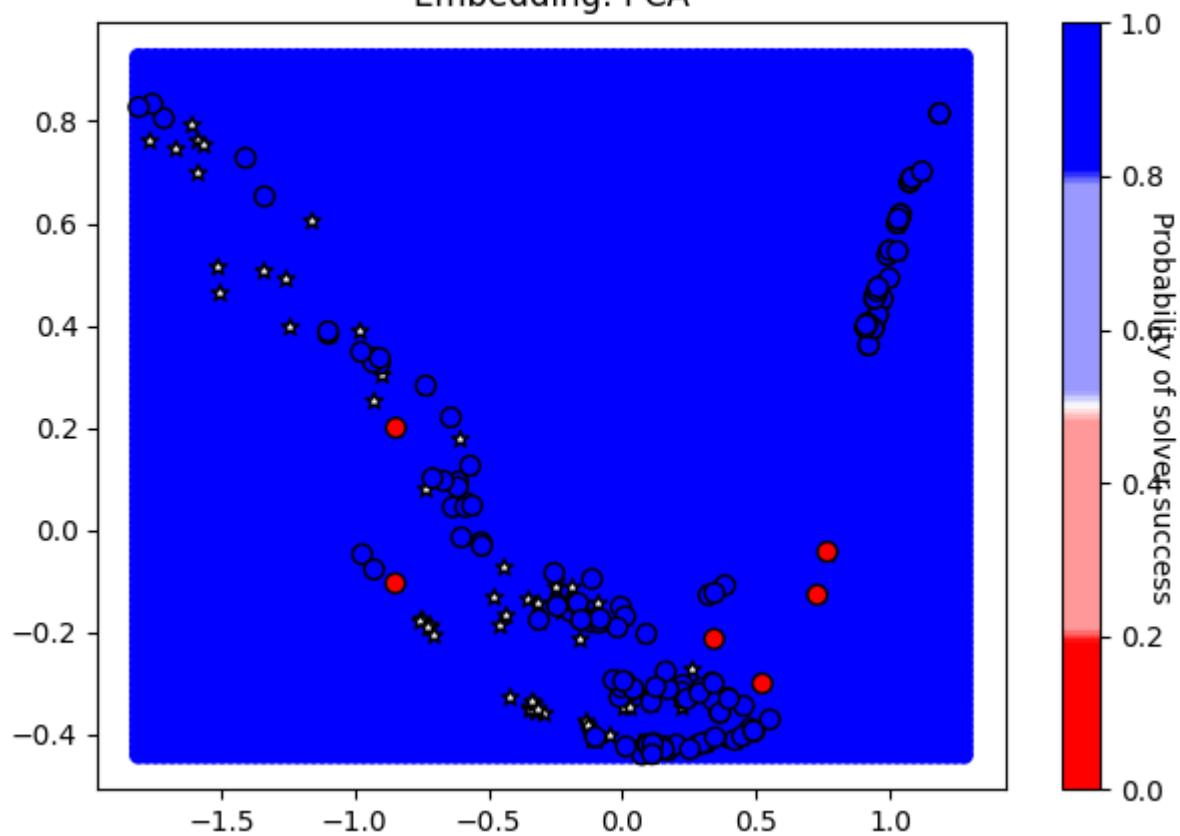
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_opt/2dde72...

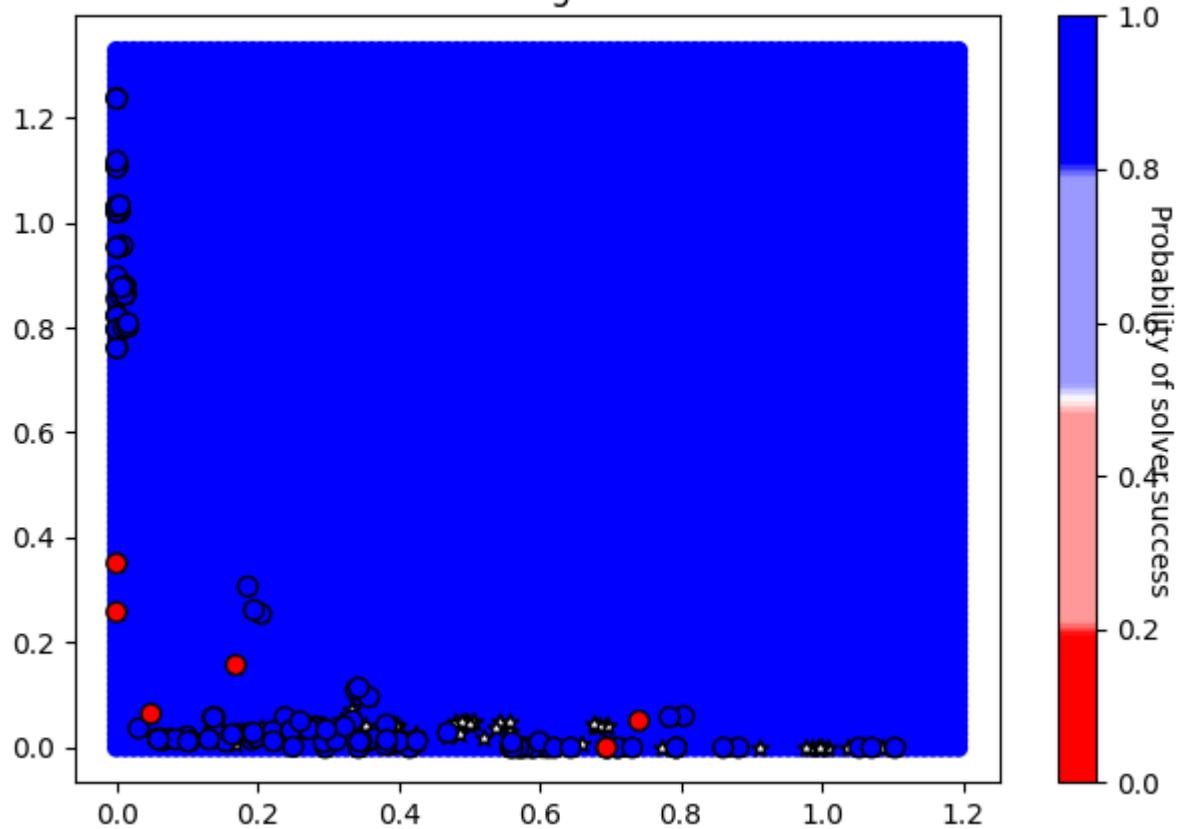
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



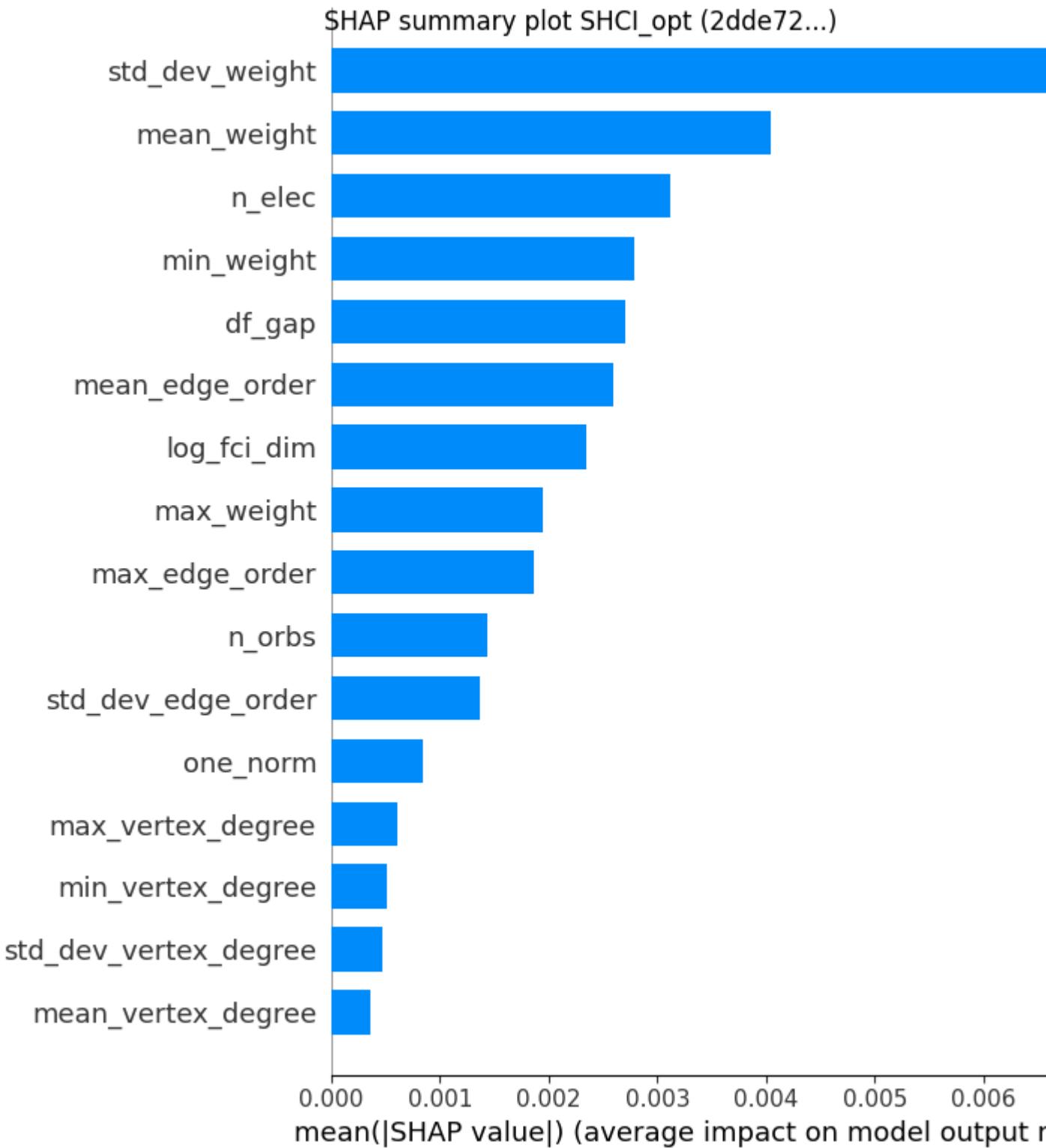
Solver SHCI\_opt (2dde72...)  
Embedding: PCA



Solver SHCI\_opt (2ddee72...)  
Embedding: NMF



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, f6b36bde-be4a-4eee-975b-2c5f7e553f5f

solver\_uuid:f6b36bde-be4a-4eee-975b-2c5f7e553f5f

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': '1.3.6'}, {'software\_name': 'qb-gsee-benchmark', 'software\_version': '0.1.0a3.dev68+g2b90efd'}, {'software\_name': 'Python', 'software\_version': '3.10.12 (main, Feb 4 2025, 14:57:36) [GCC 11.4.0]'}, {'software\_name': 'qualtran', 'software\_version': '0.4.0'}]

quantum.hardware\_details:{'quantum.hardware\_description': 'Ultra-optimistic hardware model based on the superconducting architecture described in https://arxiv.org/abs/2011.03494.'}, 'quantum.hardware\_parameters': {'num\_factories': 4, 'physical\_error\_rate': 1e-06, 'cycle\_time\_microseconds': 0.1, 'parallelize\_shots': False}}

logical\_resource\_estimate\_solution\_uuid:7d2dadd5-bec8-46e0-b3d2-82d5f8111940

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

performance\_metrics\_uuid: 7d048a2f-ab25-4e49-884f-54f3f312cd08

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 24

number\_of\_problem\_instances\_solved: 4

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 137

number\_of\_tasks\_solved: 5

number\_of\_tasks\_solved\_within\_run\_time\_limit: 5

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

max\_run\_time\_of\_attempted\_tasks: 7188148035230.209

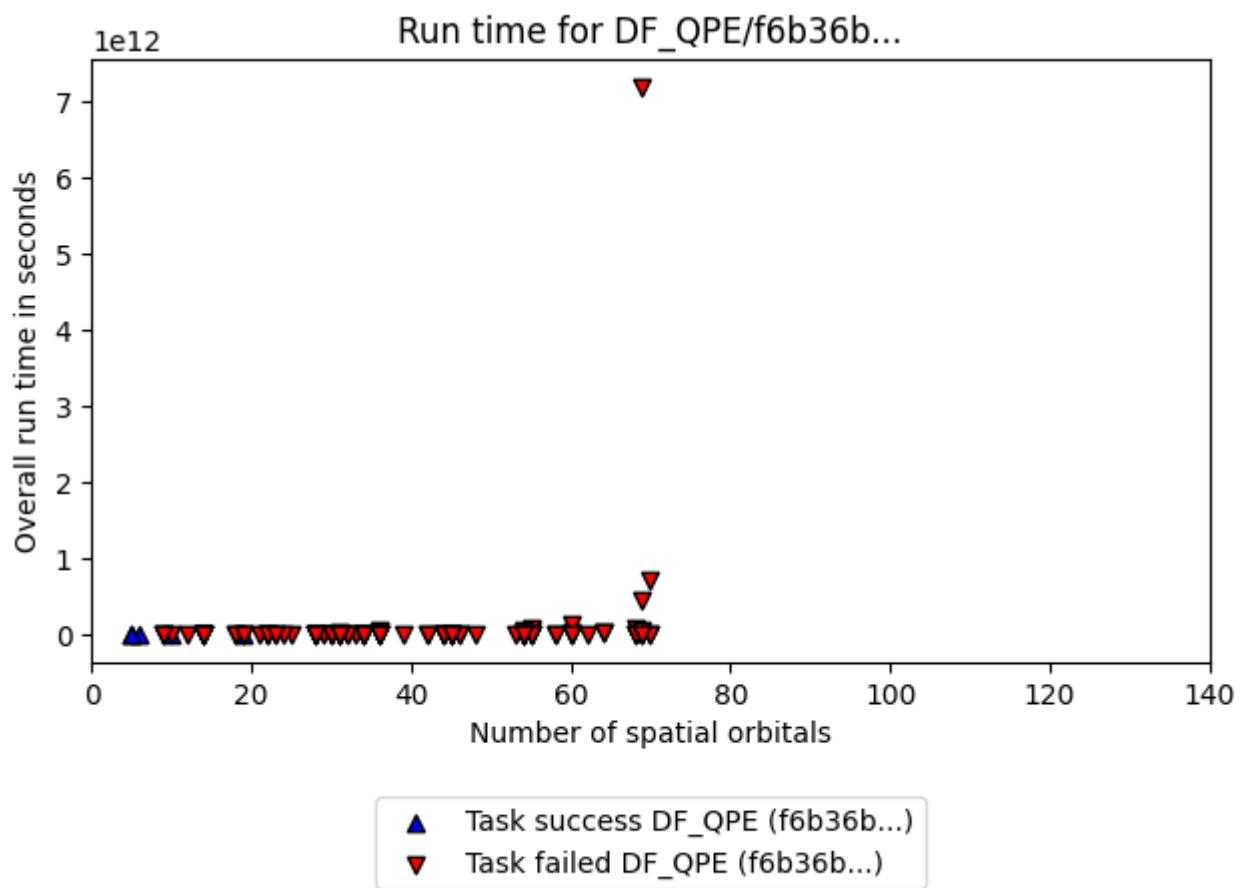
sum\_of\_run\_time\_of\_attempted\_tasks: 9230378074762.195

solvability\_ratio: 0.013

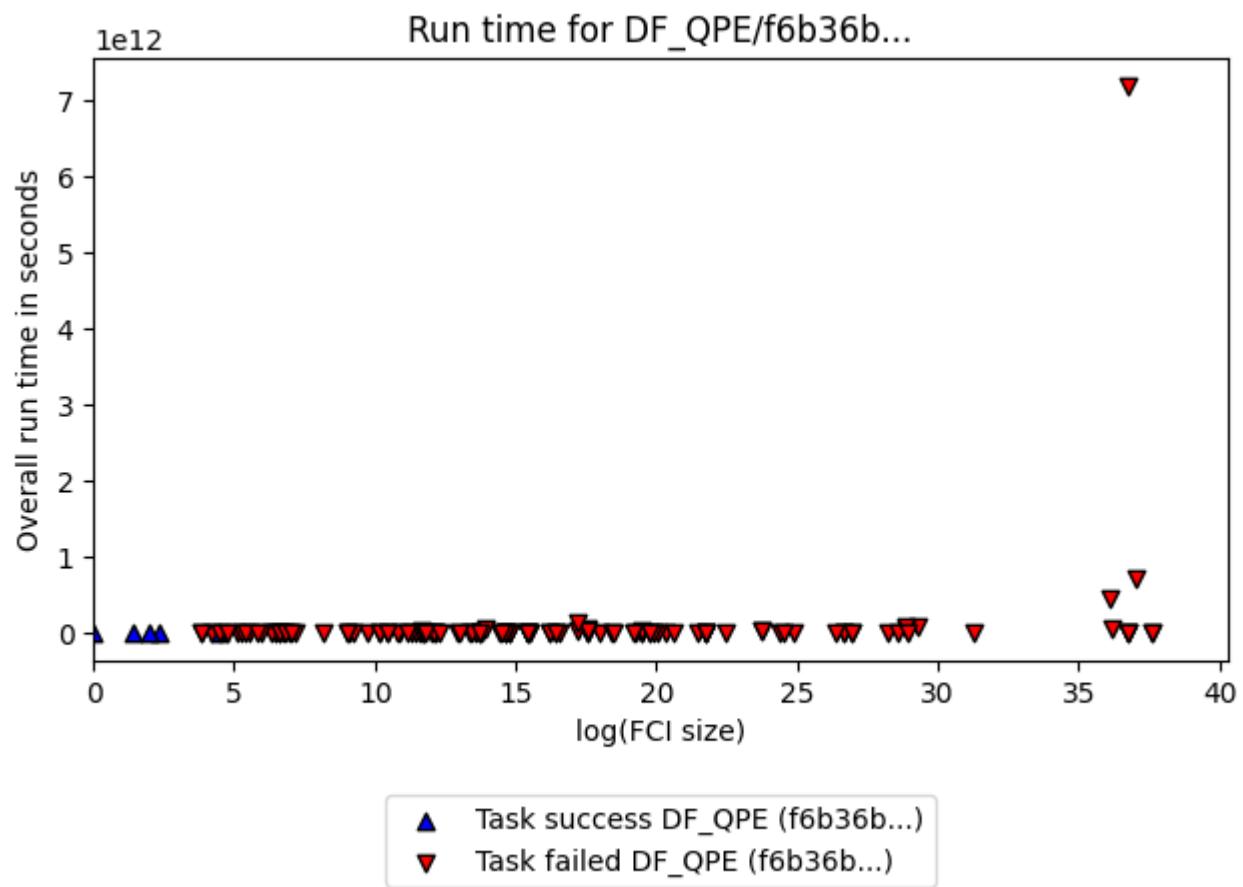
comments: solvability ratio based on PCA embedding.

f1\_score: [0.9931972789115646, 0.8333333333333334]

ml\_metrics\_calculator\_version: 1



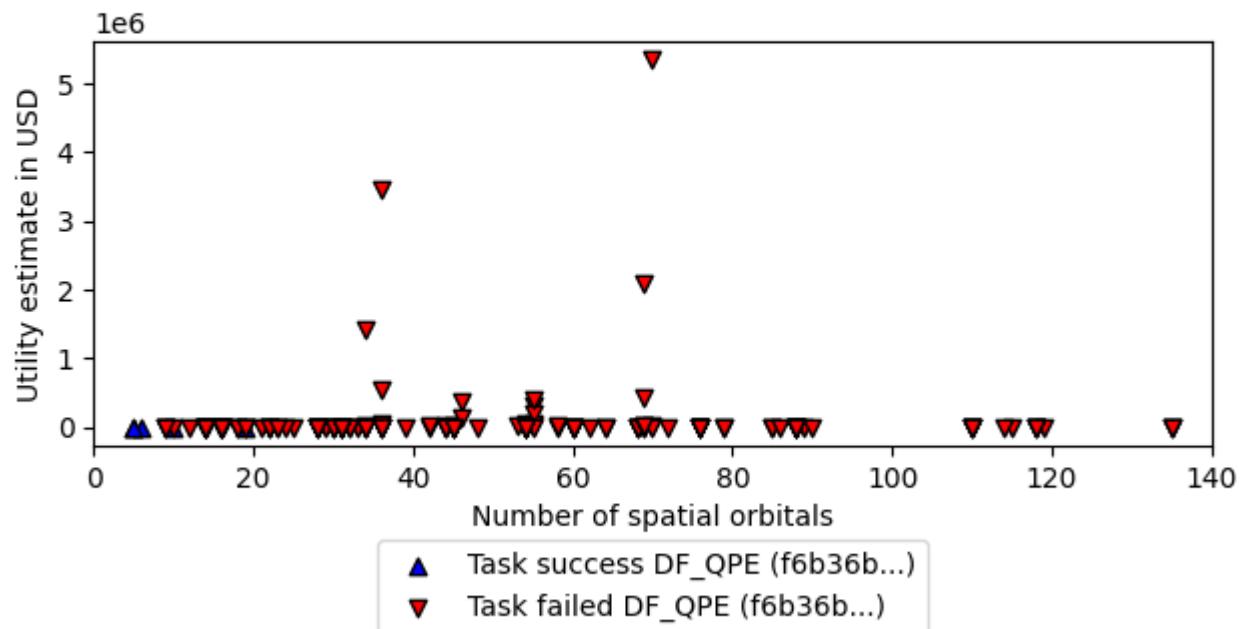
Note: plot only contains attempted tasks.



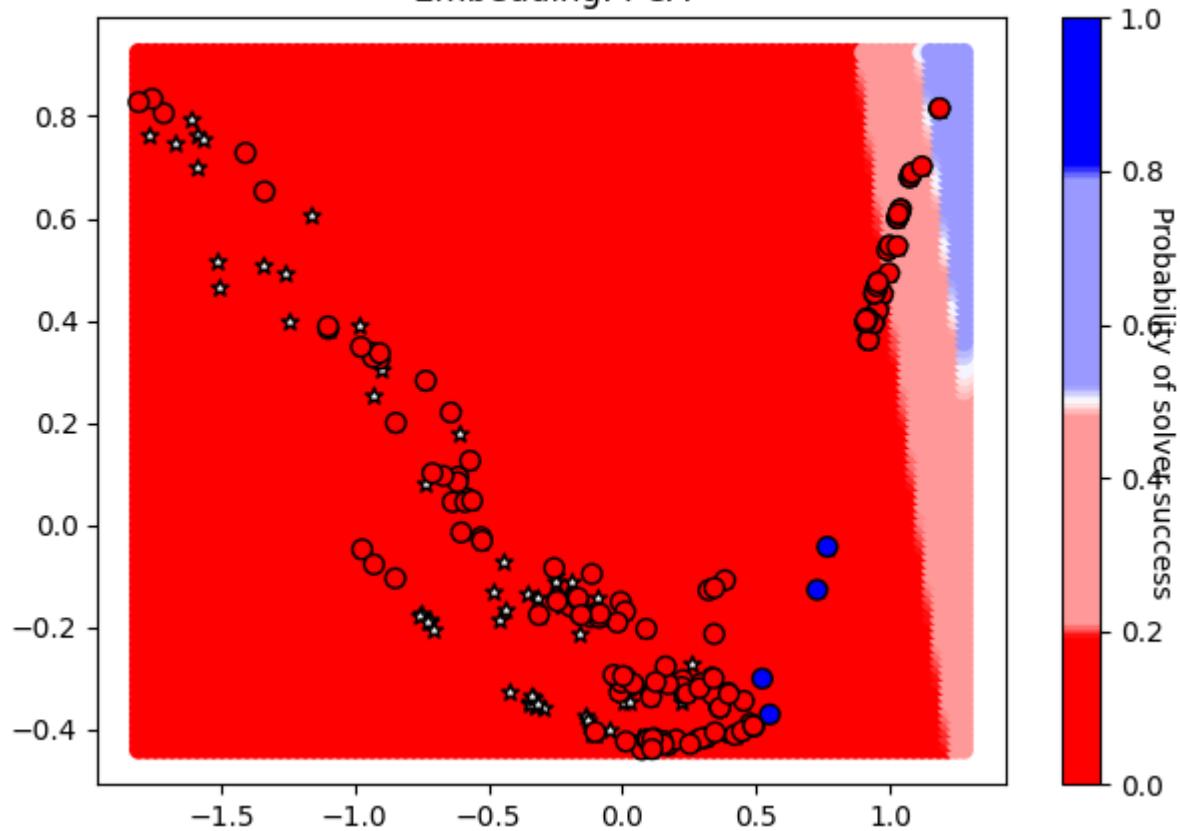
Note: plot only contains attempted tasks.

## Utility capture from DF\_QPE/f6b36b...

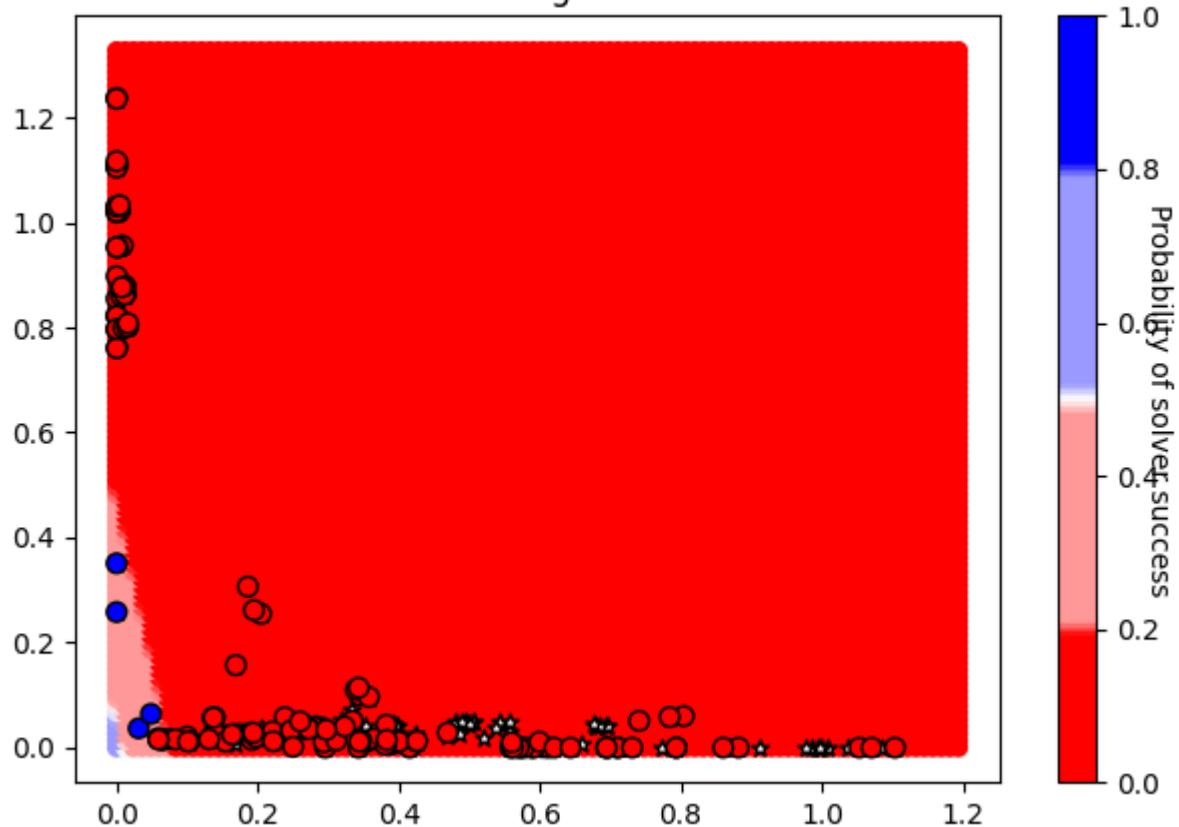
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



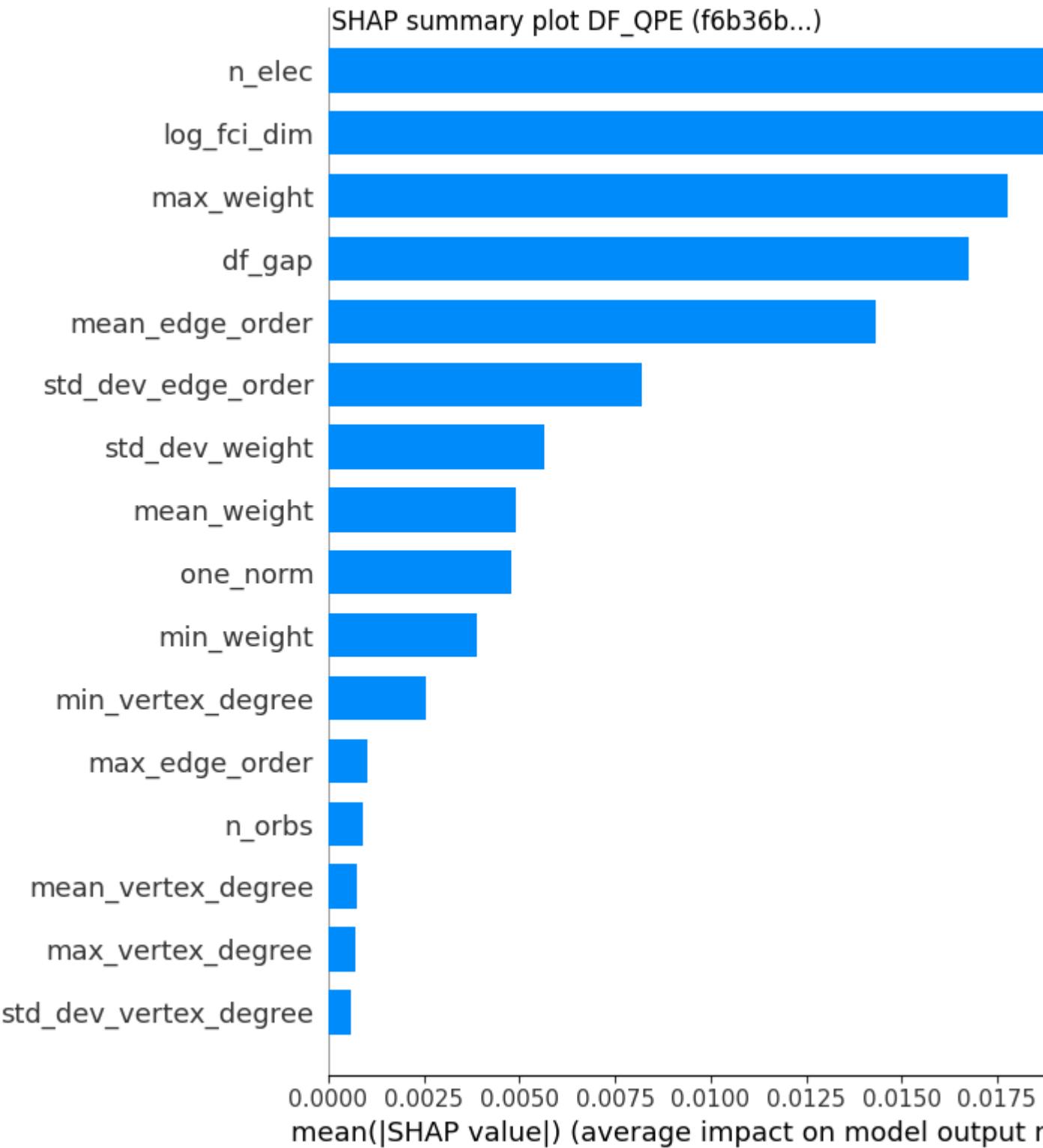
Solver DF\_QPE (f6b36b...)  
Embedding: PCA



Solver DF\_QPE (f6b36b...)  
Embedding: NNMF



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.

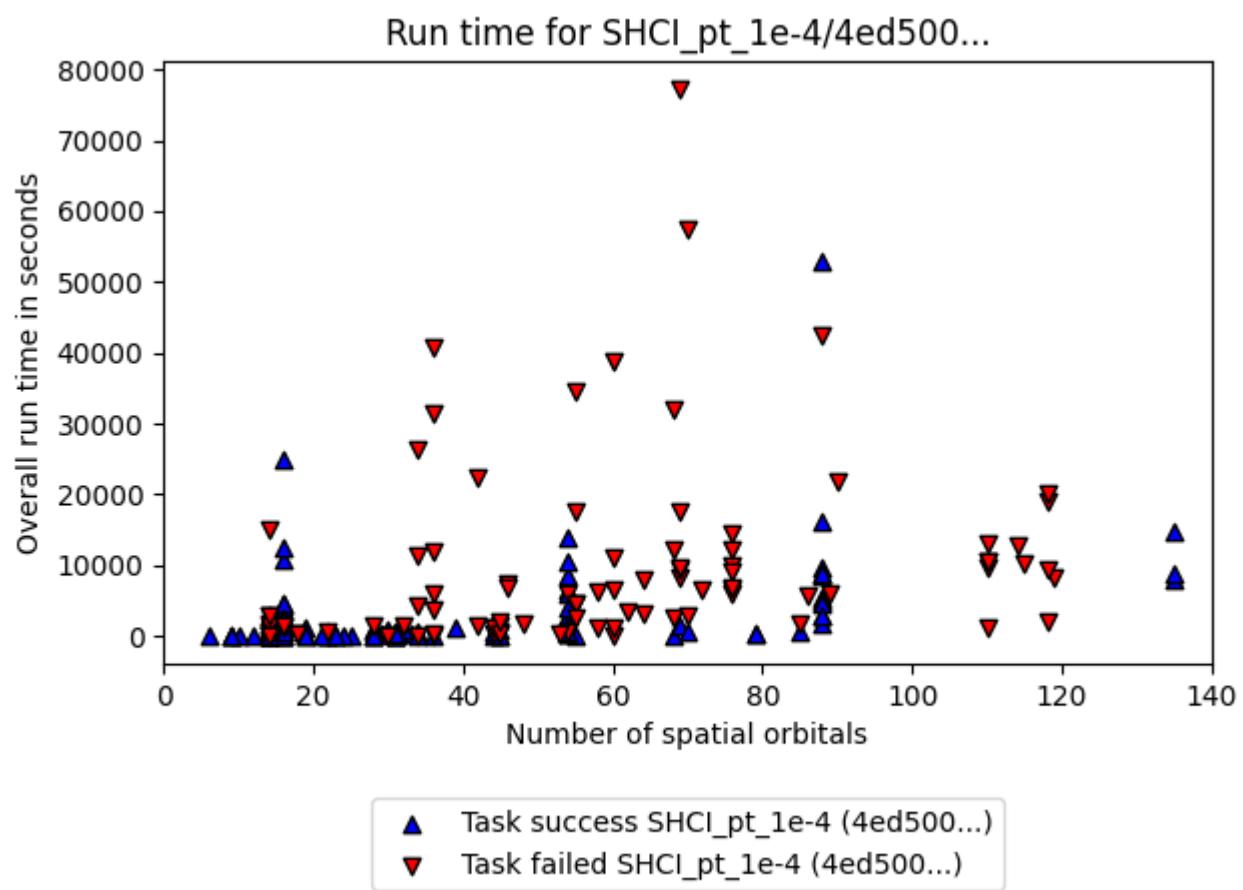


## Solver SHCI\_pt\_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4

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

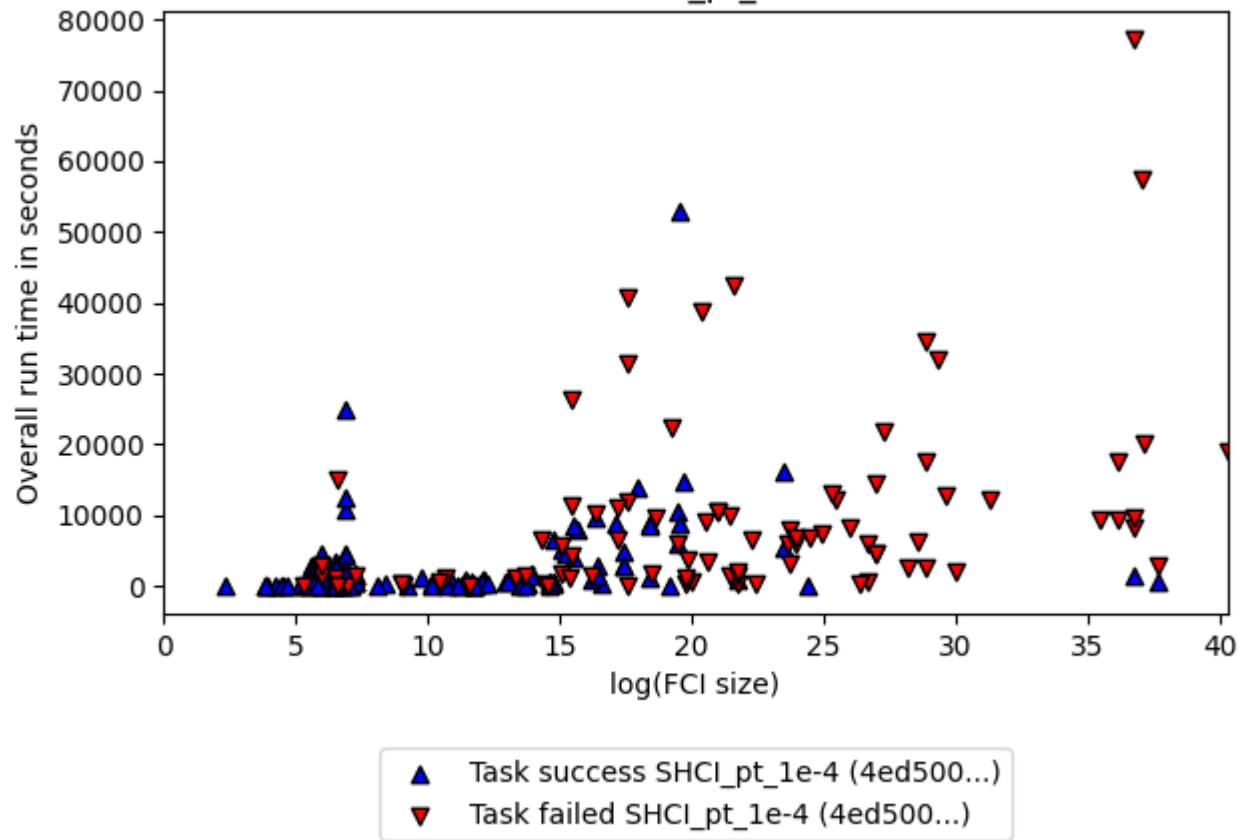
solver\_short\_name:SHCI\_pt\_1e-4

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: 8f072bd2-7e0b-4675-9d9c-78057f8de690  
creation.timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 22  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 131  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 131  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 1.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.7058823529411765, 0.9632352941176471]  
ml.metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

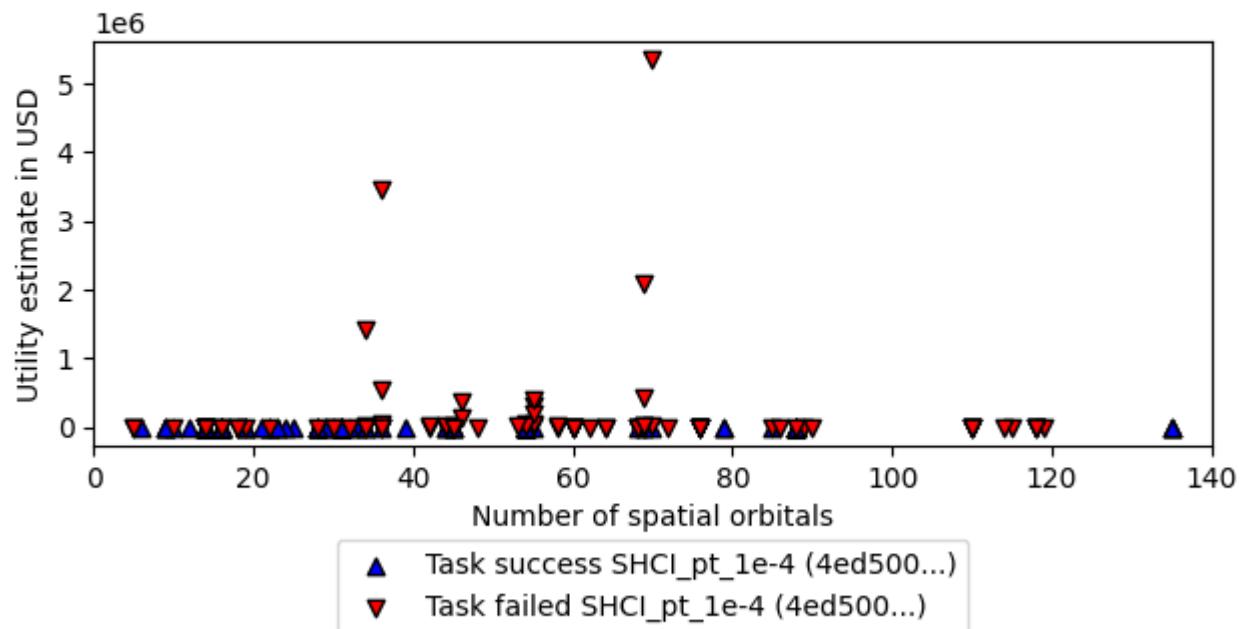
### Run time for SHCI\_pt\_1e-4/4ed500...



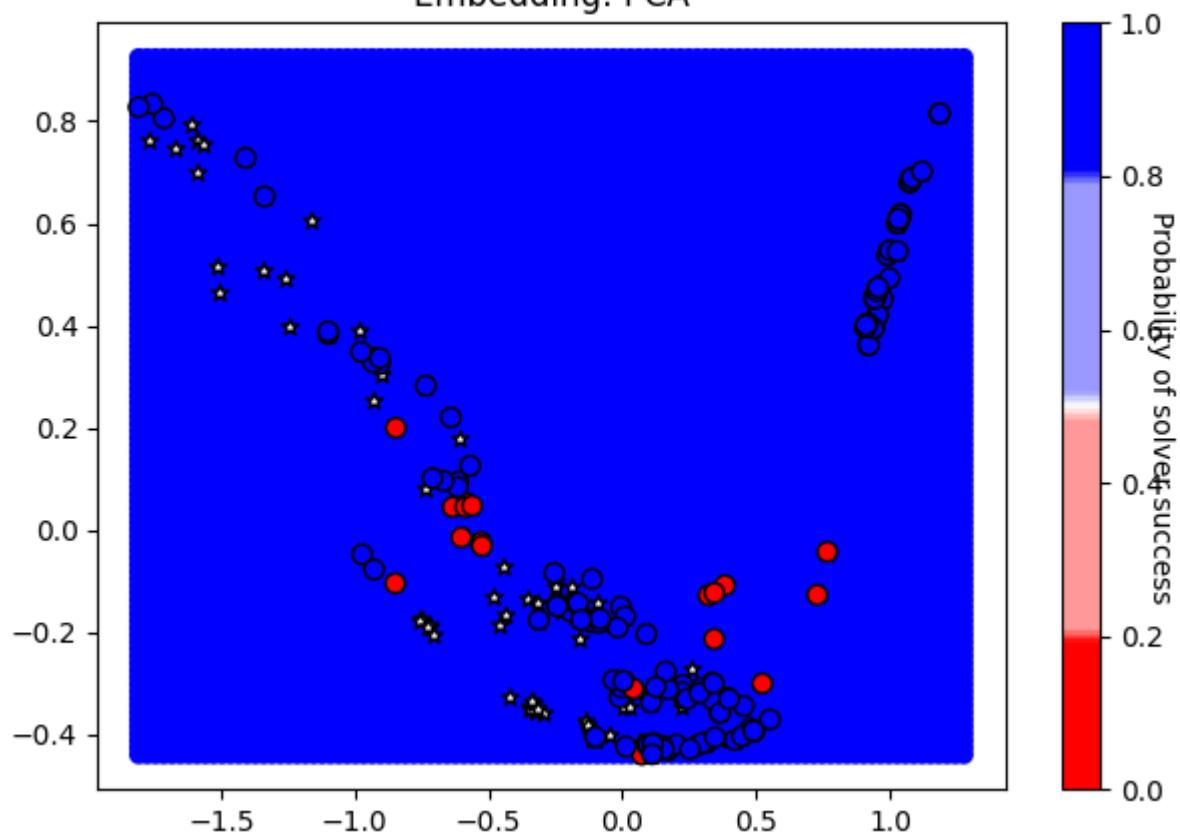
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_pt\_1e-4/4ed500...

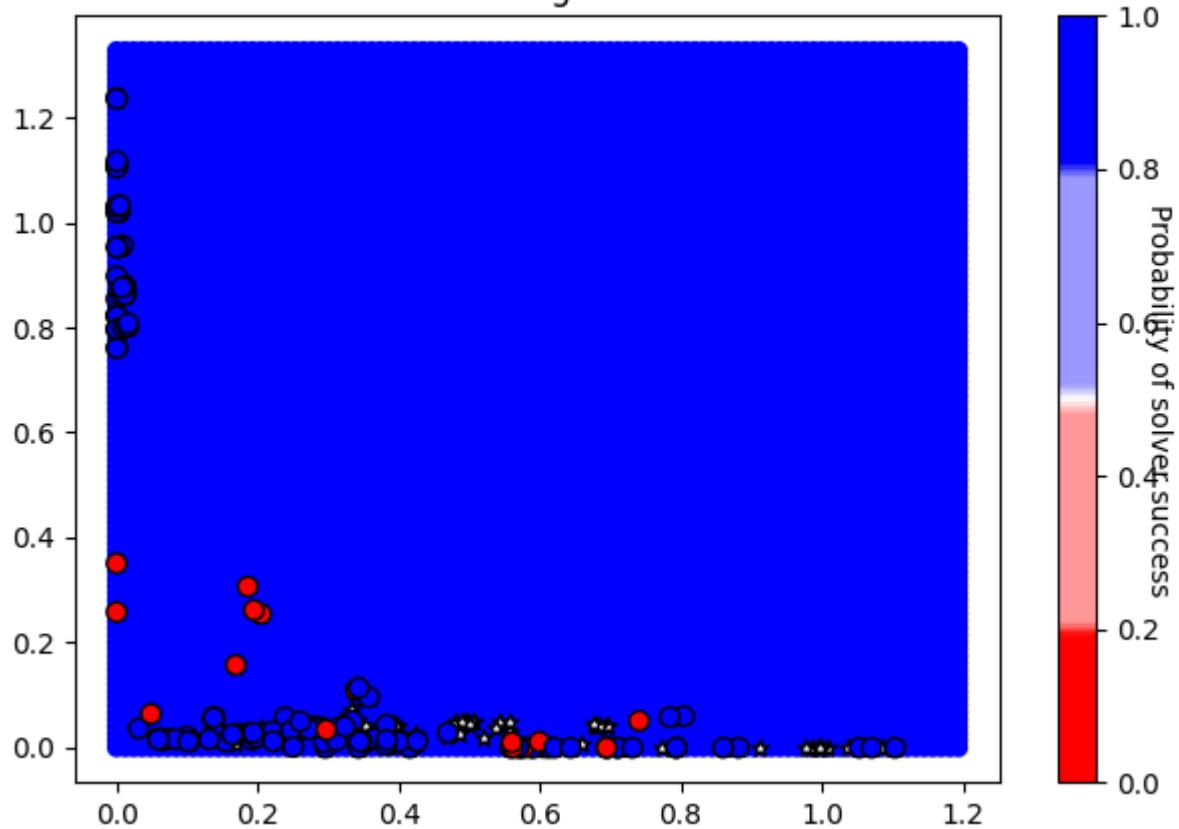
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



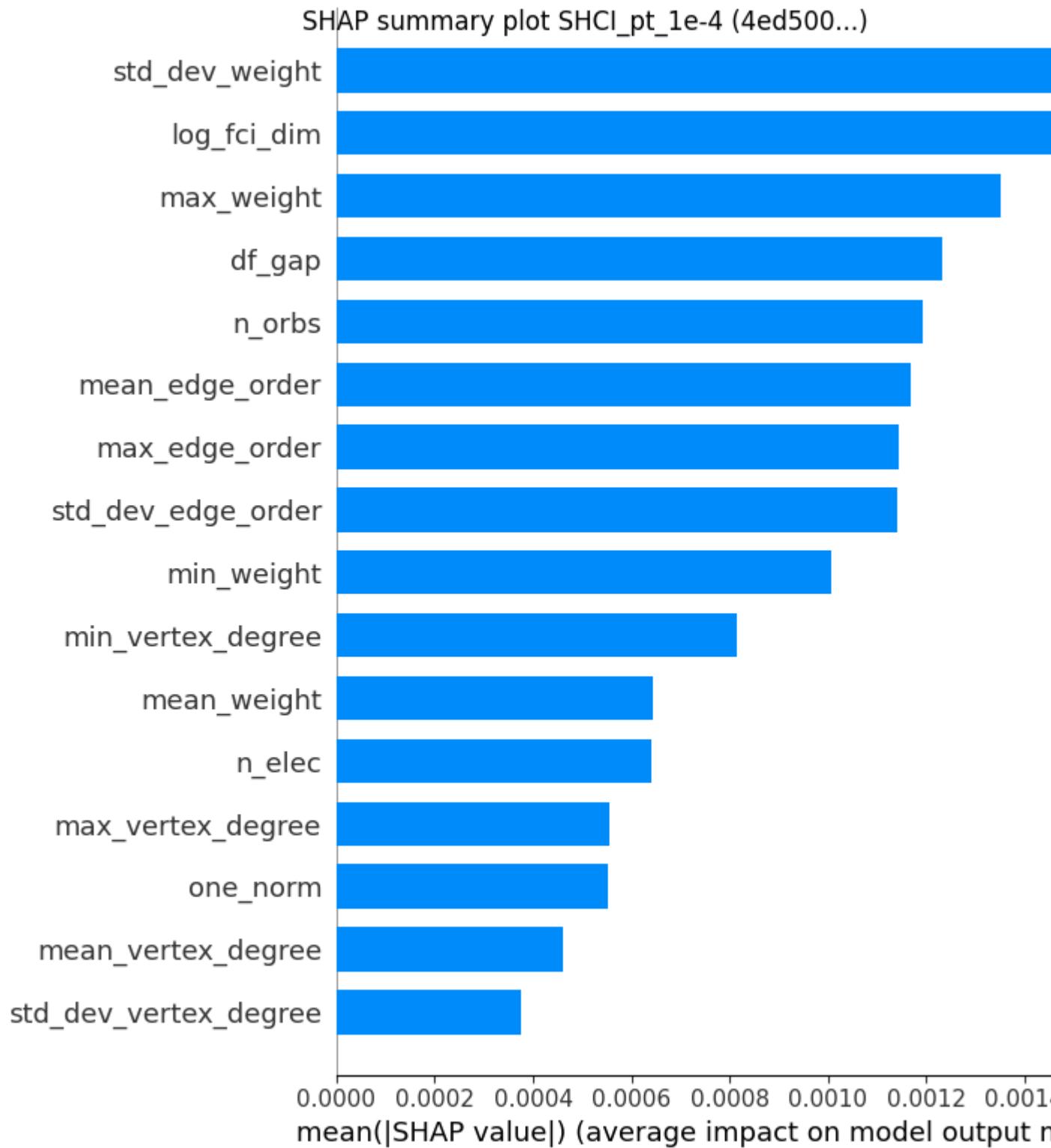
Solver SHCI\_pt\_1e-4 (4ed500...)  
Embedding: PCA



Solver SHCI\_pt\_1e-4 (4ed500...)  
Embedding: NMF



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.

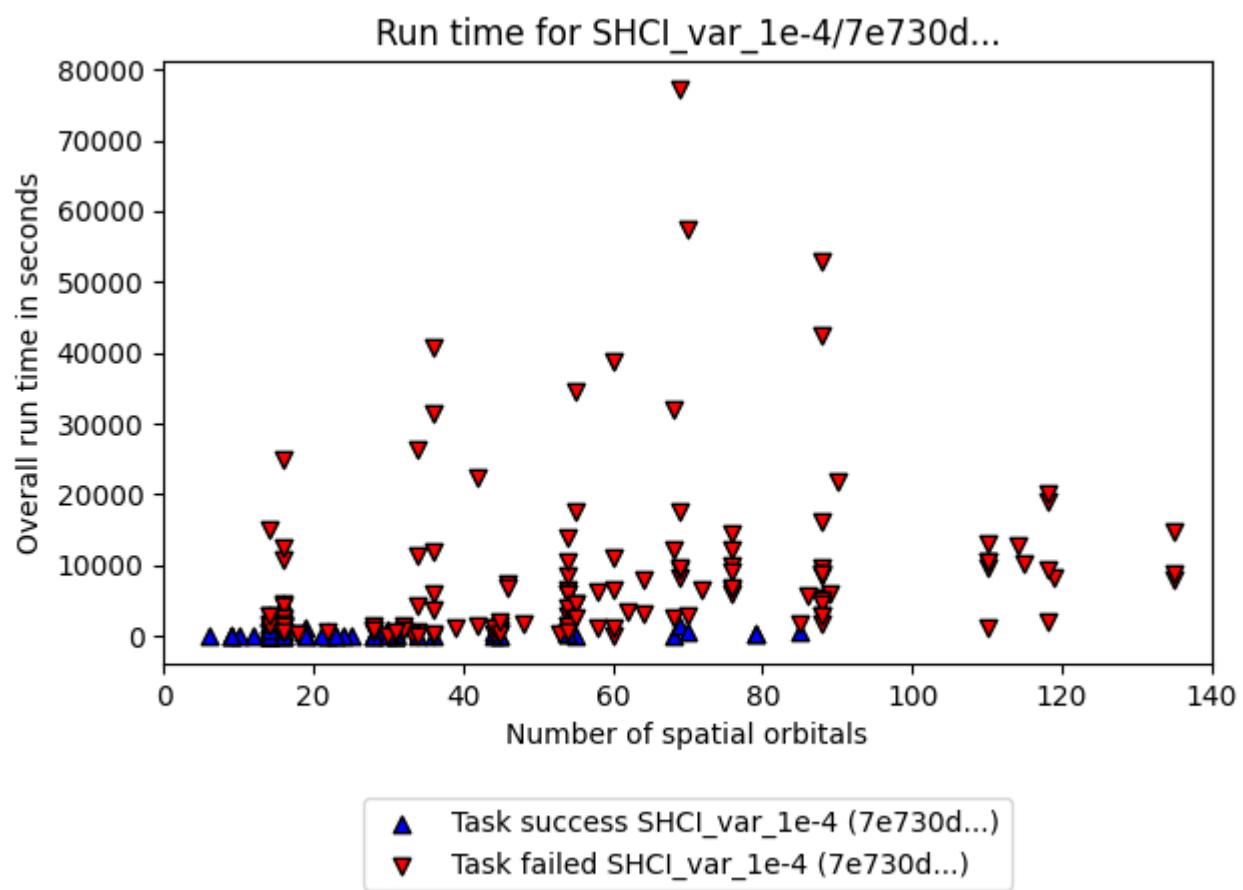


## Solver SHCI\_var\_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54

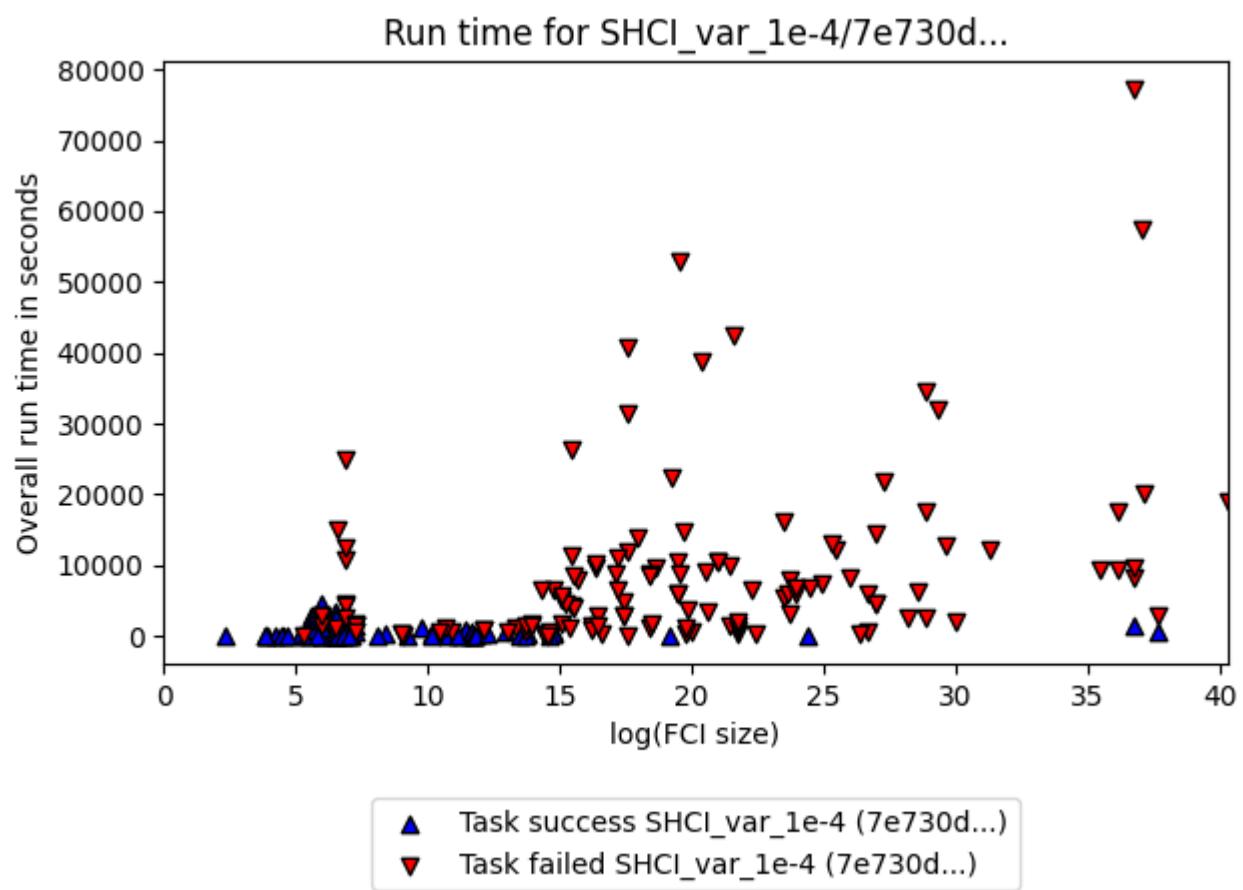
solver\_uuid:7e730dfb-57ee-480b-a8a1-4b73f5f07c54

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: 2089931f-a1de-4271-b8e7-90eb29a8575c  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 13  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 87  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 87  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 0.6661  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.98484848484849, 0.9885057471264368]  
ml\_metrics\_calculator\_version: 1



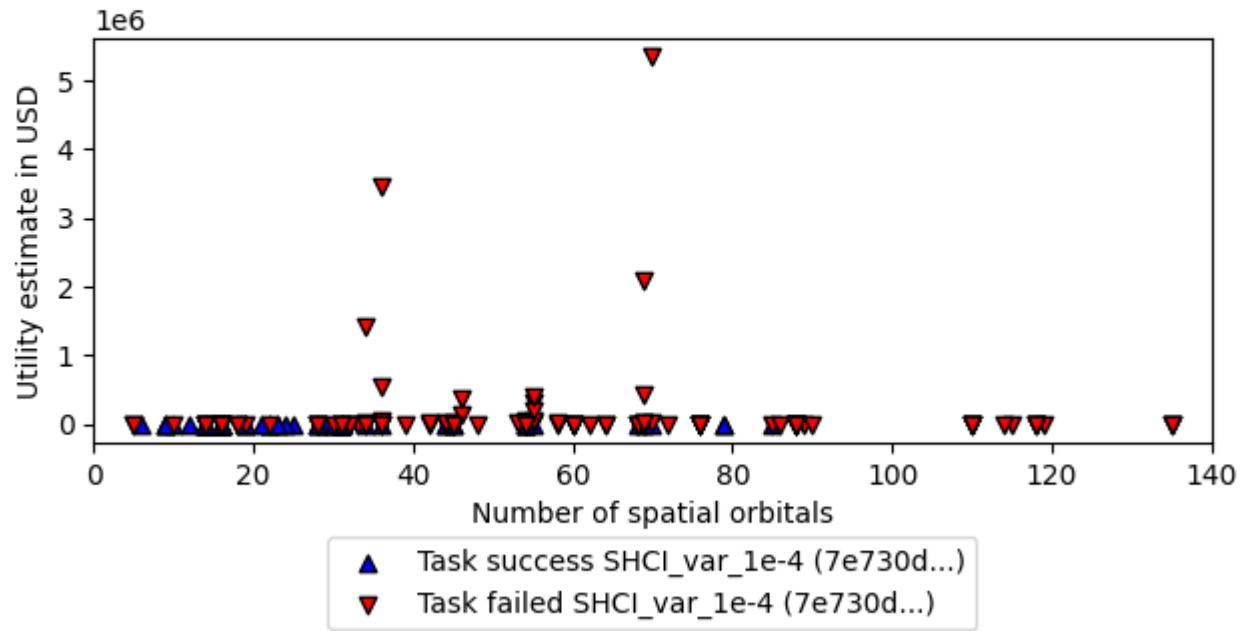
Note: plot only contains attempted tasks.



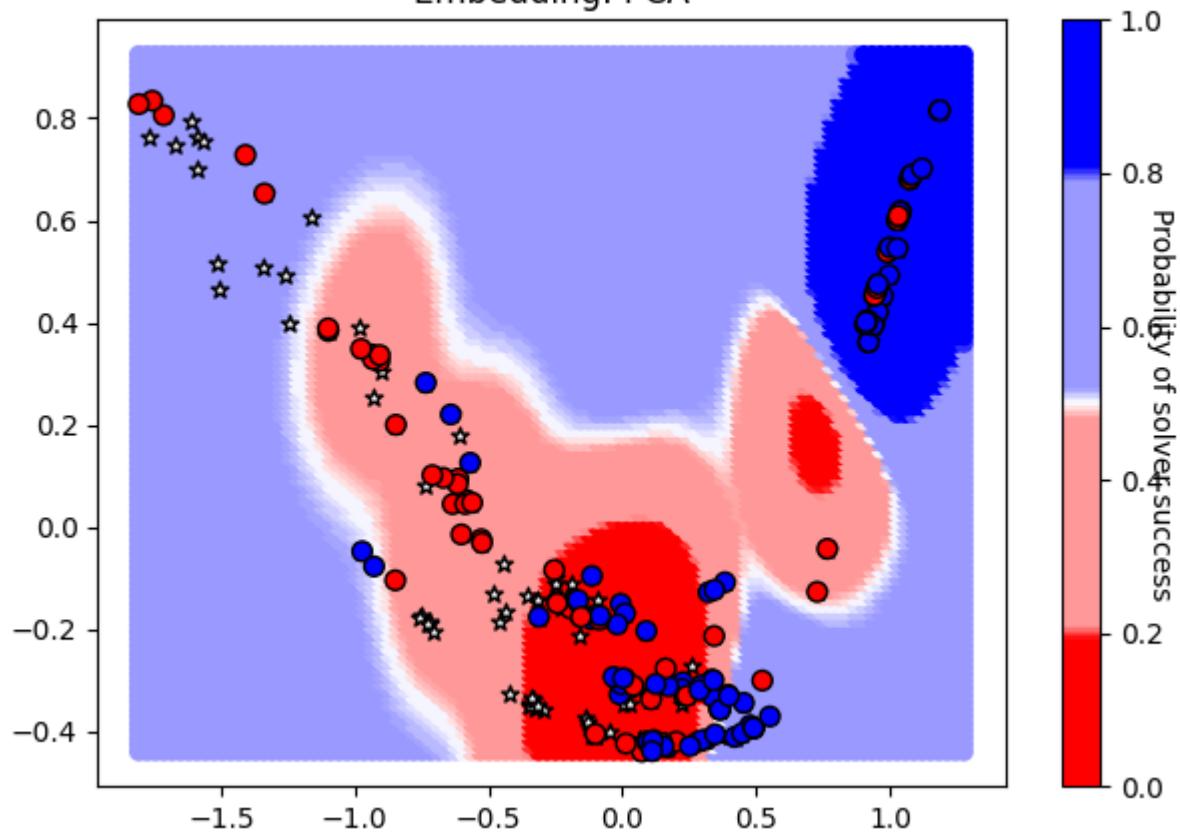
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_var\_1e-4/7e730d...

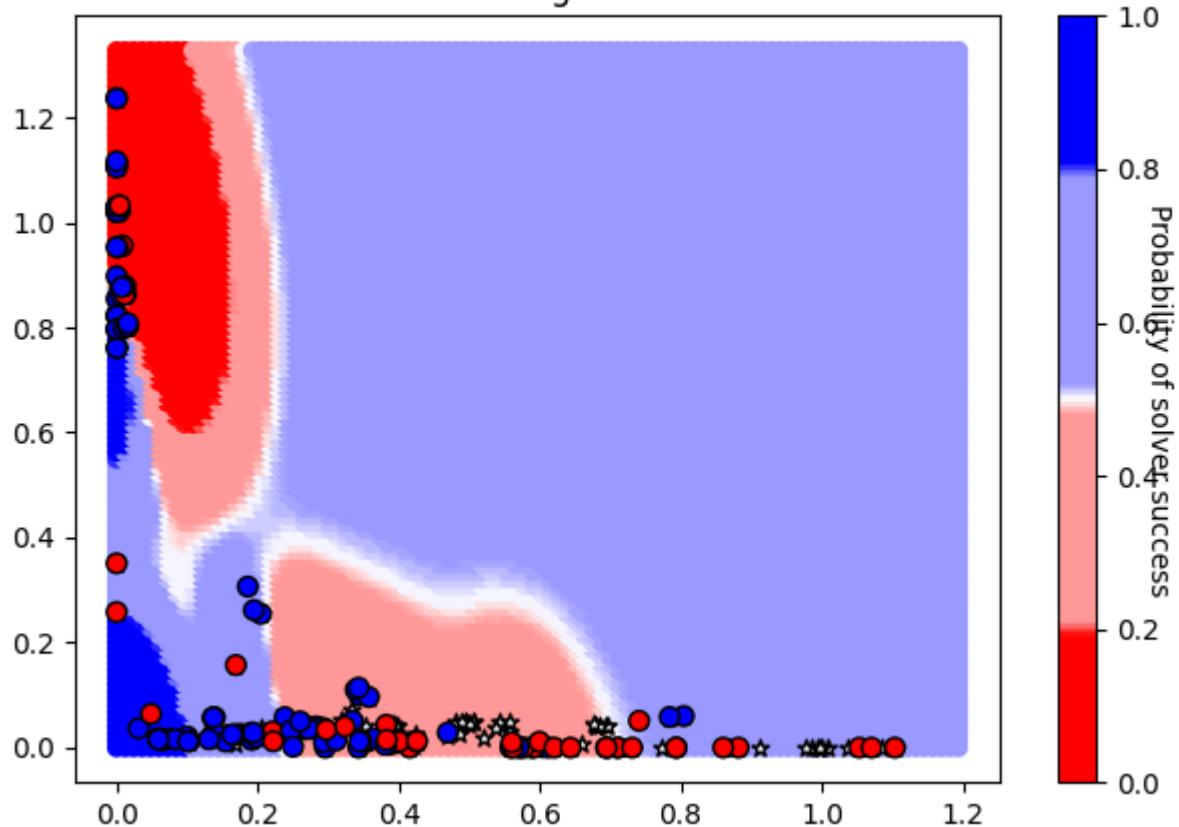
(captured: \$1.0e+02/1.5e+07, approximately 6.8e-04%)



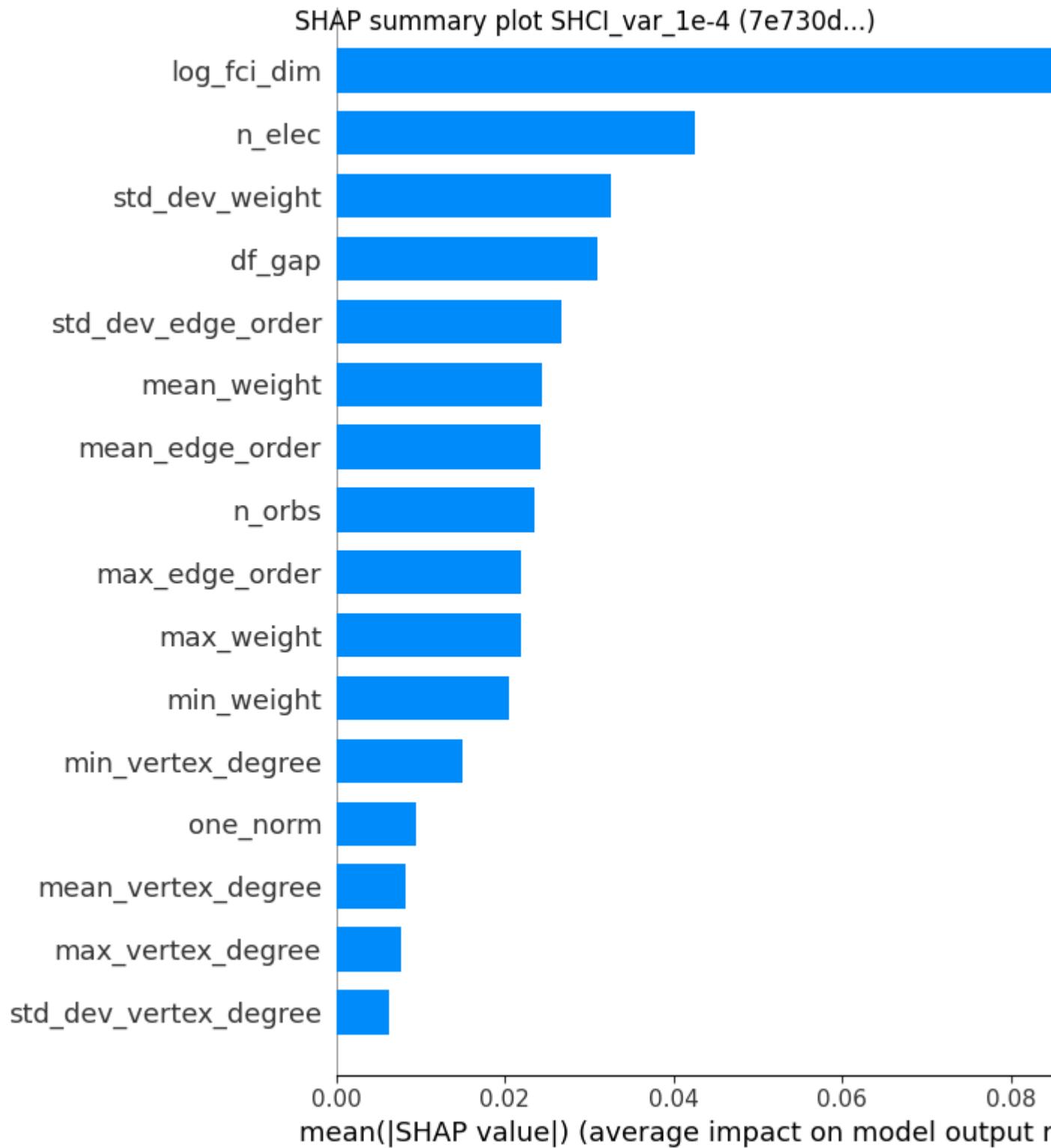
Solver SHCI\_var\_1e-4 (7e730d...)  
Embedding: PCA



Solver SHCI\_var\_1e-4 (7e730d...)  
Embedding: NMF



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.

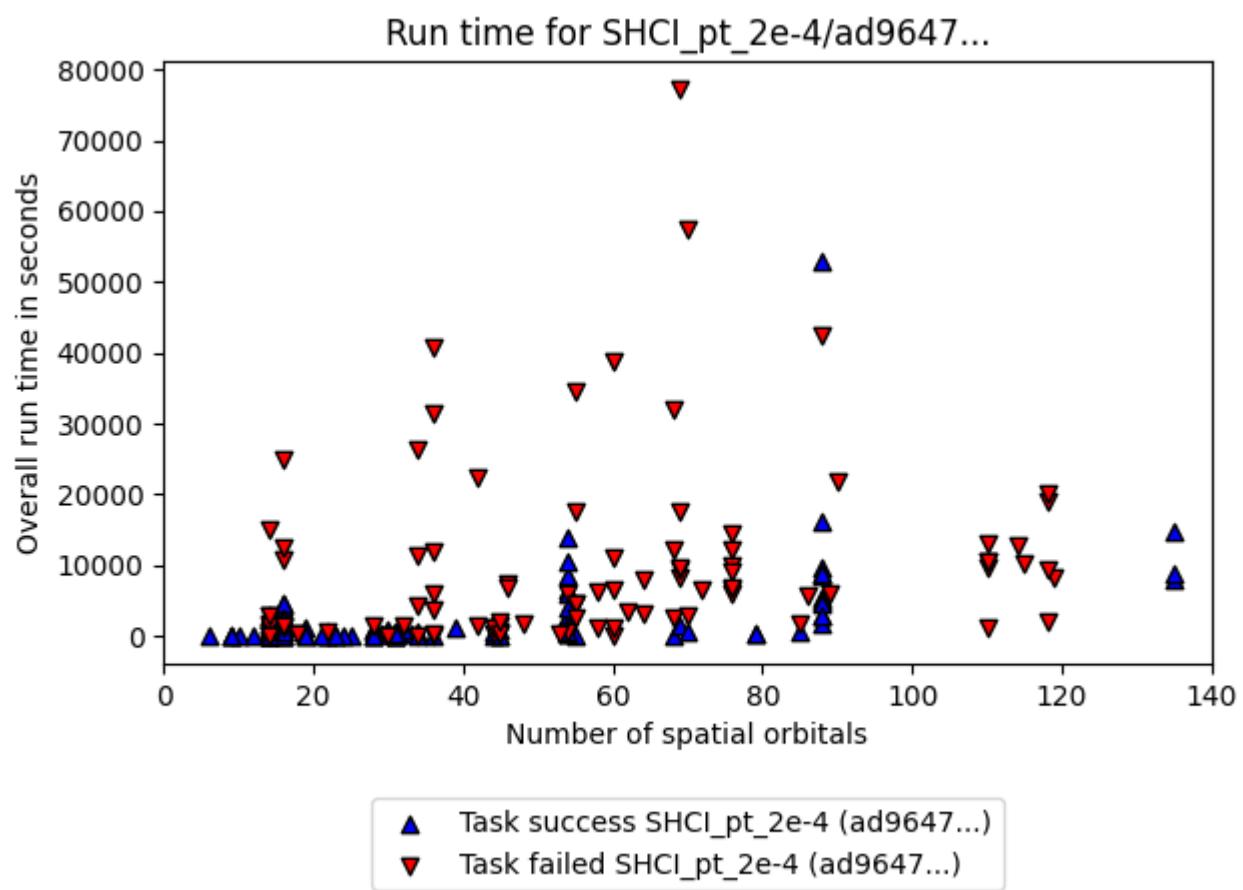


## Solver SHCI\_pt\_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb

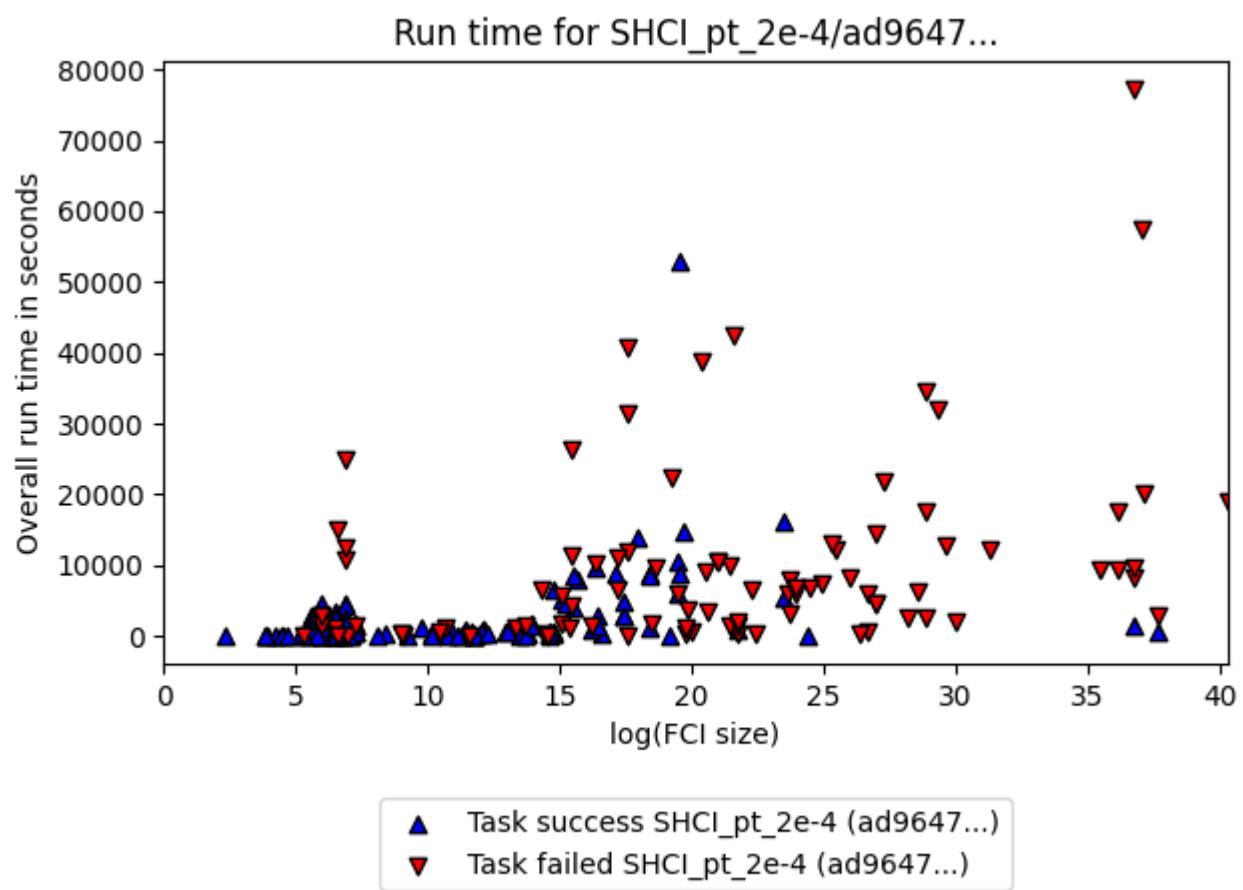
solver\_uuid:ad964781-302e-4728-a26d-39918e0a6cdb

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: 707e7860-ed13-484d-8542-aa8a0cde5a97  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 22  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 128  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 128  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 1.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.6486486486486487, 0.9516728624535316]  
ml\_metrics\_calculator\_version: 1



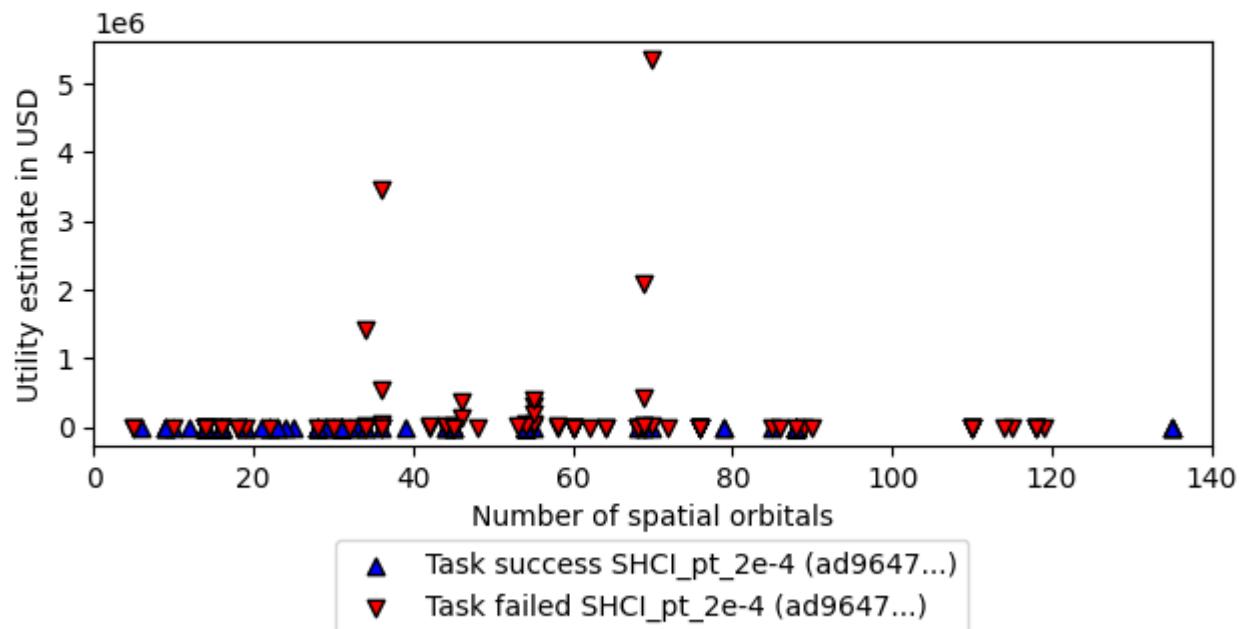
Note: plot only contains attempted tasks.



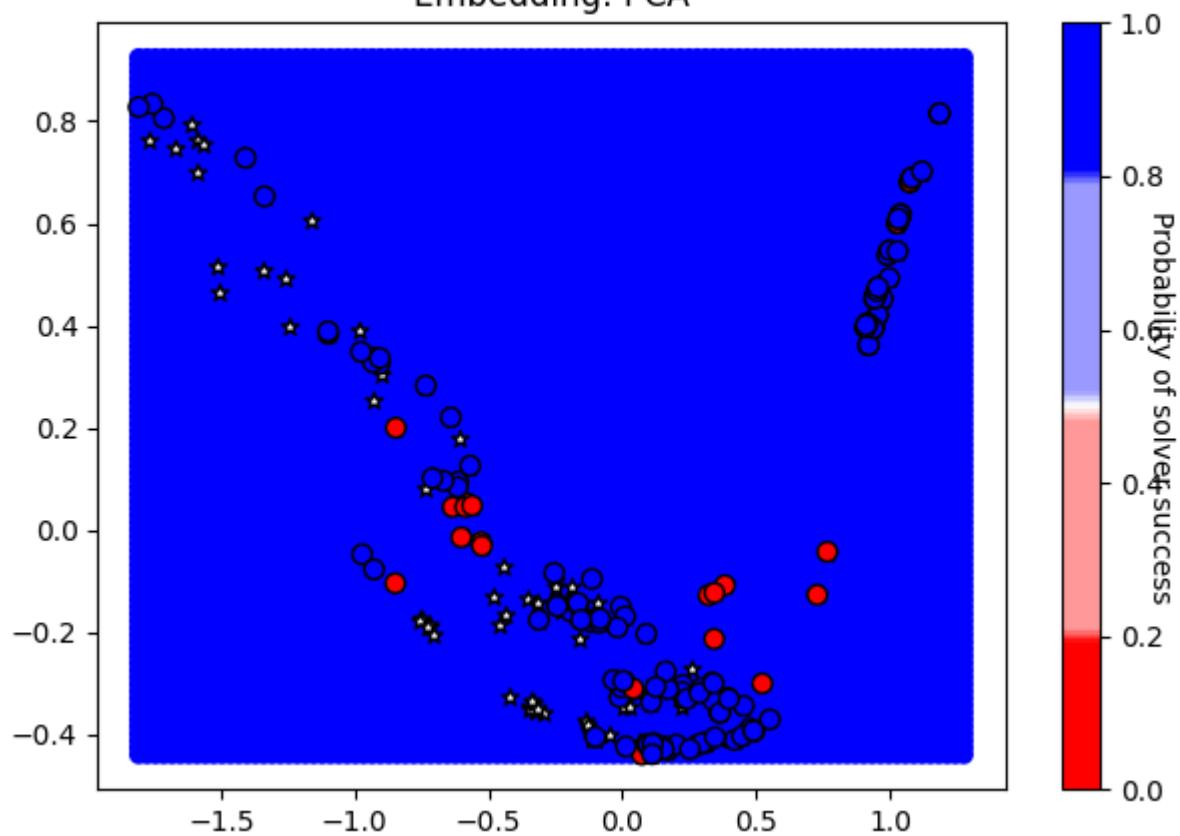
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_pt\_2e-4/ad9647...

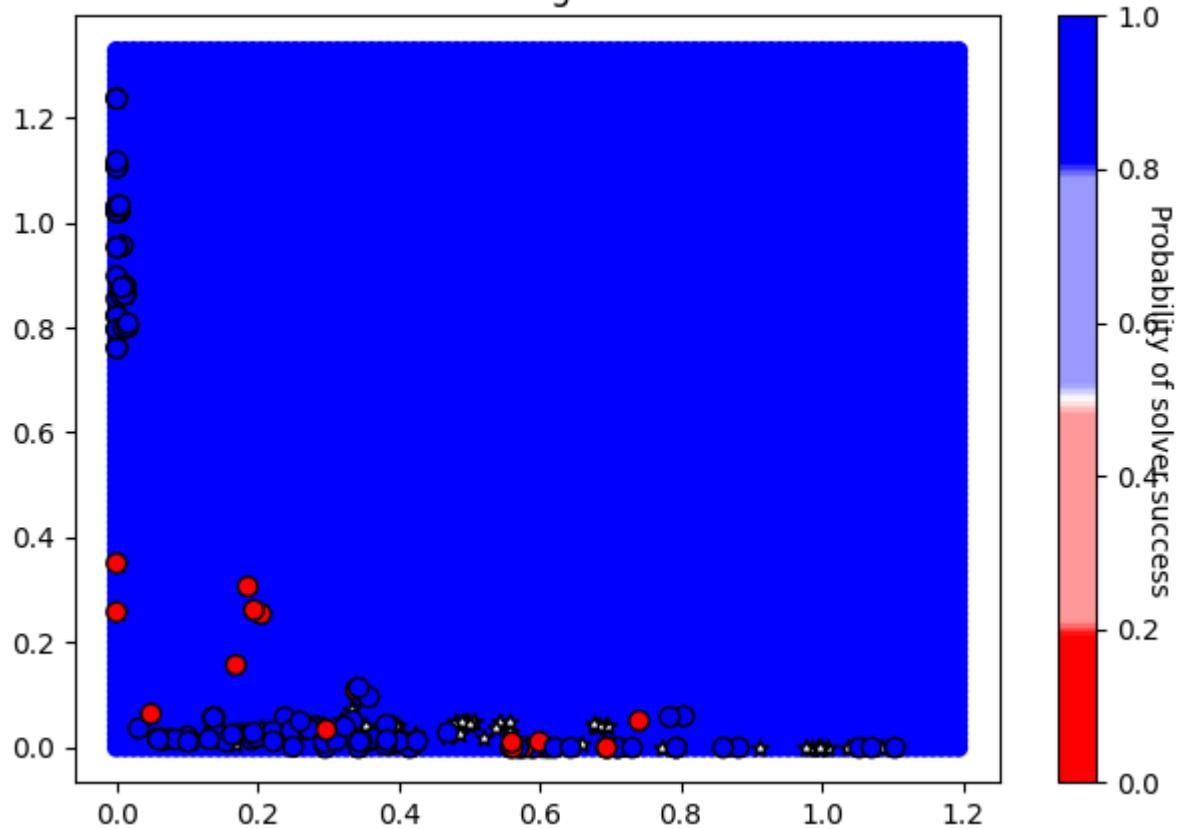
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



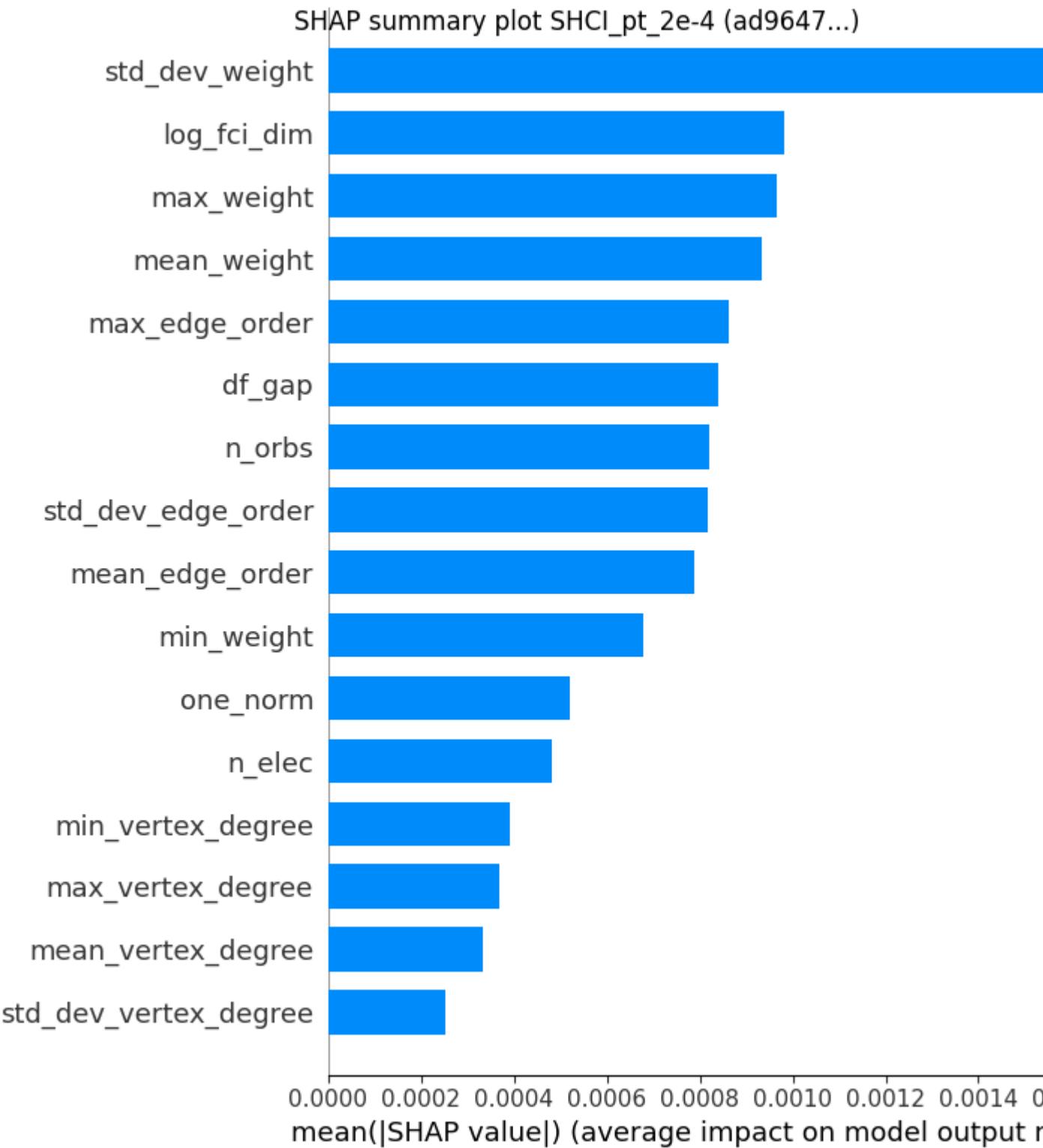
Solver SHCI\_pt\_2e-4 (ad9647...)  
Embedding: PCA



Solver SHCI\_pt\_2e-4 (ad9647...)  
Embedding: NMF



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.

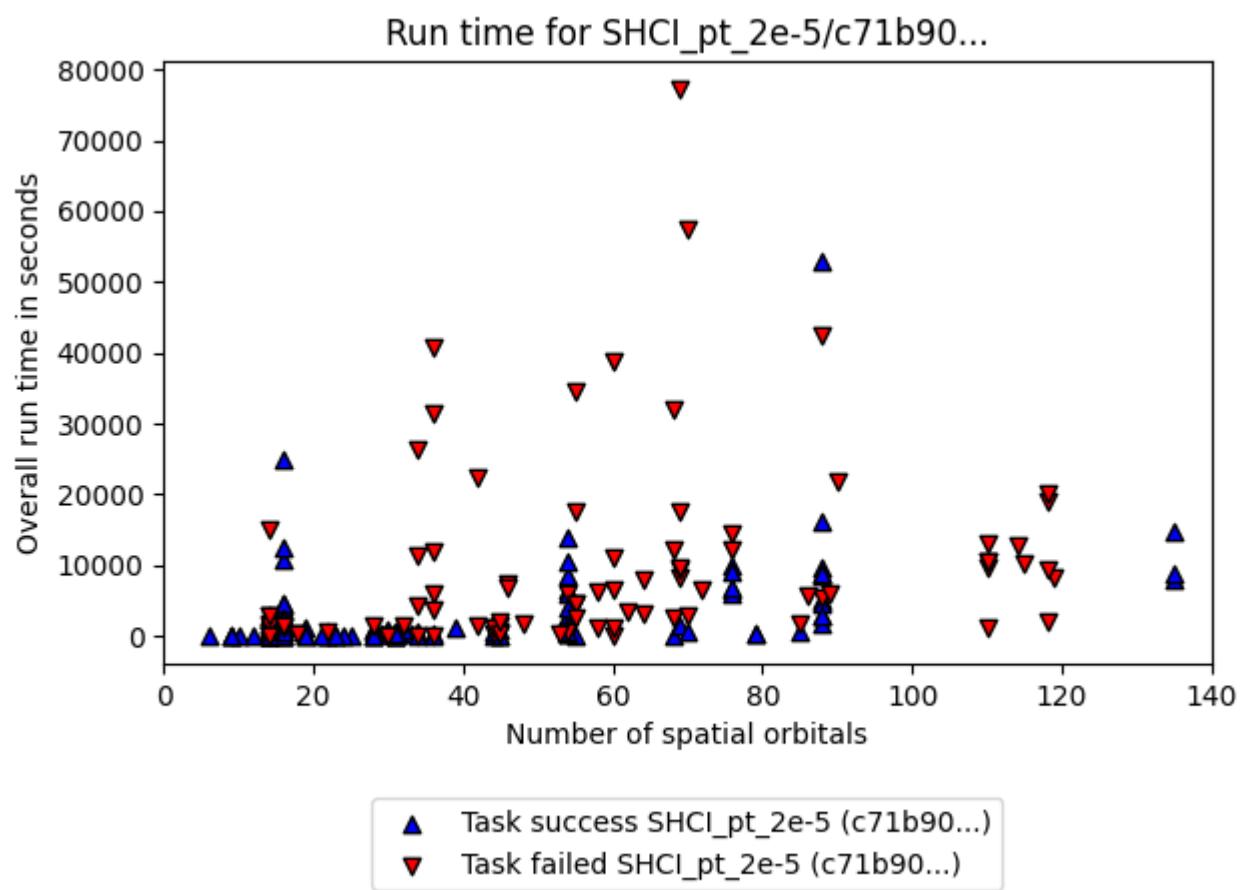


## Solver SHCI\_pt\_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6

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

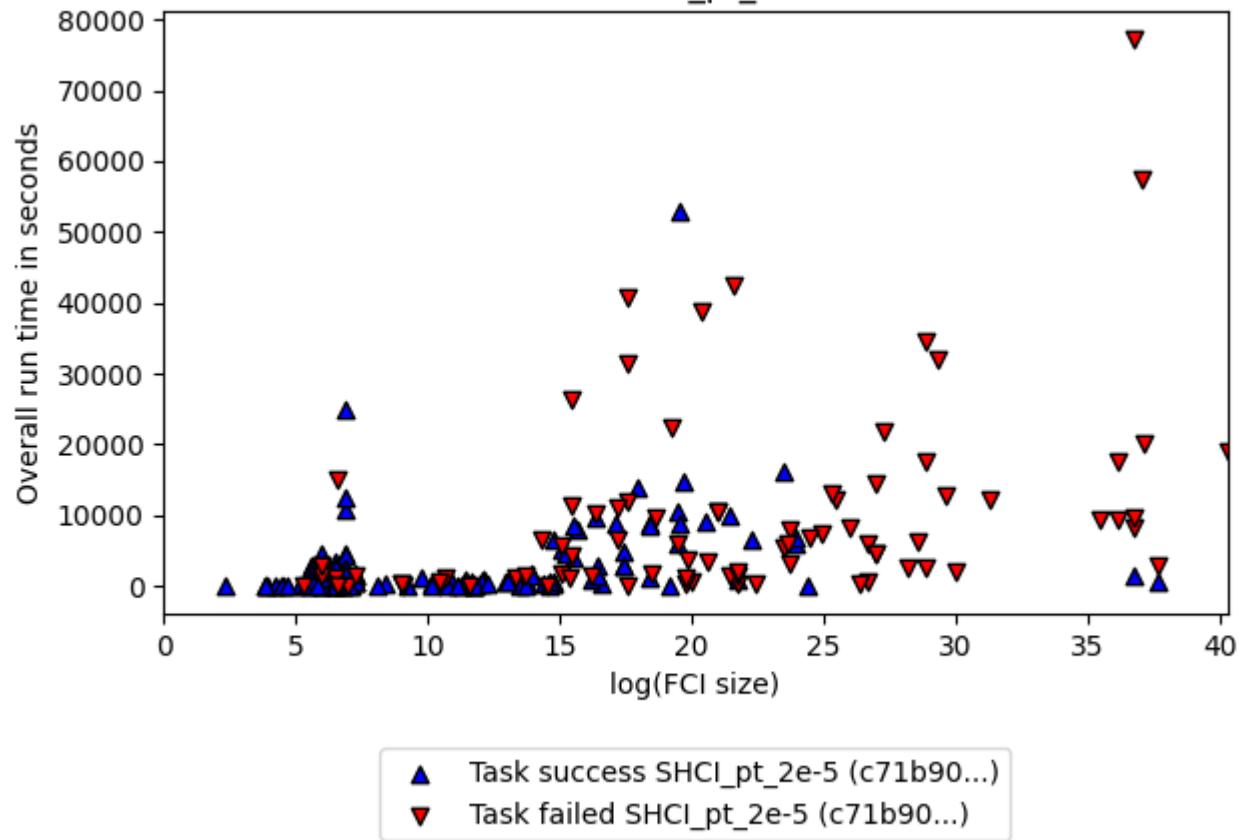
solver\_short\_name:SHCI\_pt\_2e-5

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: 18dfe585-5d46-43d4-86f3-aefd83975476  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 26  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 136  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 136  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 1.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.7428571428571429, 0.966789667896679]  
ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

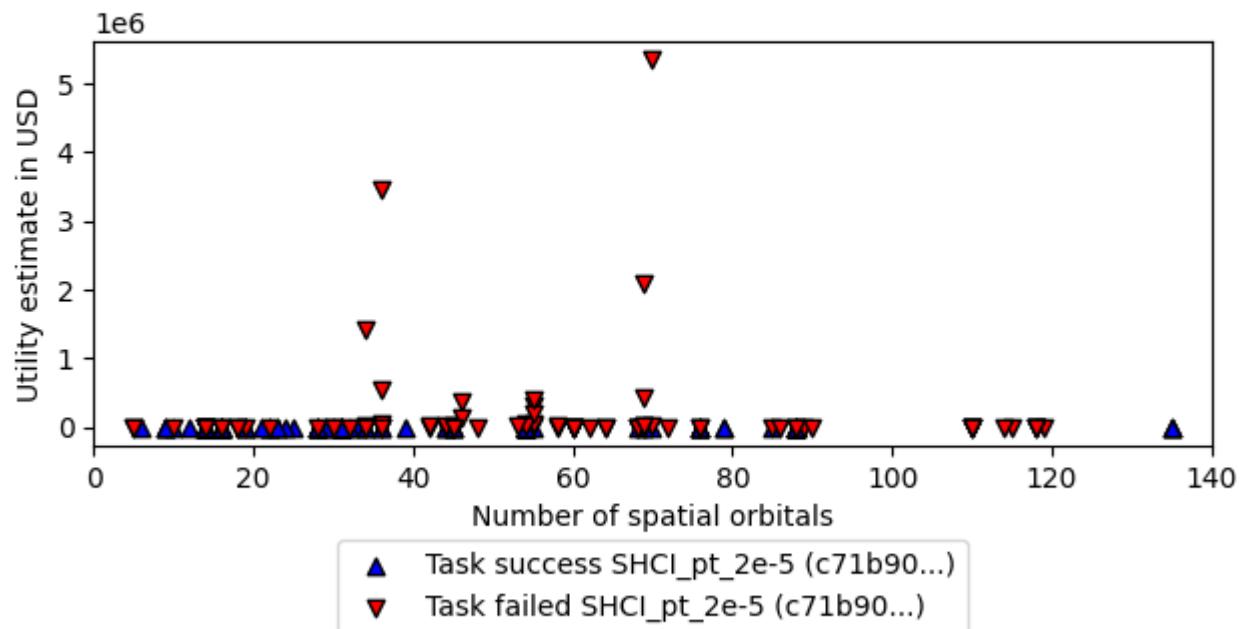
### Run time for SHCI\_pt\_2e-5/c71b90...



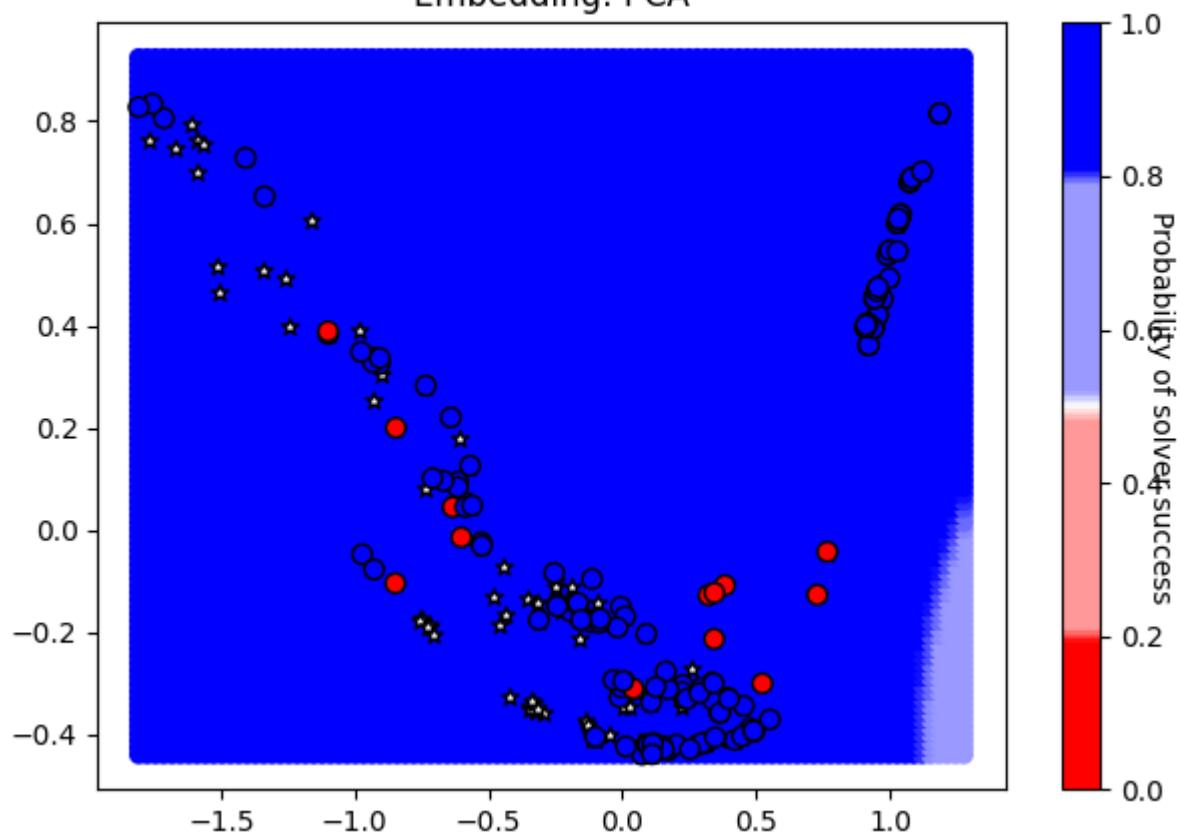
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_pt\_2e-5/c71b90...

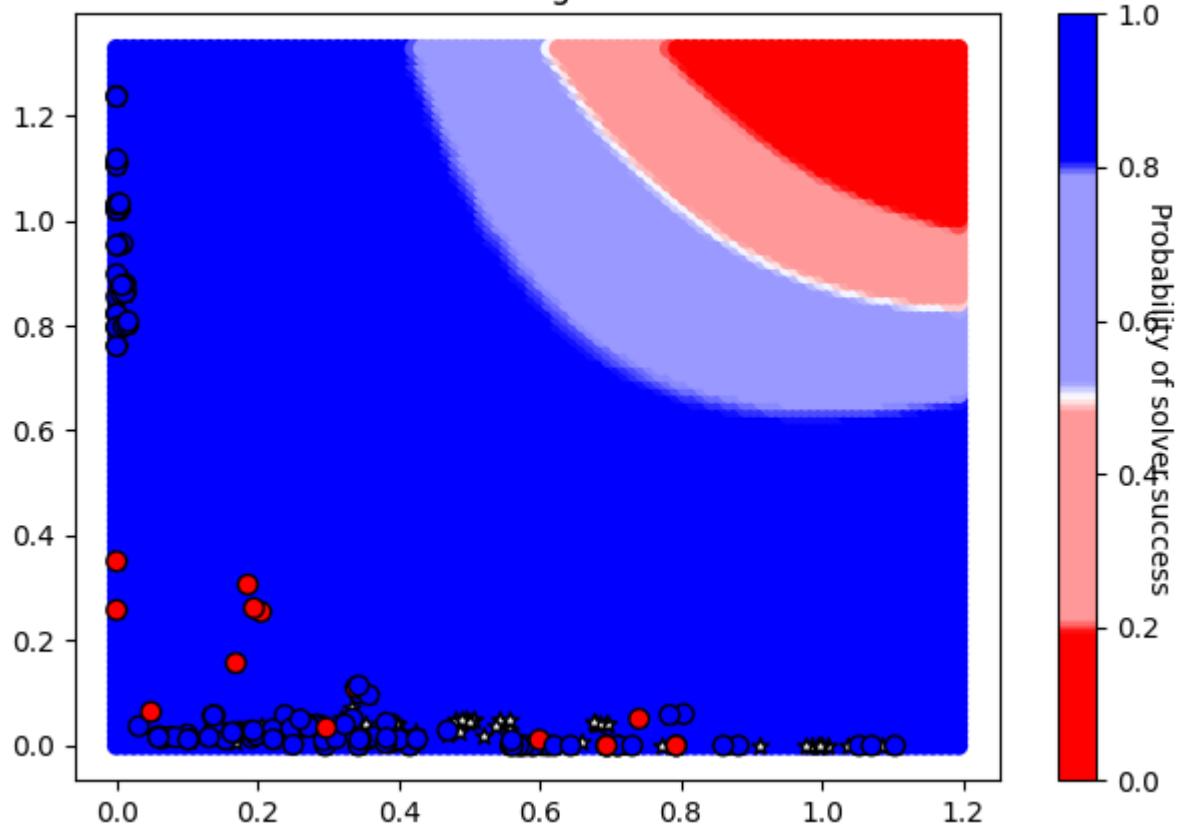
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



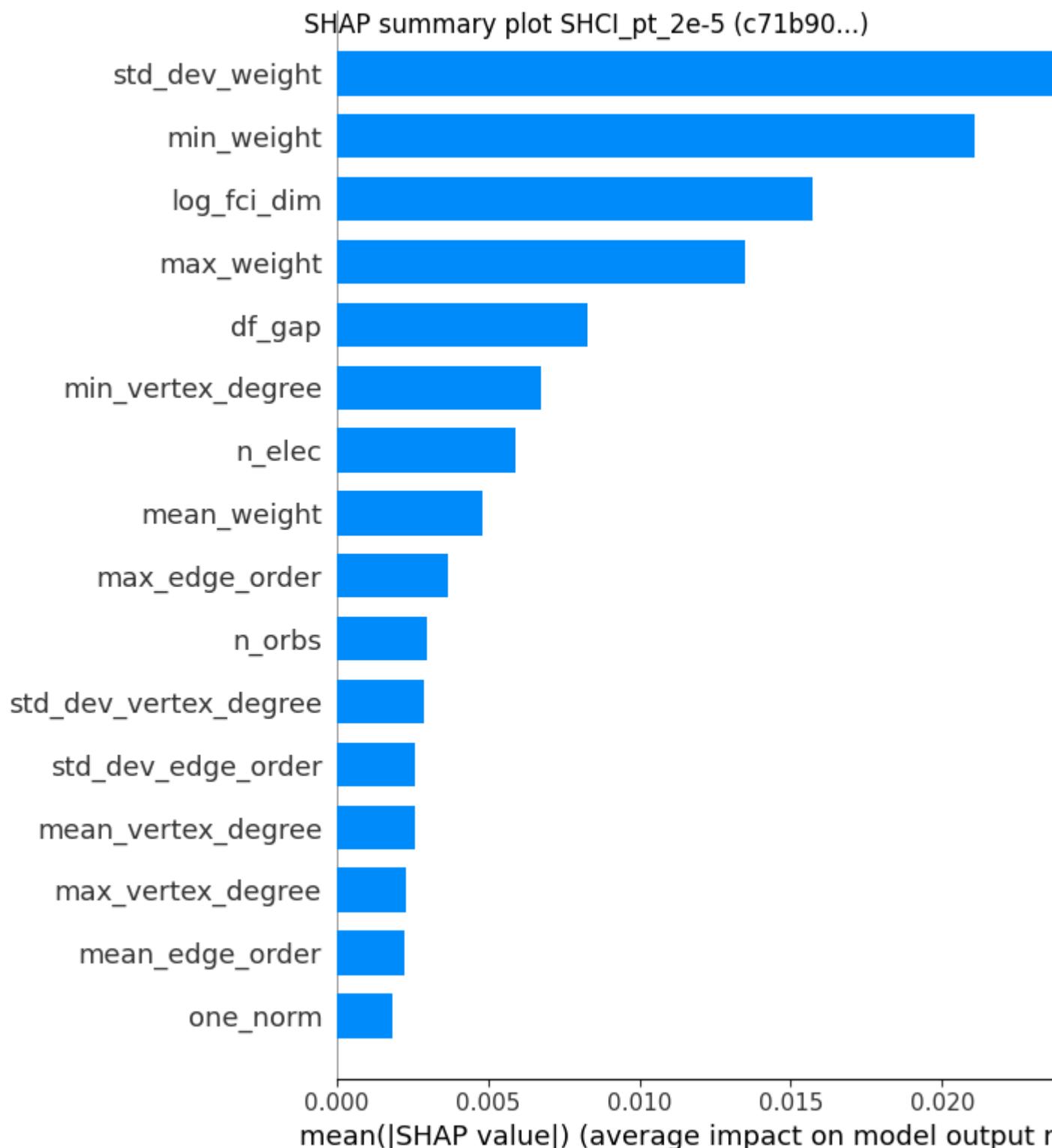
Solver SHCI\_pt\_2e-5 (c71b90...)  
Embedding: PCA



Solver SHCI\_pt\_2e-5 (c71b90...)  
Embedding: NMF



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.

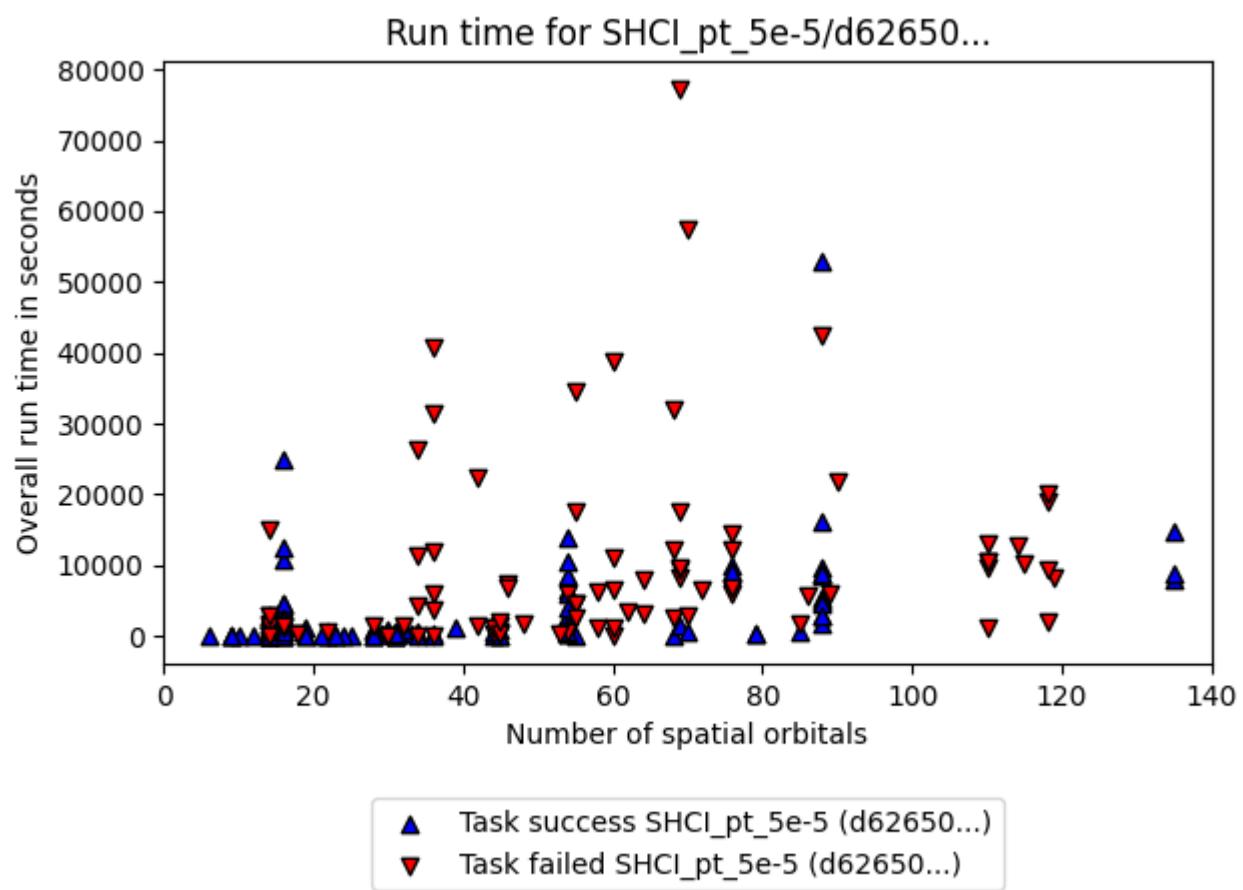


## Solver SHCI\_pt\_5e-5, d626506c-7aae-4ad6-802a-b29af5f2bb93

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

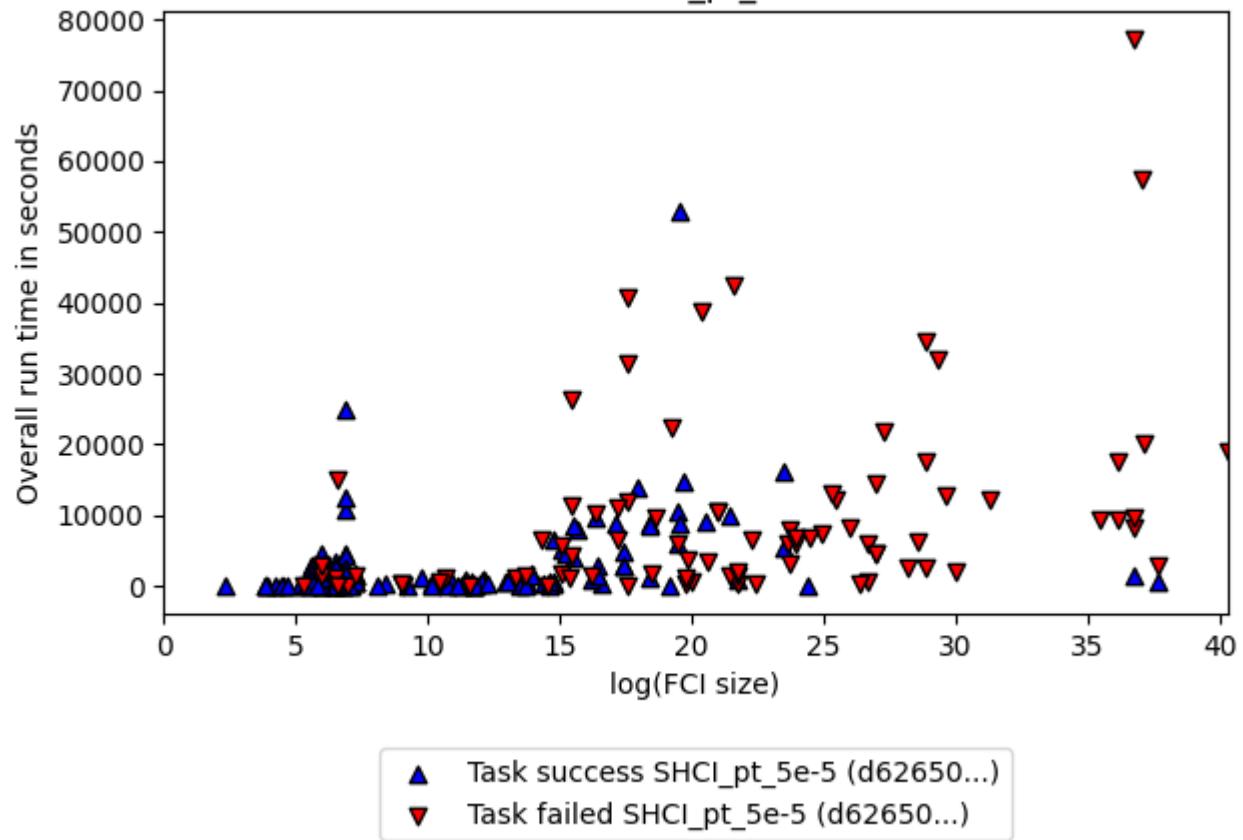
solver\_short\_name:SHCI\_pt\_5e-5

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: e3800070-0741-4d53-b19b-0e81438ad9b8  
creation.timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 24  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 134  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 134  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 1.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.8, 0.974169741697417]  
ml.metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

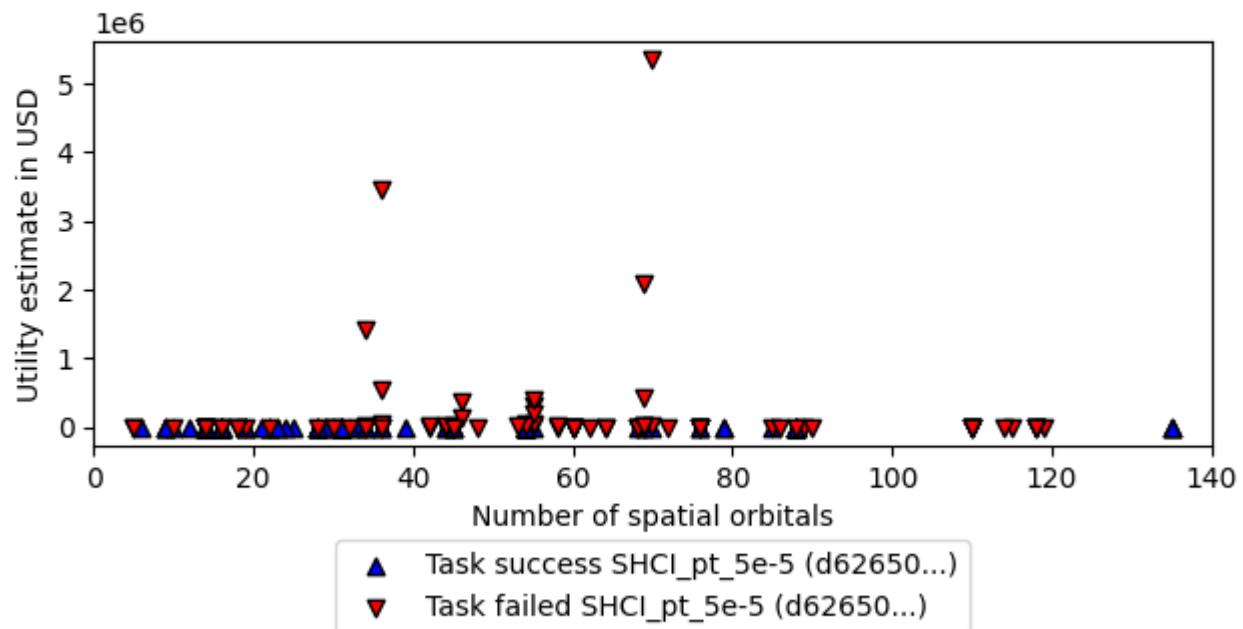
Run time for SHCI\_pt\_5e-5/d62650...



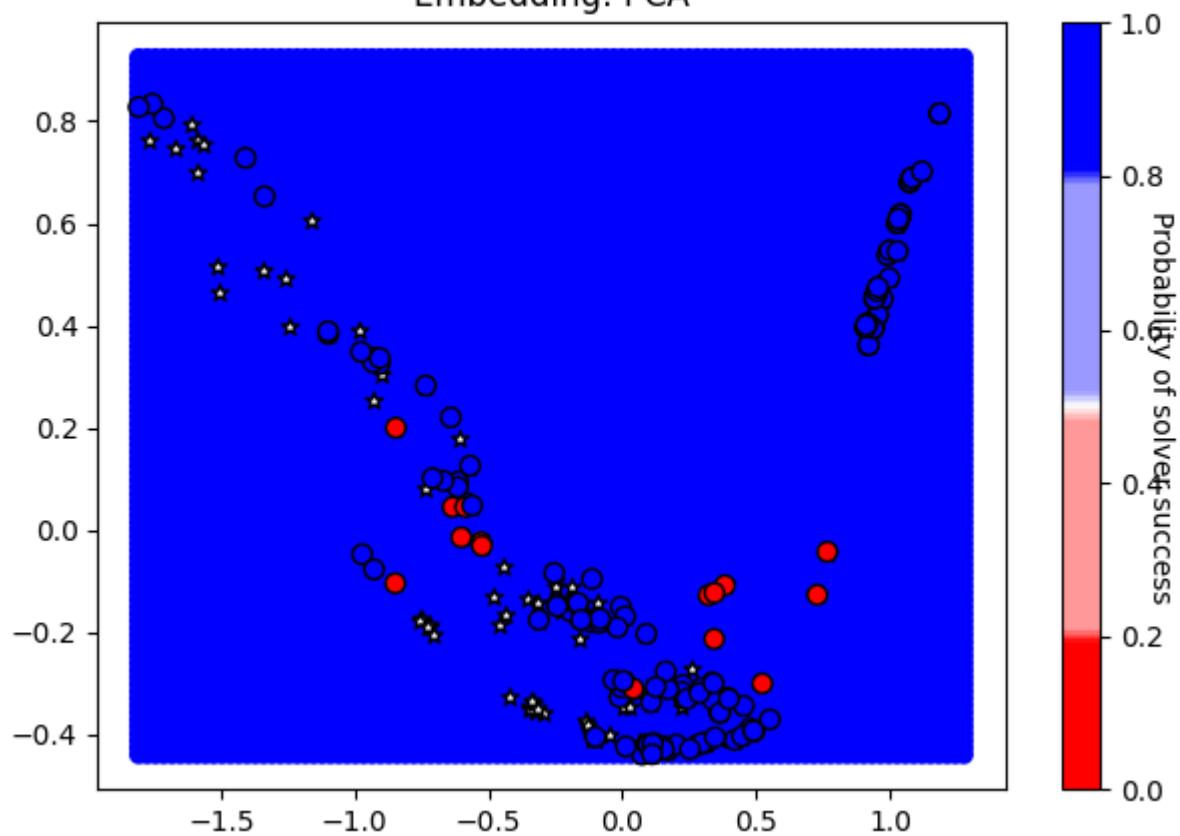
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_pt\_5e-5/d62650...

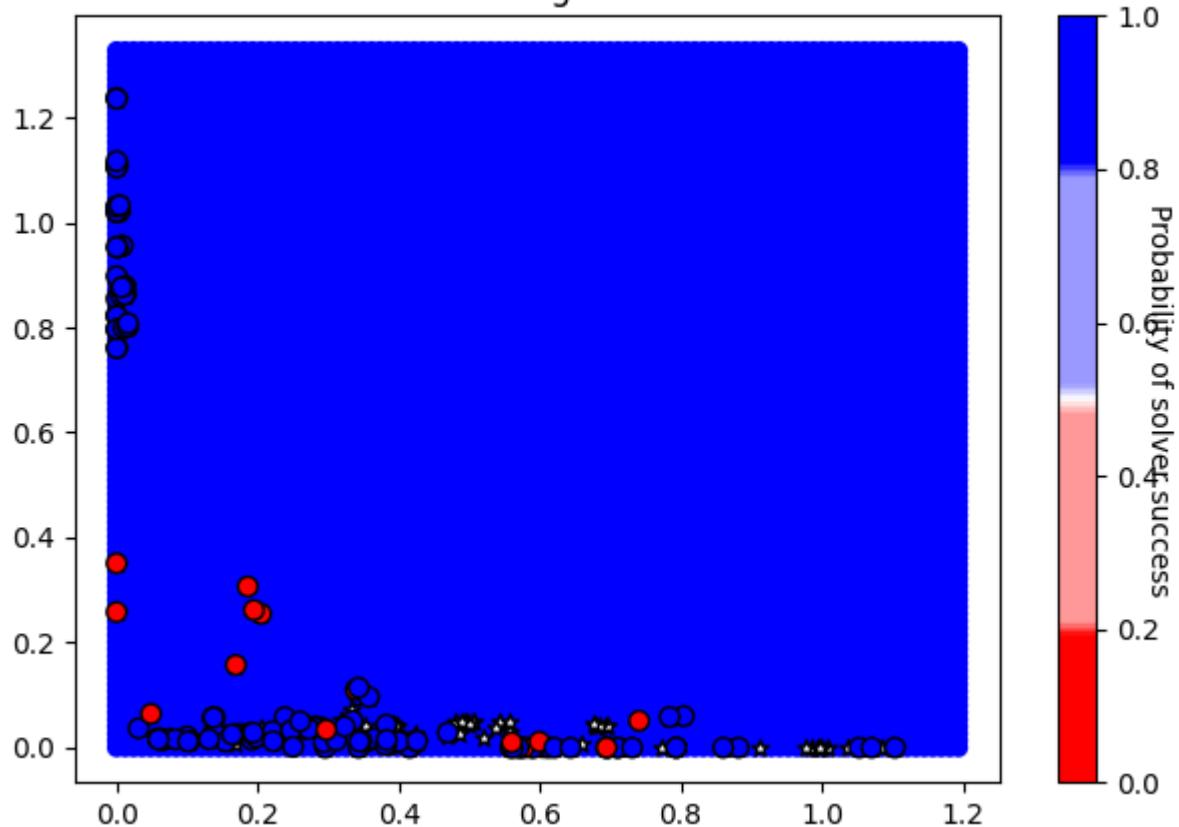
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



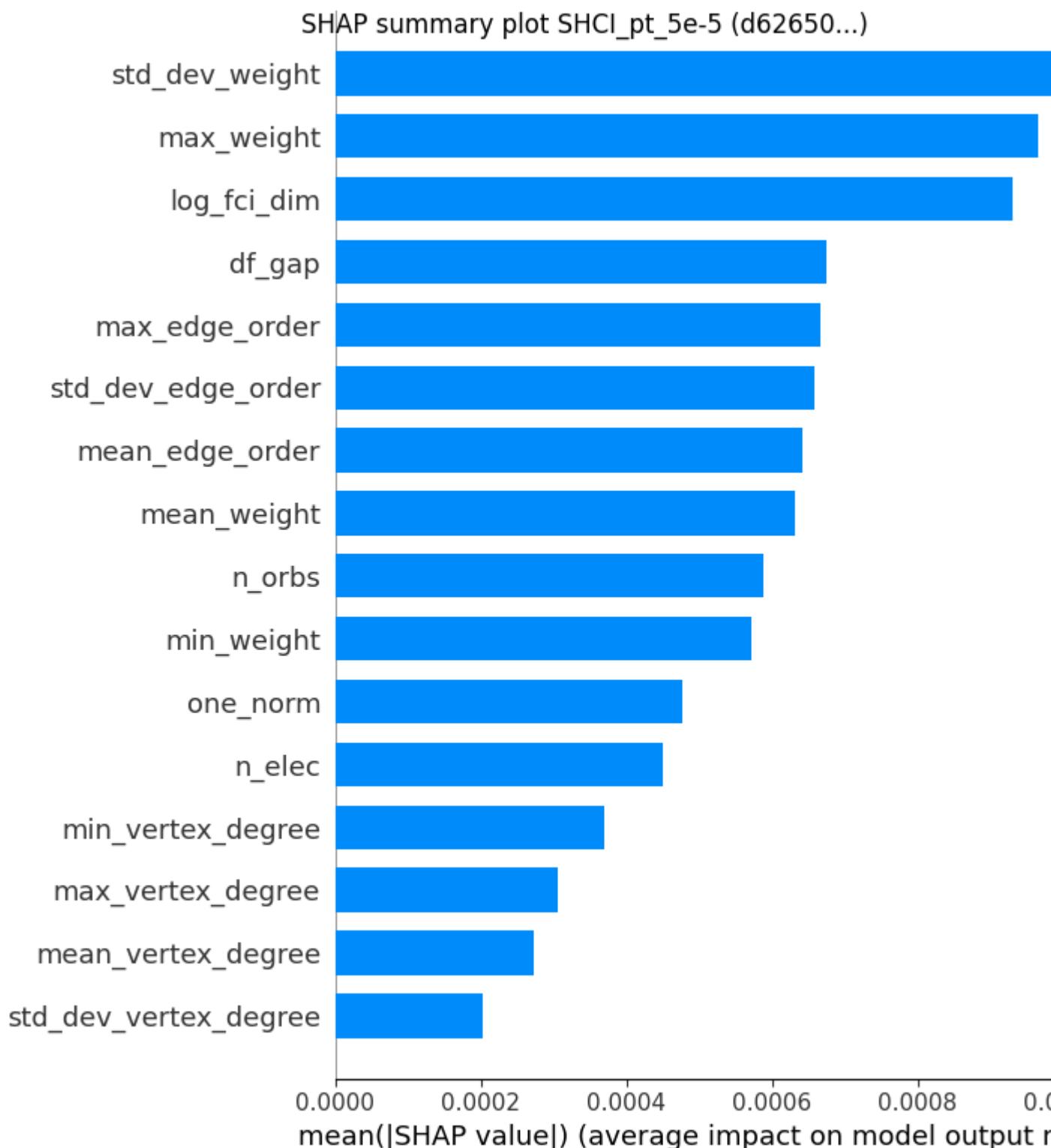
Solver SHCI\_pt\_5e-5 (d62650...)  
Embedding: PCA



Solver SHCI\_pt\_5e-5 (d62650...)  
Embedding: NMF



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.

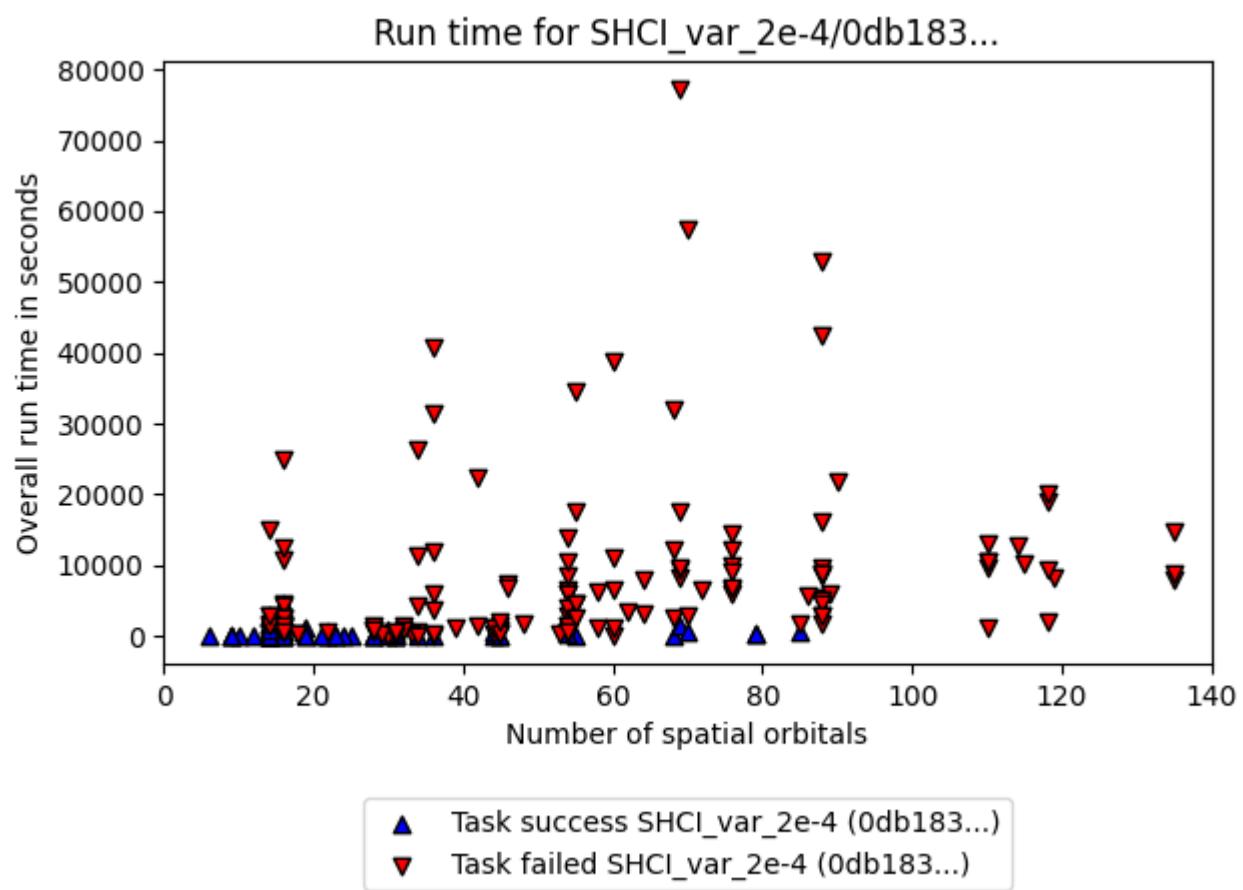


## Solver SHCI\_var\_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a

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

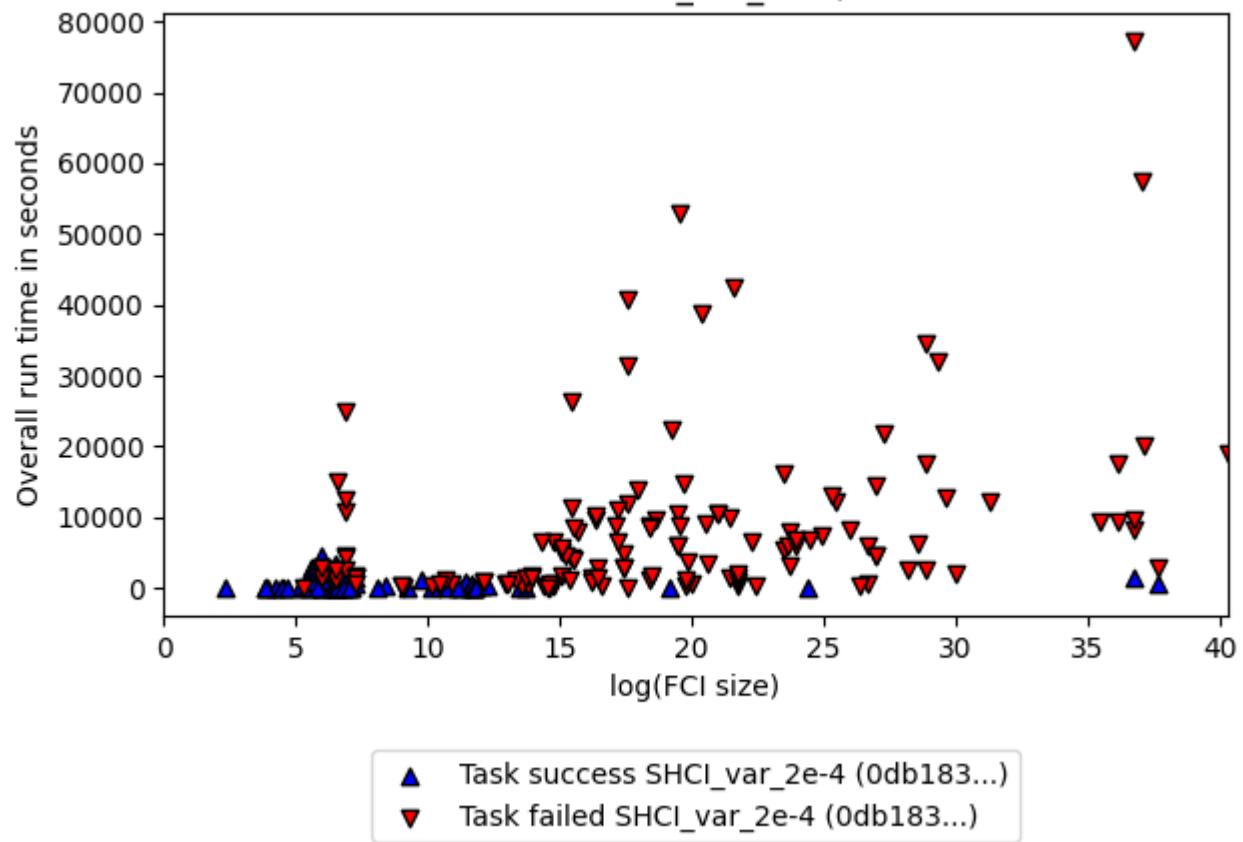
solver\_short\_name:SHCI\_var\_2e-4

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: 71409bbf-b9ac-4f18-b5f6-e84b91d95ac3  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 13  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 79  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 79  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 0.7146  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9863013698630136, 0.9875]  
ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

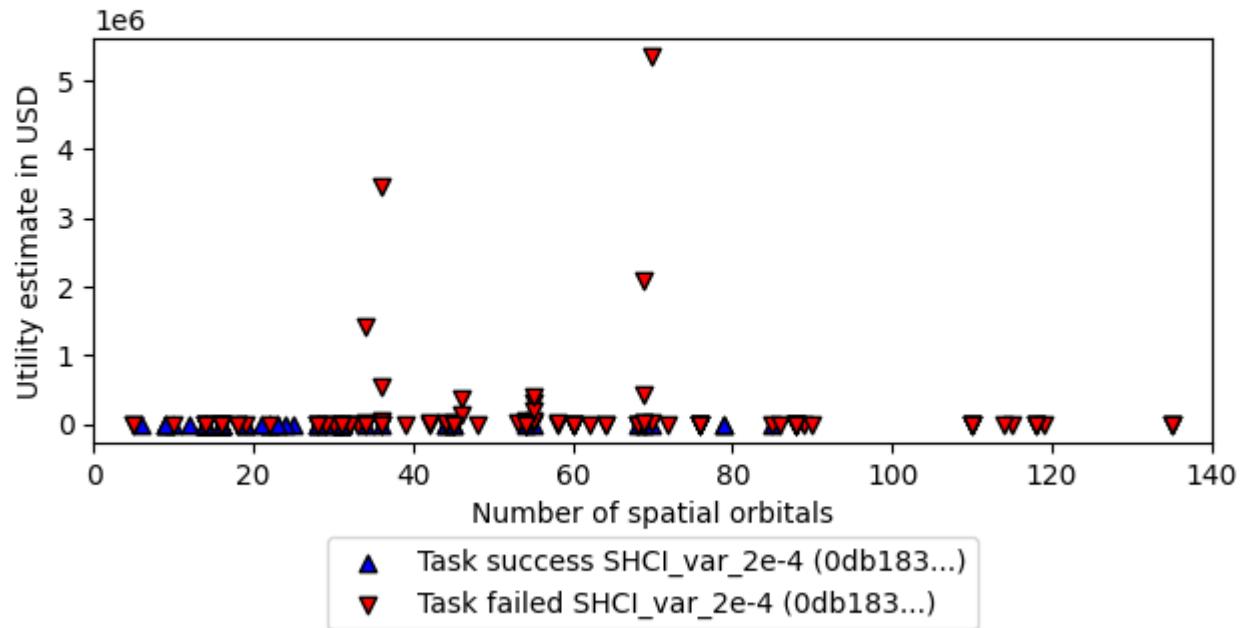
### Run time for SHCI\_var\_2e-4/0db183...



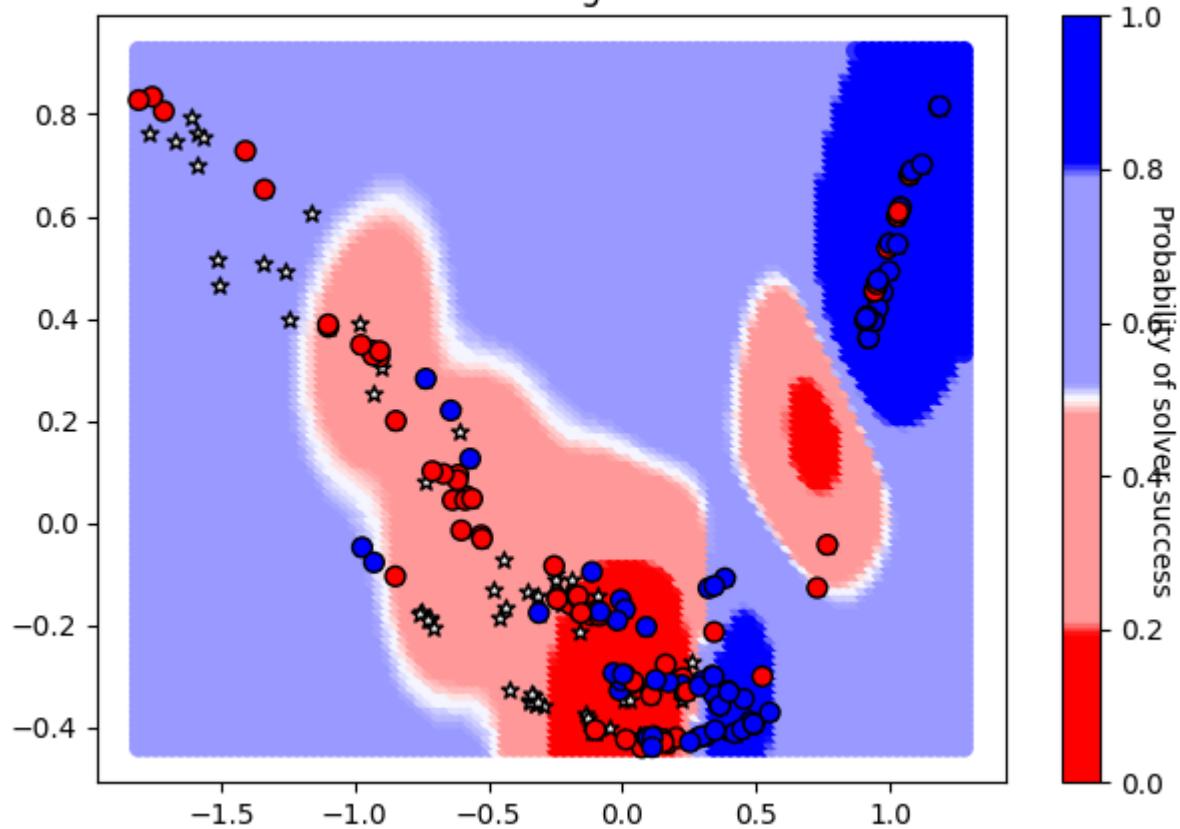
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_var\_2e-4/0db183...

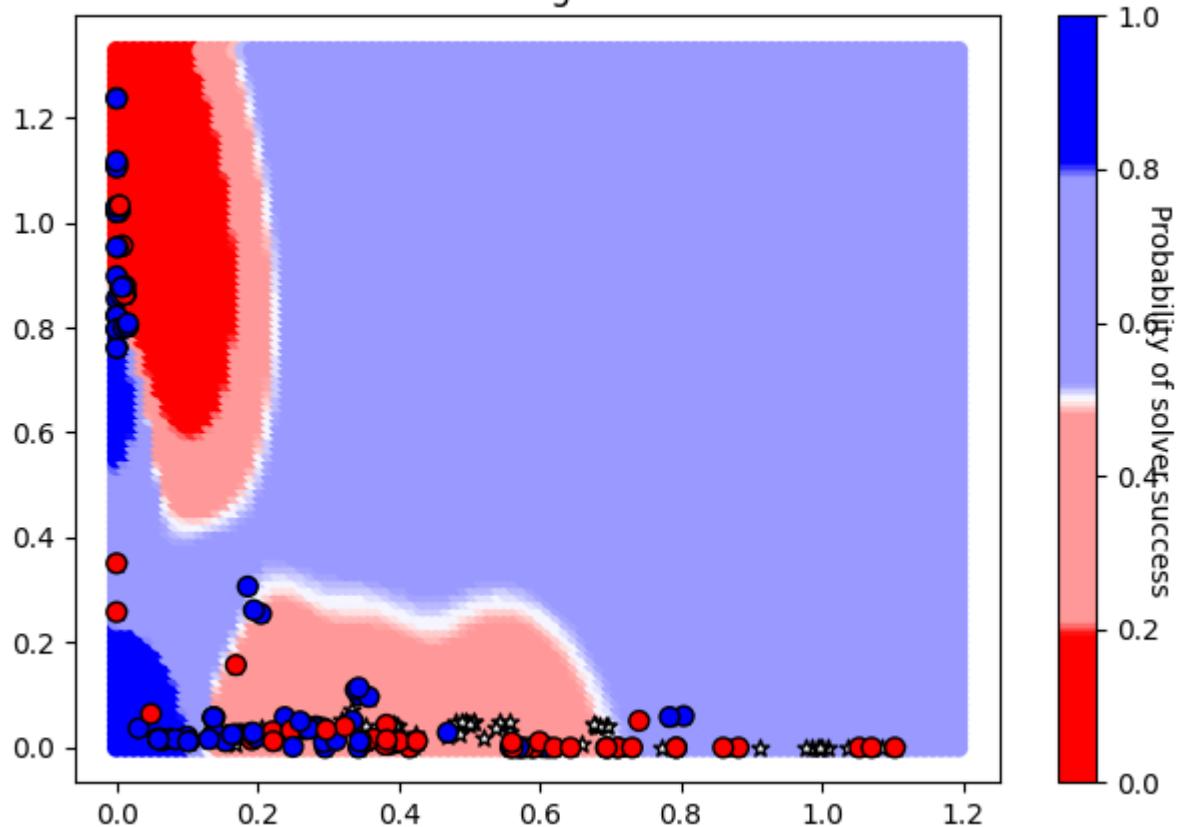
(captured: \$8.6e+01/1.5e+07, approximately 5.8e-04%)



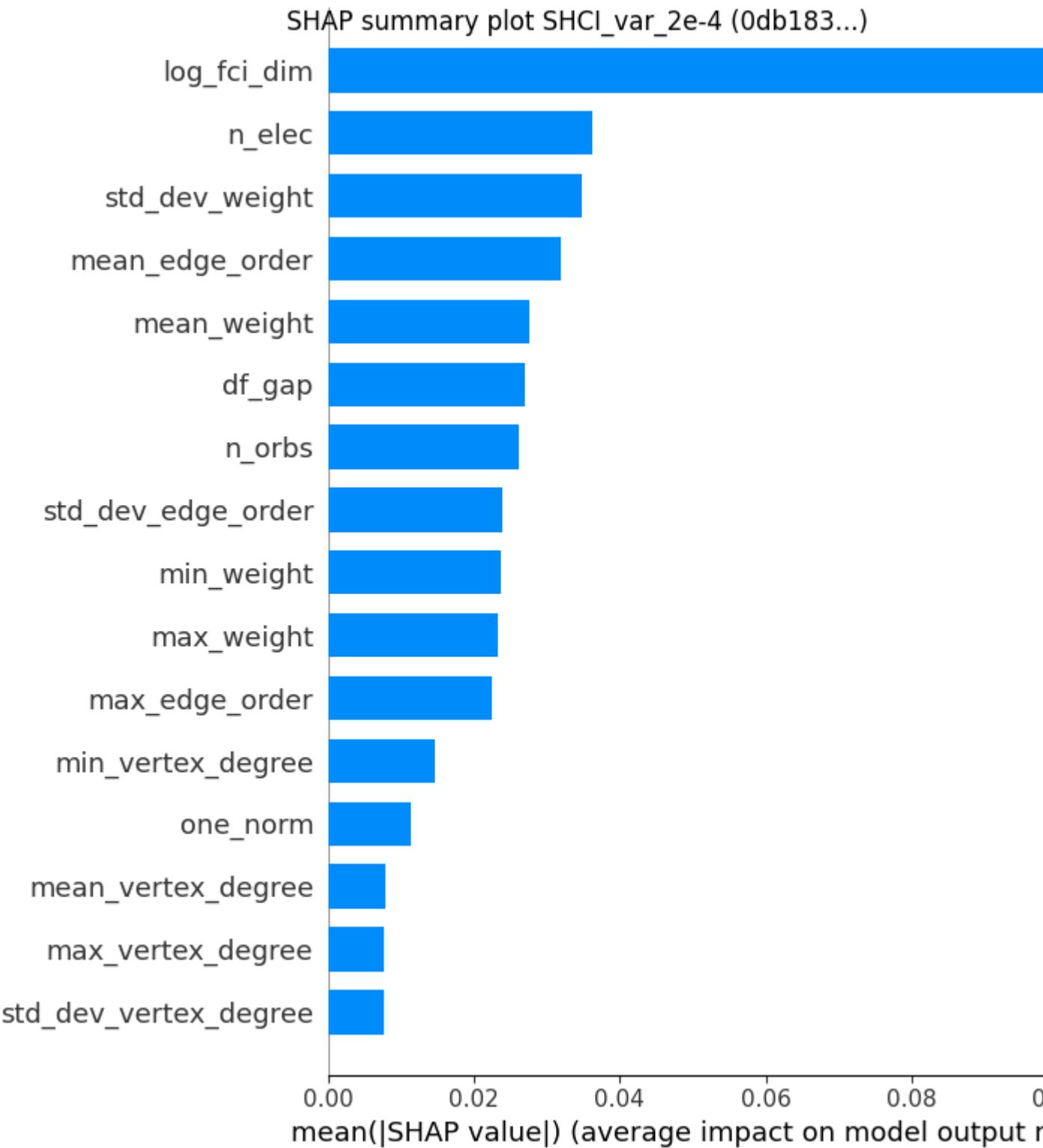
Solver SHCI\_var\_2e-4 (0db183...)  
Embedding: PCA



Solver SHCI\_var\_2e-4 (0db183...)  
Embedding: NMF



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.

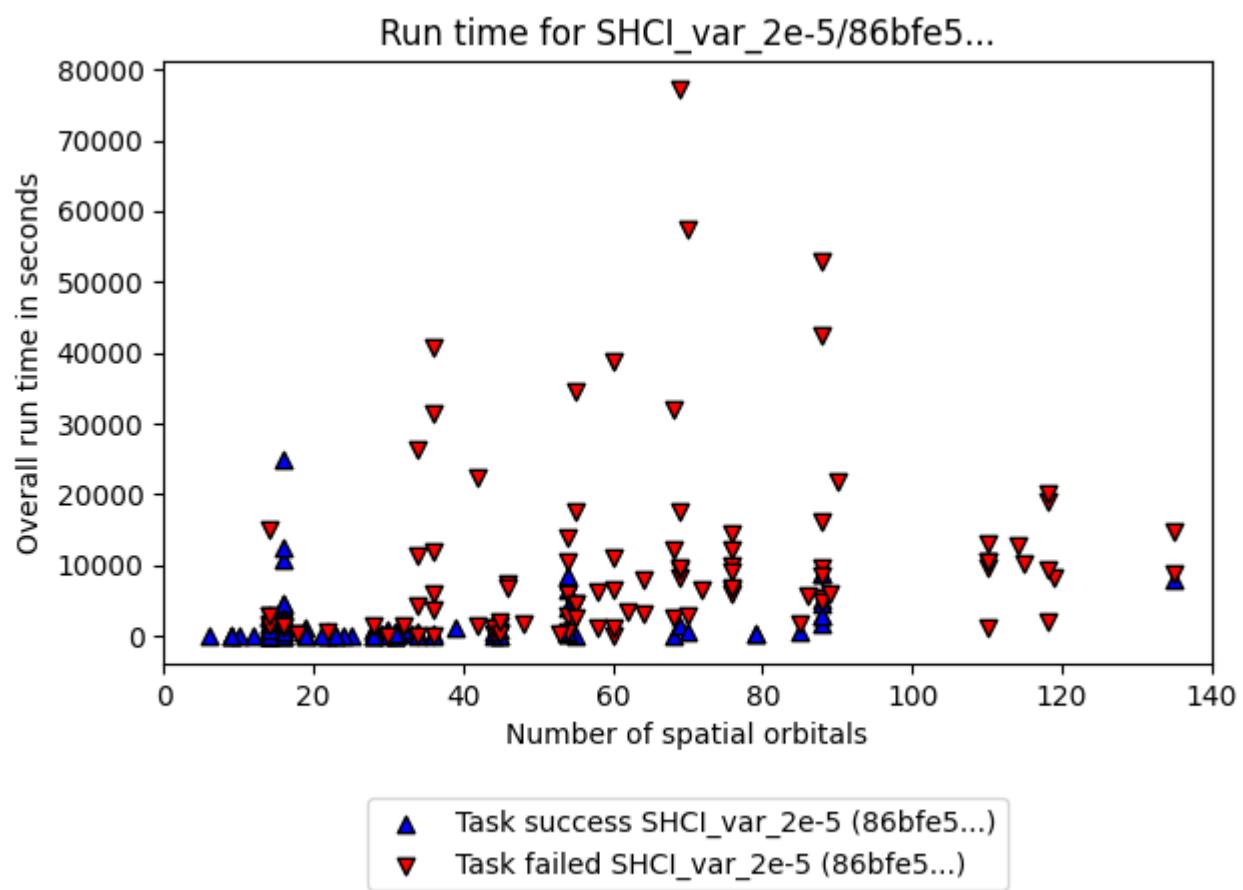


## Solver SHCI\_var\_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688

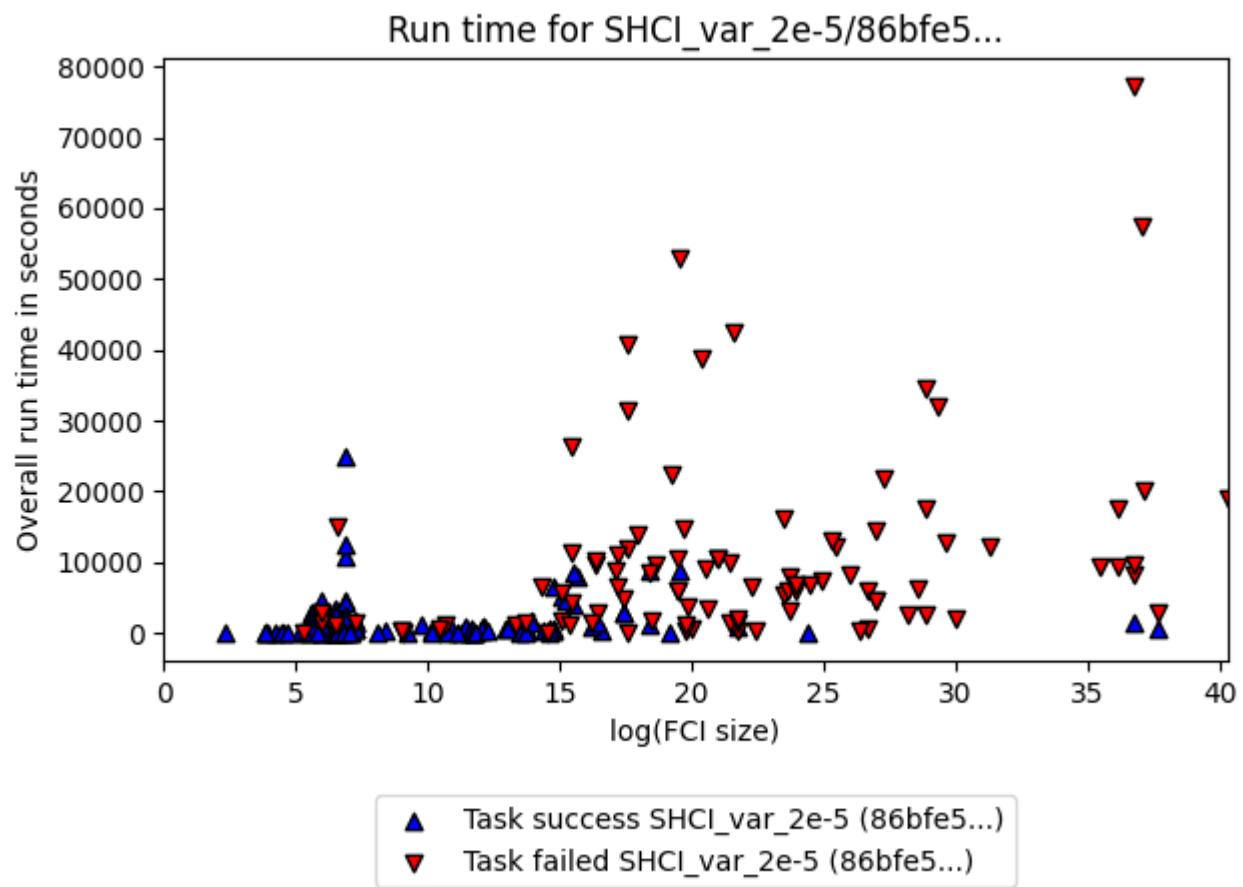
solver\_uuid:86bfe50c-9342-4d54-bb68-abc8abd95688

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: 0c9d9379-36be-4f3d-92ec-fc566d0d8d6a  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 18  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 124  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 124  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 0.5598  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.819672131147541, 0.9551020408163265]  
ml\_metrics\_calculator\_version: 1



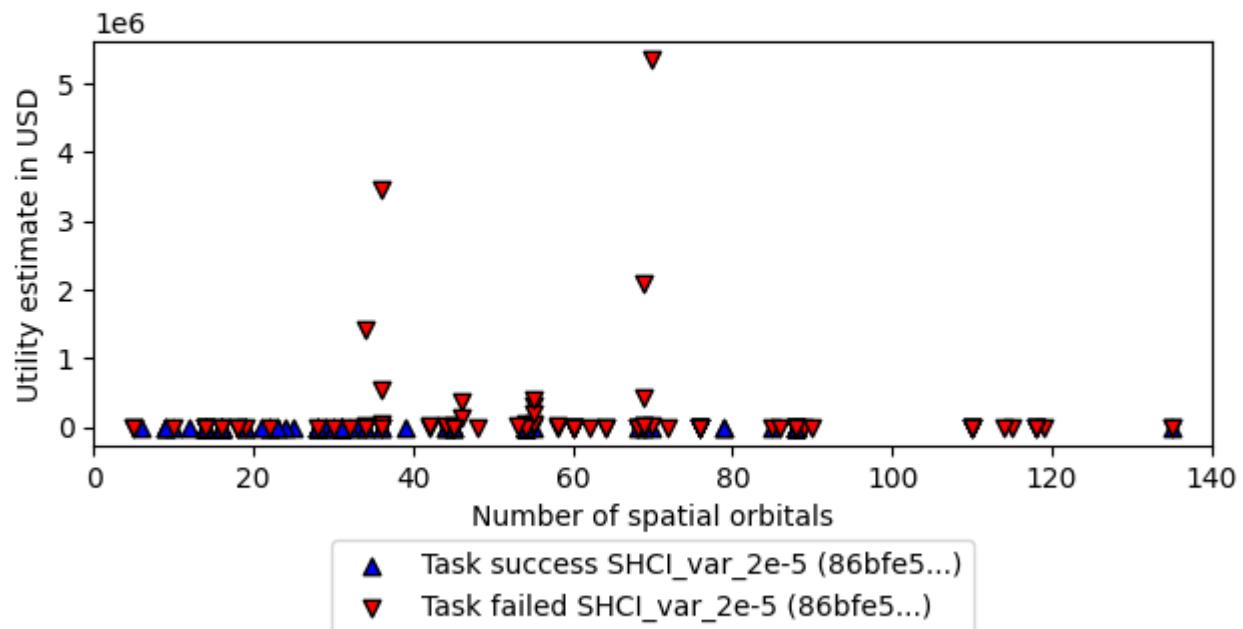
Note: plot only contains attempted tasks.



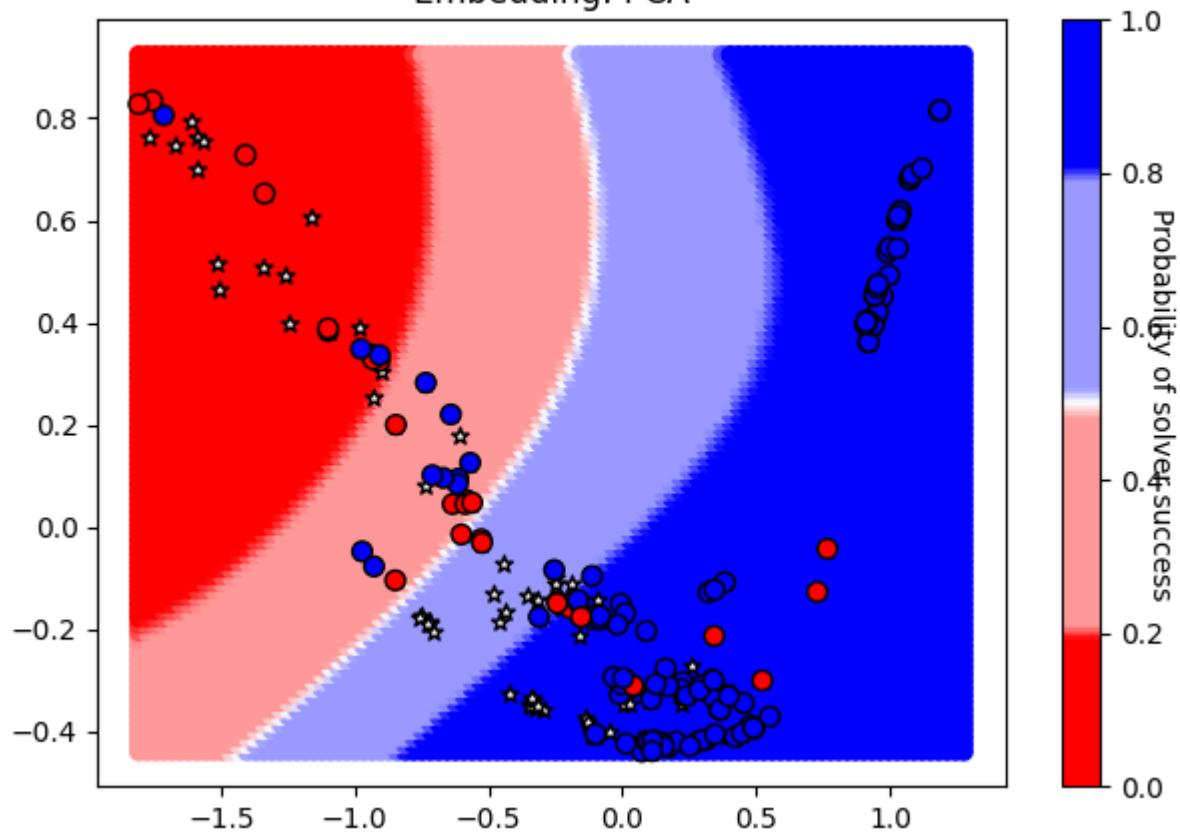
Note: plot only contains attempted tasks.

## Utility capture from SHCI\_var\_2e-5/86bfe5...

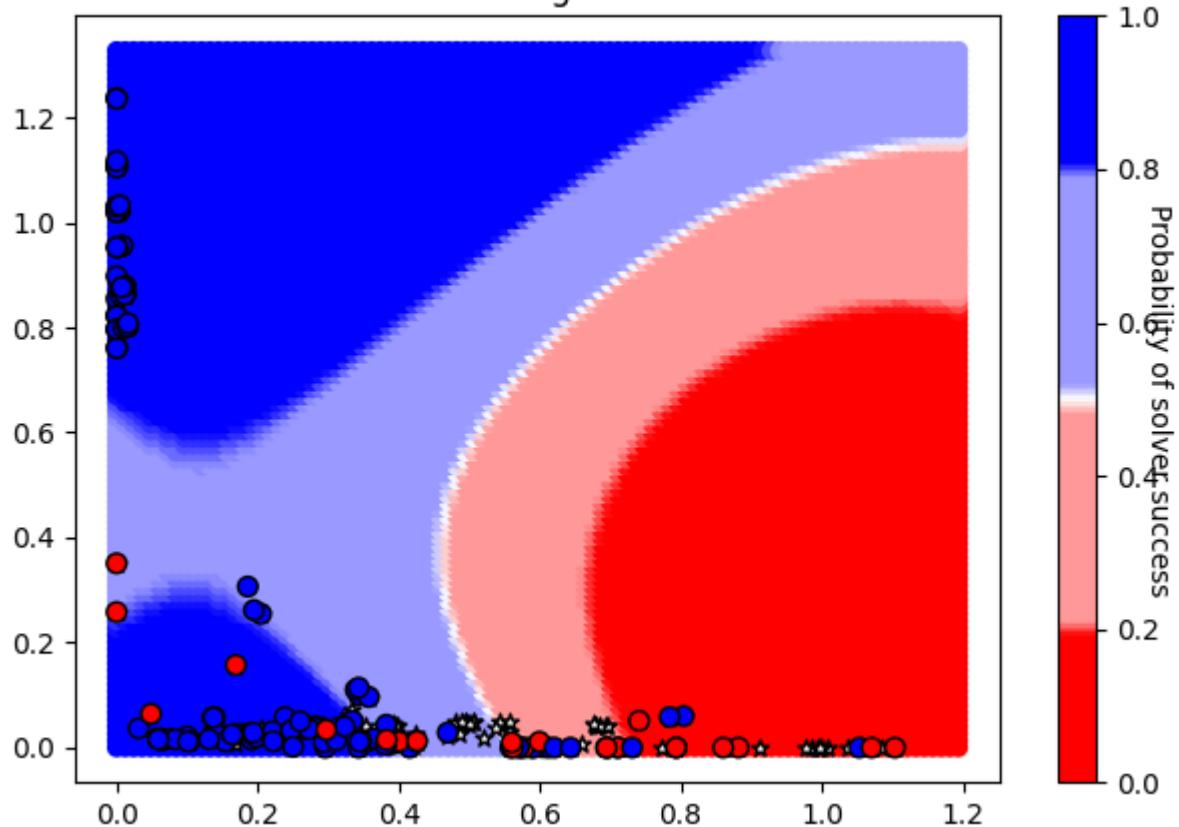
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



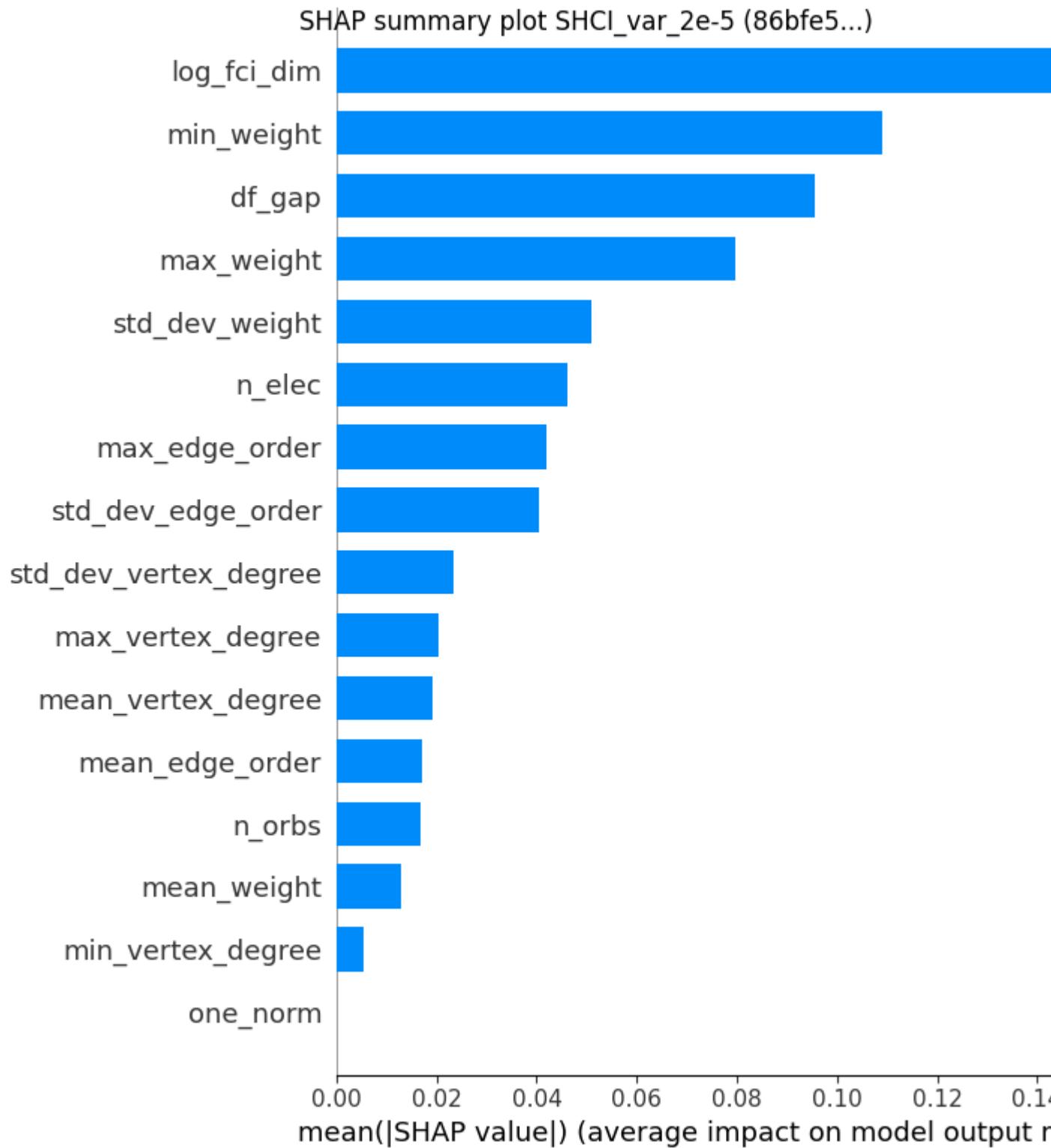
Solver SHCI\_var\_2e-5 (86bfe5...)  
Embedding: PCA



Solver SHCI\_var\_2e-5 (86bfe5...)  
Embedding: NMF



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.

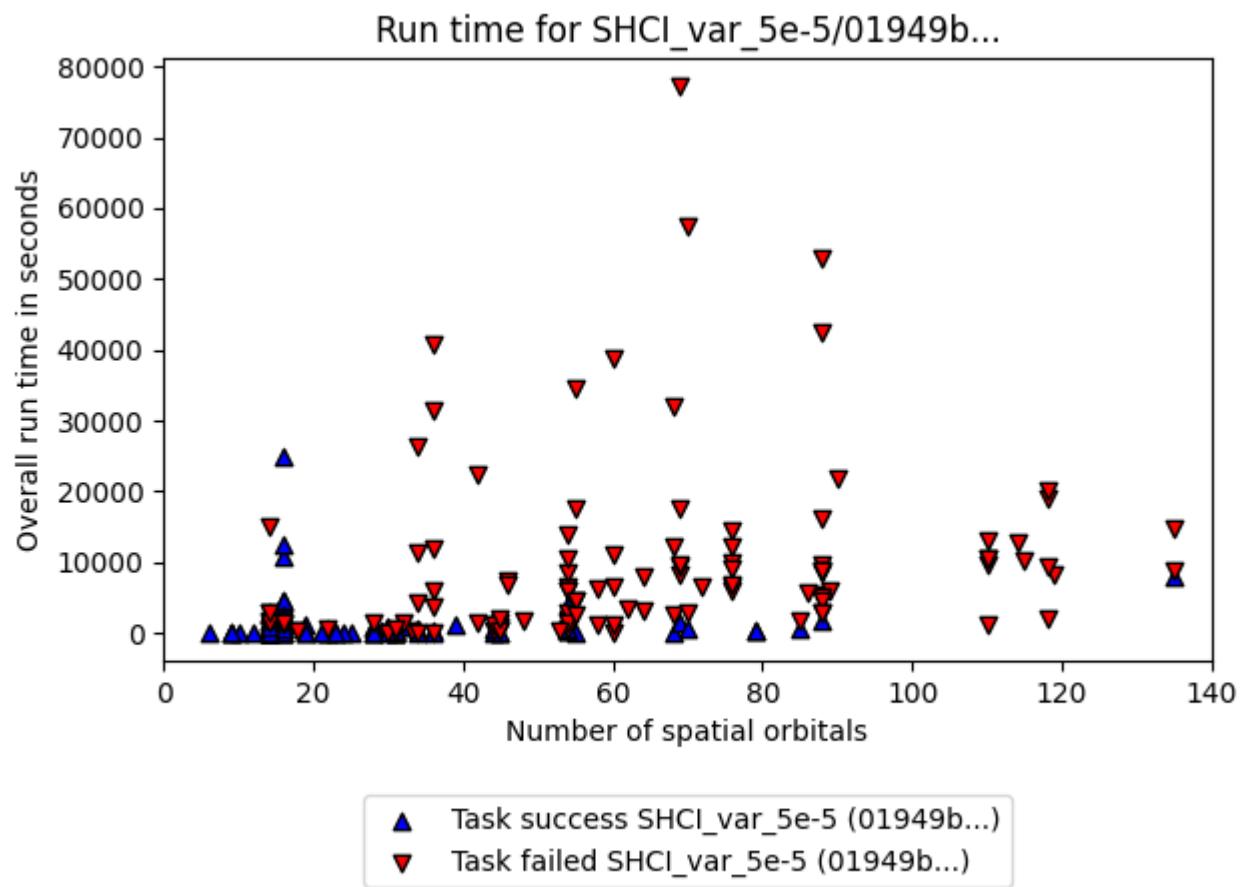


## Solver SHCI\_var\_5e-5, 01949b95-c427-4693-9134-01f47f688c09

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

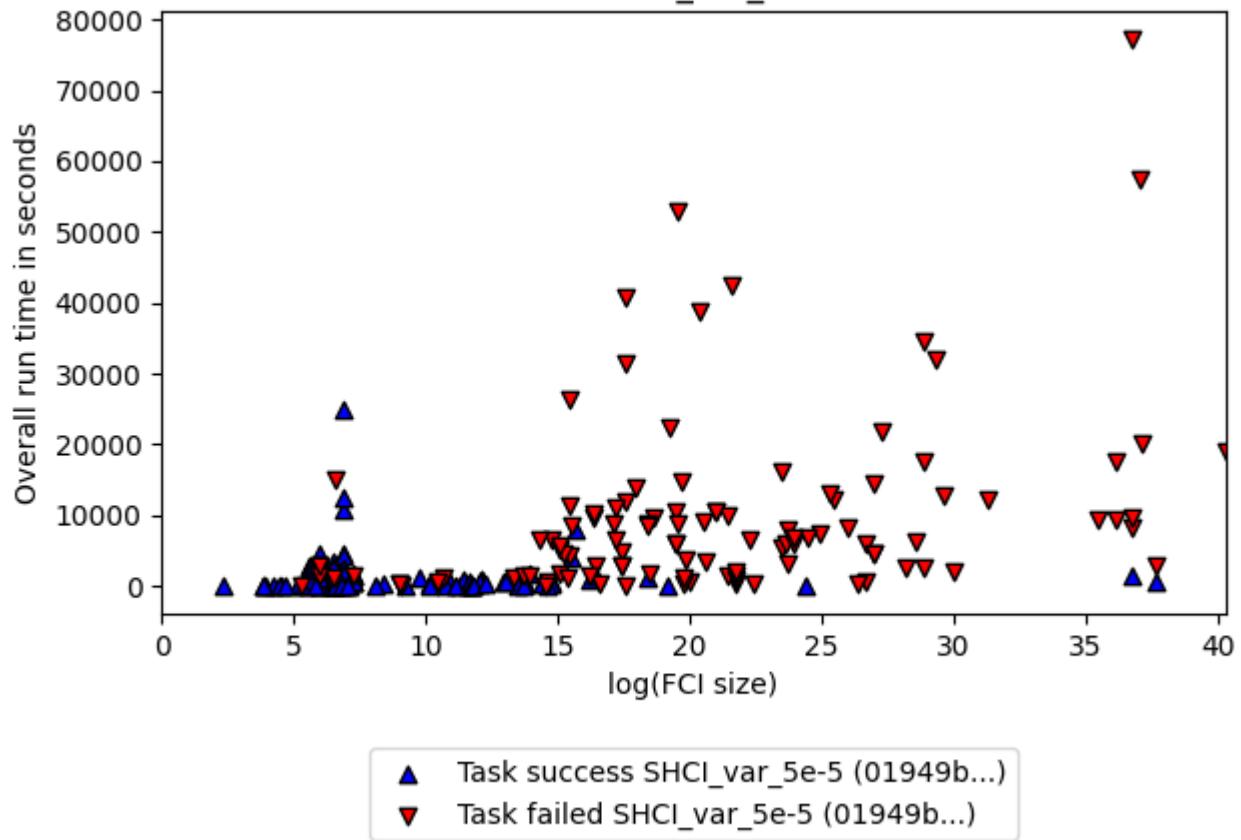
solver\_short\_name:SHCI\_var\_5e-5

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: 81362f75-9818-4625-ae5a-18bbea5e5607  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 14  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 111  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 223  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 111  
max\_run\_time\_of\_attempted\_tasks: 77244.15200000002  
sum\_of\_run\_time\_of\_attempted\_tasks: 1220720.12  
solvability\_ratio: 0.9462  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9545454545454546, 0.981651376146789]  
ml\_metrics\_calculator\_version: 1



Note: plot only contains attempted tasks.

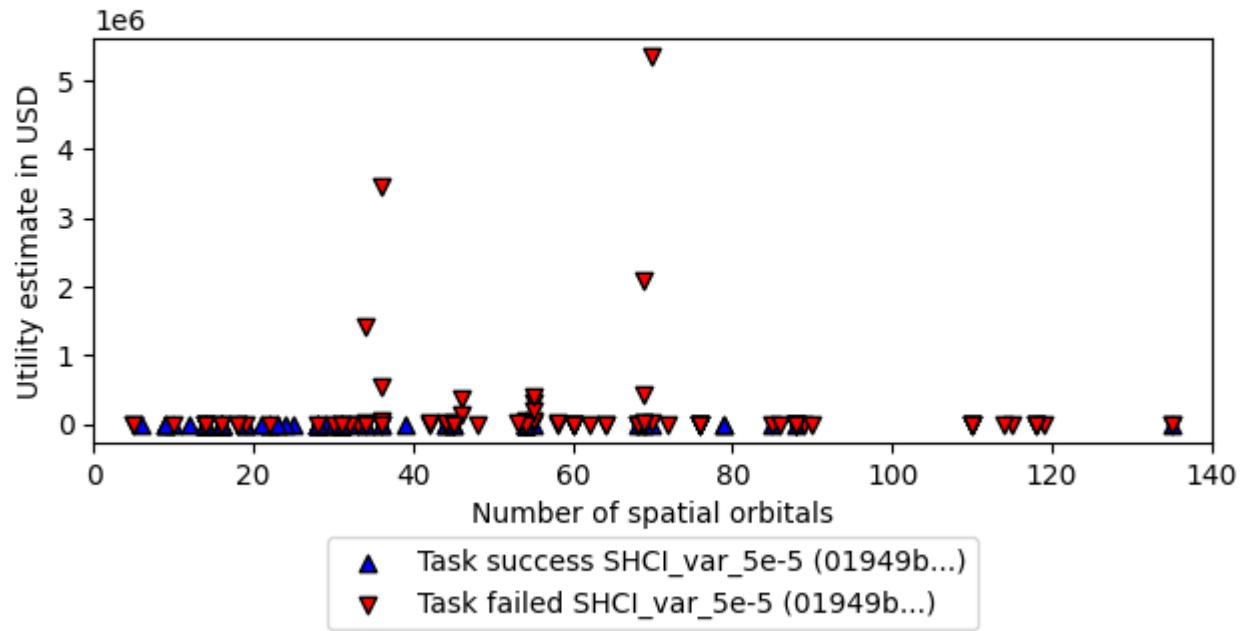
Run time for SHCI\_var\_5e-5/01949b...



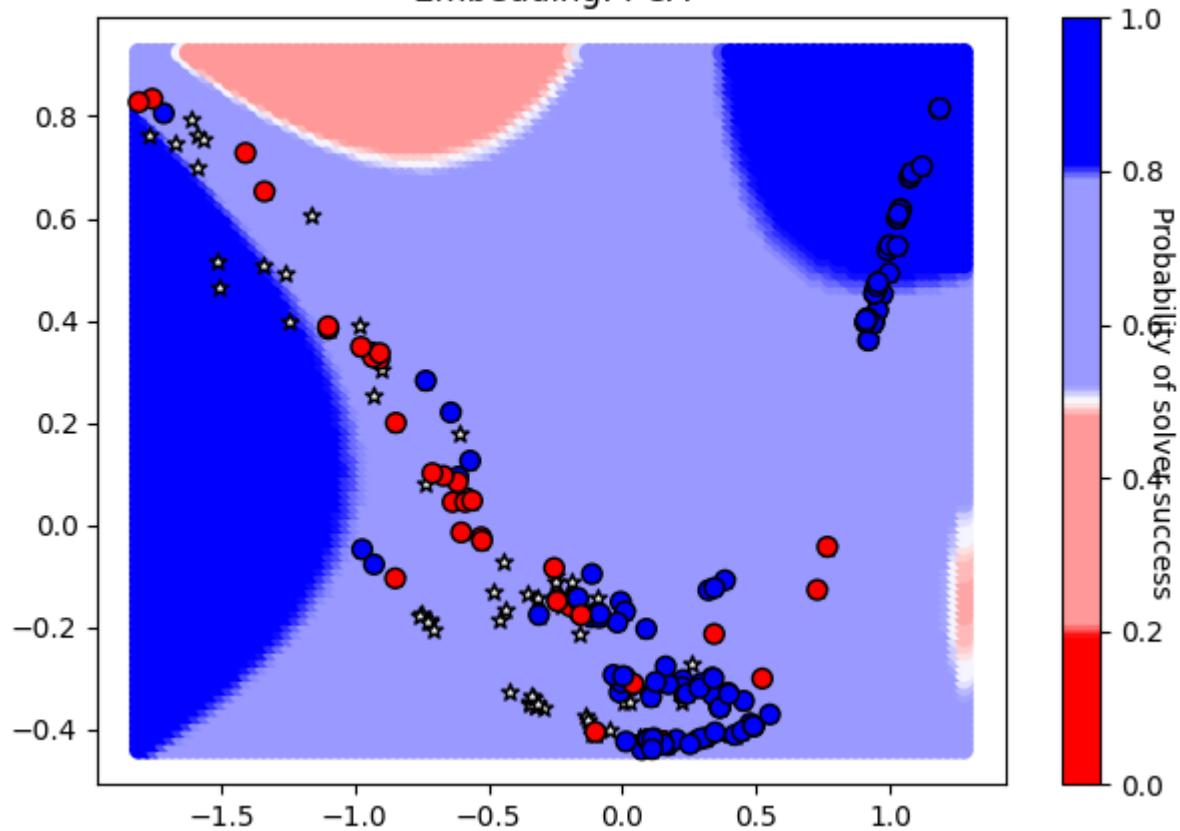
Note: plot only contains attempted tasks.

# Utility capture from SHCI\_var\_5e-5/01949b...

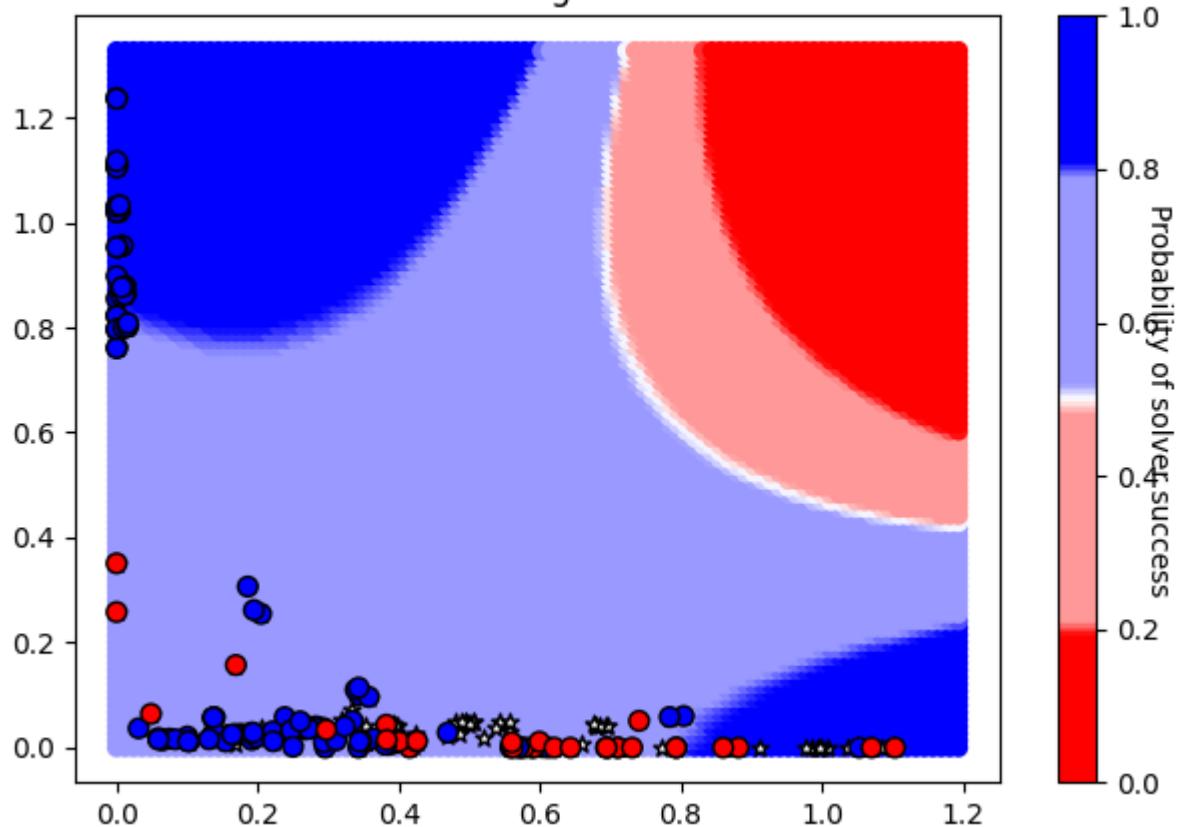
(captured:  $\$4.5\text{e+}02/1.5\text{e+}07$ , approximately  $3.0\text{e-}03\%$ )



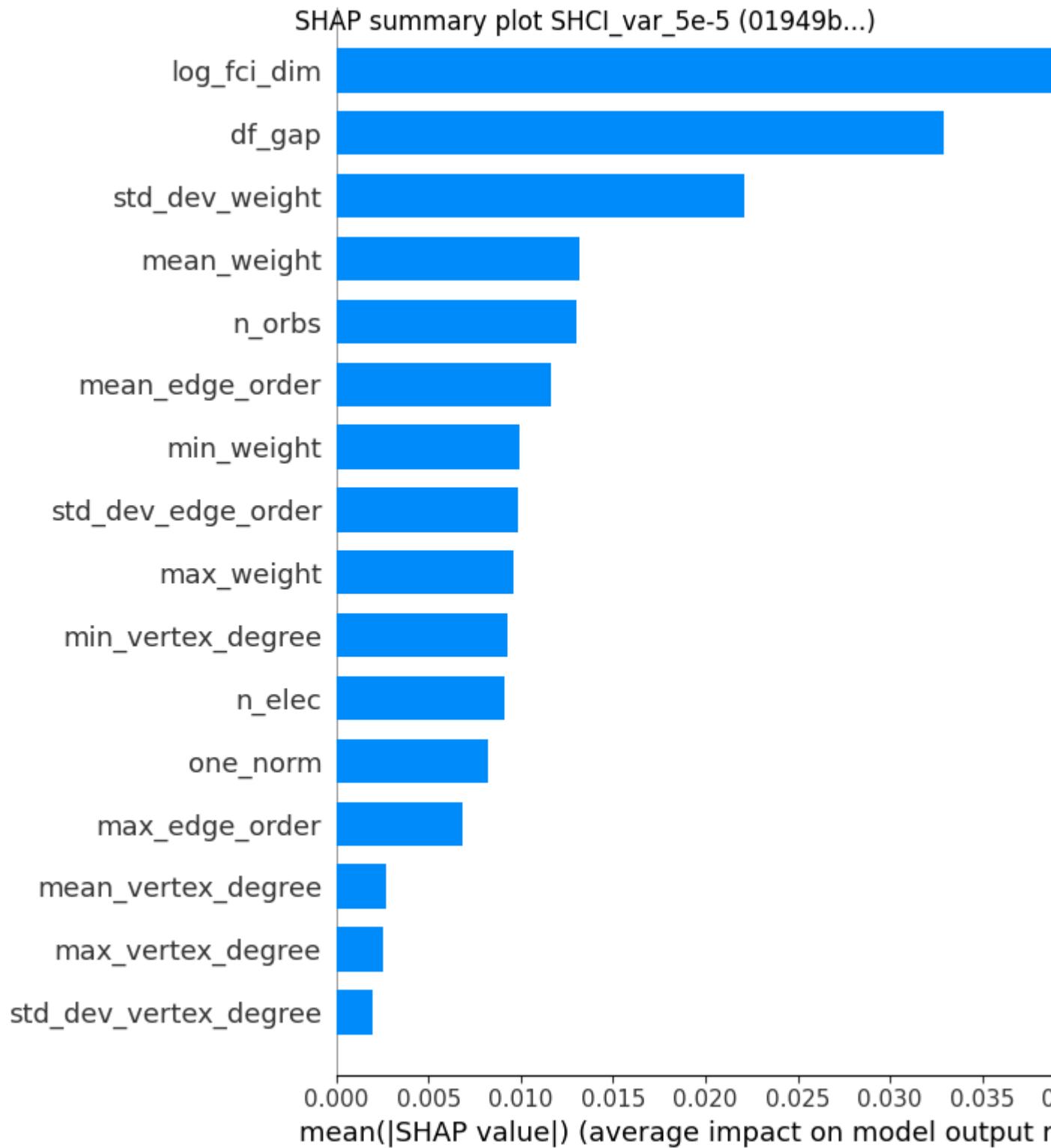
Solver SHCI\_var\_5e-5 (01949b...)  
Embedding: PCA



Solver SHCI\_var\_5e-5 (01949b...)  
Embedding: NMF



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, 4b07b89f-c66f-4e72-8c24-df3e4222cb41

solver\_uuid:4b07b89f-c66f-4e72-8c24-df3e4222cb41

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': '1.3.6'}, {'software\_name': 'qb-gsee-benchmark', 'software\_version': '0.1.0a3.dev68+g2b90efd'}, {'software\_name': 'Python', 'software\_version': '3.10.12 (main, Feb 4 2025, 14:57:36) [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. Assumes that enough QPUs are available to run all shots in parallel.'}, 'quantum.hardware\_parameters': {'num\_factories': 4, 'physical\_error\_rate': 0.0001, 'cycle\_time\_microseconds': 1, 'parallelize\_shots': True}}

logical\_resource\_estimate\_solution\_uuid:5ed24527-1892-46f9-8a7a-a9fe92993b48

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

performance\_metrics\_uuid: 56cd16fe-2625-4646-b8af-5f99a6c9bbca

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 22

number\_of\_problem\_instances\_solved: 3

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 131

number\_of\_tasks\_solved: 3

number\_of\_tasks\_solved\_within\_run\_time\_limit: 3

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 131

max\_run\_time\_of\_attempted\_tasks: 26774753292.953506

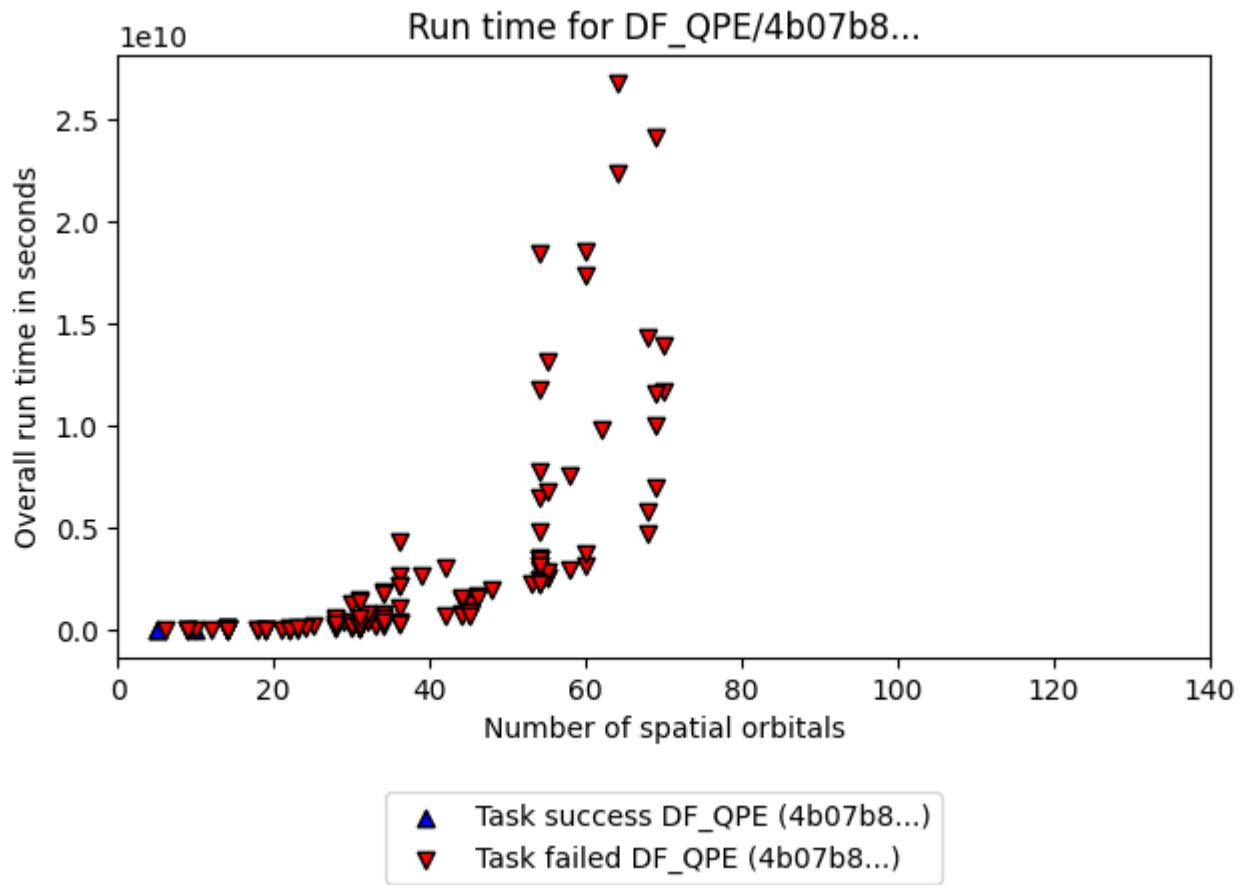
sum\_of\_run\_time\_of\_attempted\_tasks: 381759348210.49603

solvability\_ratio: 0.0

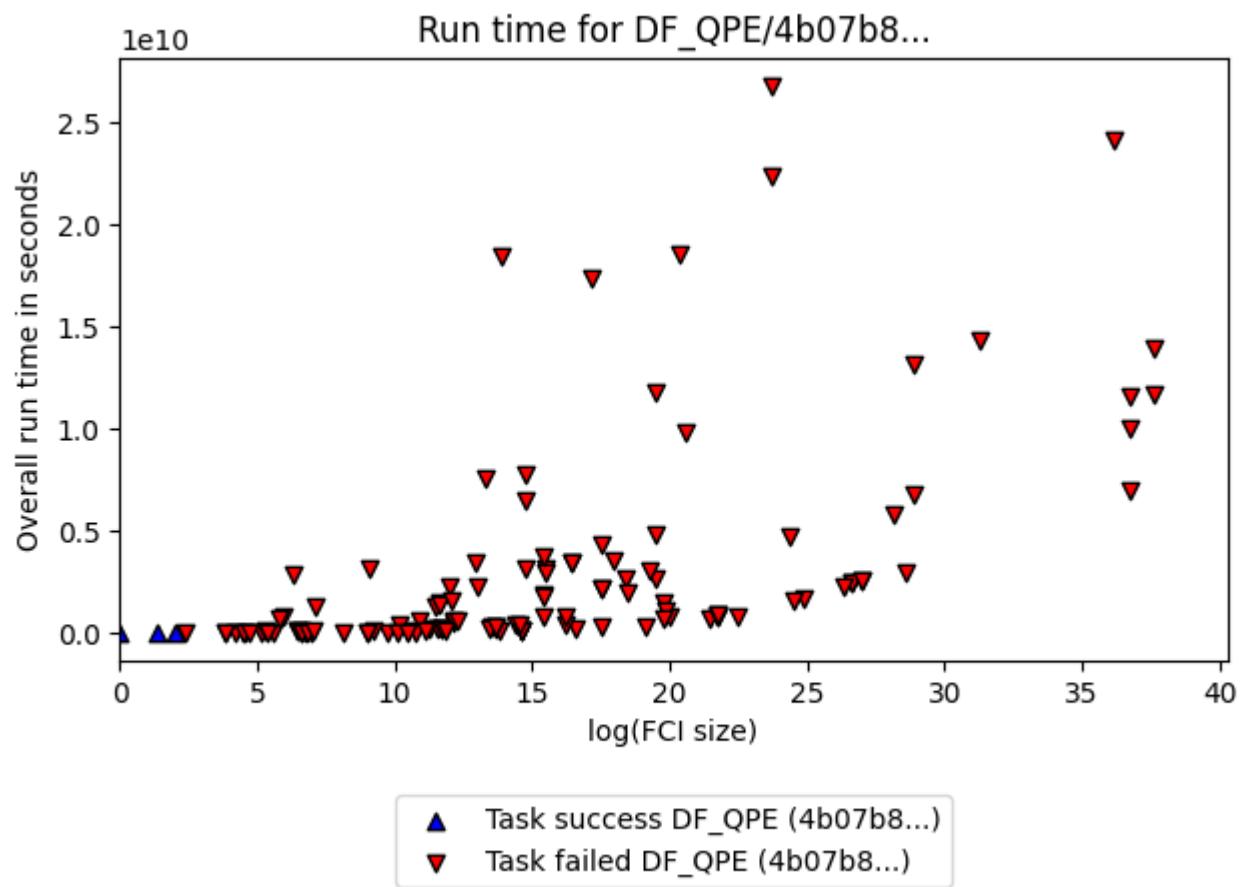
comments: solvability ratio based on PCA embedding.

f1\_score: [1.0, 1.0]

ml\_metrics\_calculator\_version: 1



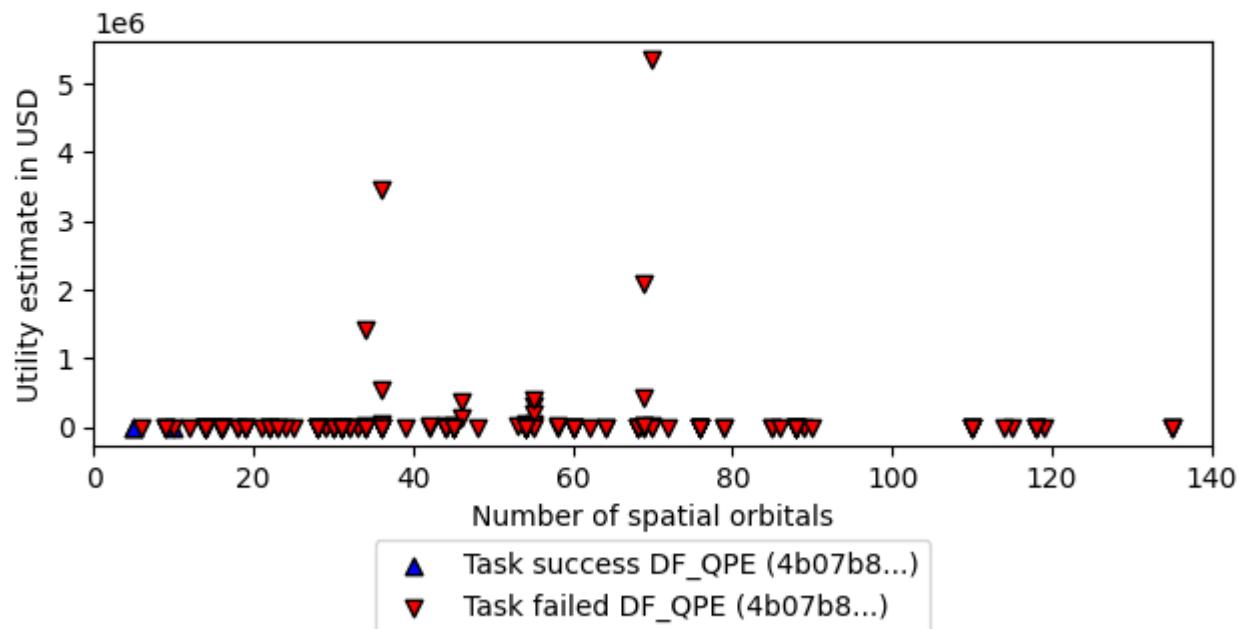
Note: plot only contains attempted tasks.



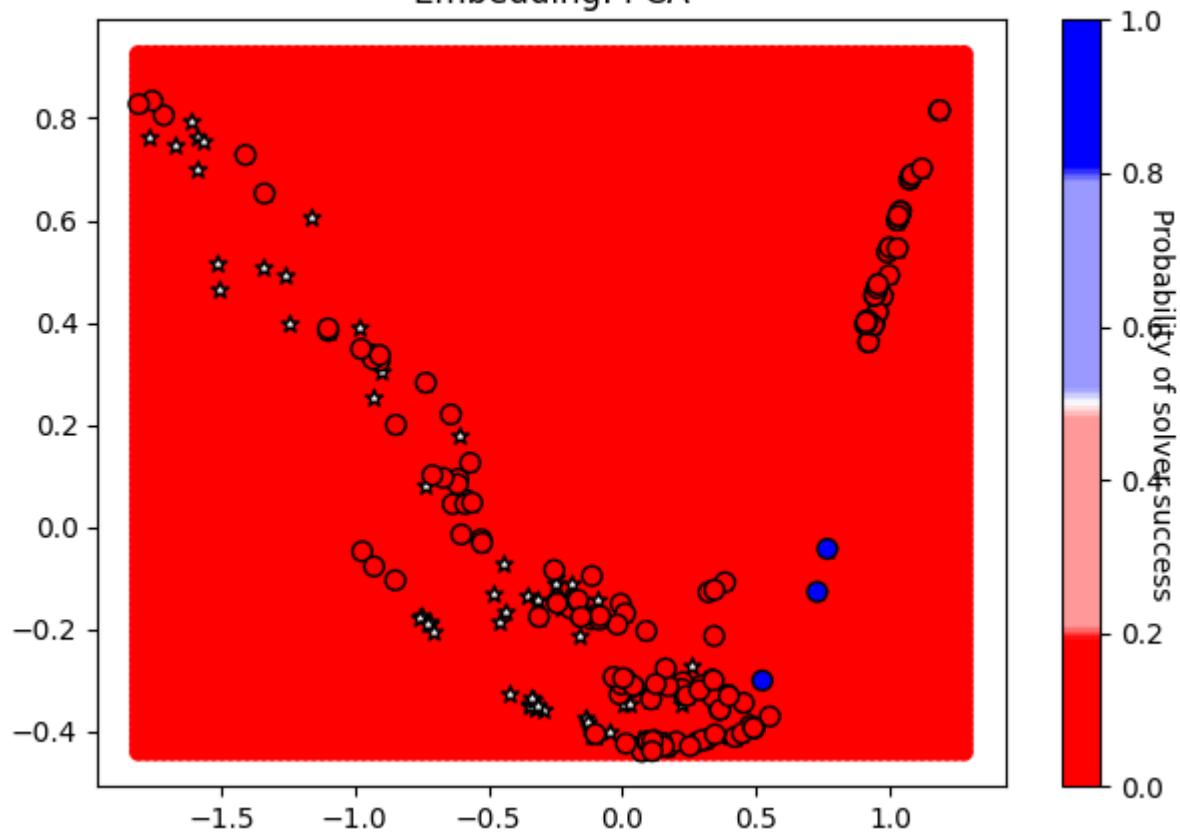
Note: plot only contains attempted tasks.

## Utility capture from DF\_QPE/4b07b8...

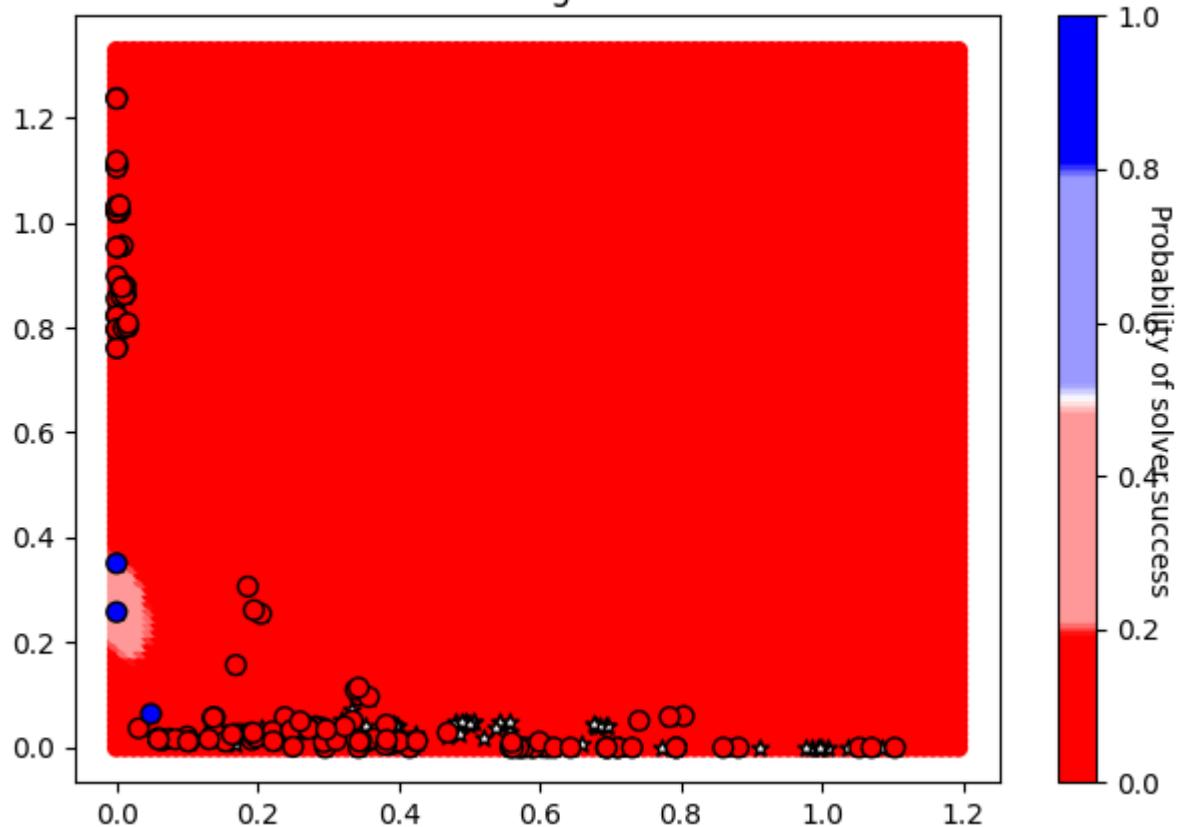
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



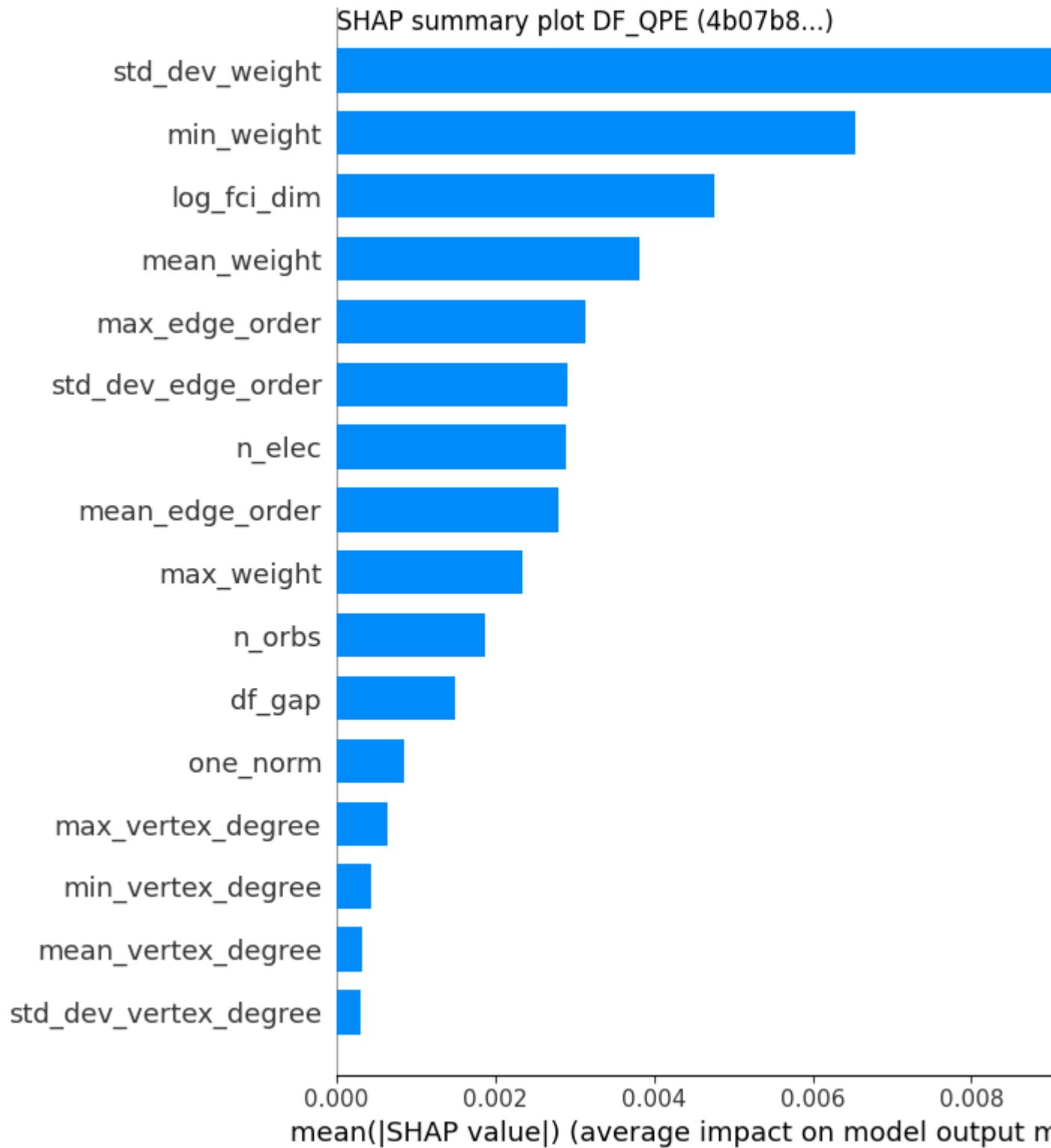
Solver DF\_QPE (4b07b8...)  
Embedding: PCA



Solver DF\_QPE (4b07b8...)  
Embedding: NNMF



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': '1.3.6'}, {'software\_name': 'qb-gsee-benchmark', 'software\_version': '0.1.0a3.dev68+g2b90efd'}, {'software\_name': 'Python', 'software\_version': '3.10.12 (main, Feb 4 2025, 14:57:36) [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, 'parallelize\_shots': False}}

logical\_resource\_estimate\_solution\_uuid:b38ef522-b636-4e49-9e75-b3dc9955f58b

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

performance\_metrics\_uuid: ddccbfbe-b3be-4ba1-9904-43ee85f2b17b

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 22

number\_of\_problem\_instances\_solved: 2

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 131

number\_of\_tasks\_solved: 2

number\_of\_tasks\_solved\_within\_run\_time\_limit: 2

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 131

max\_run\_time\_of\_attempted\_tasks: 1394057080220.9934

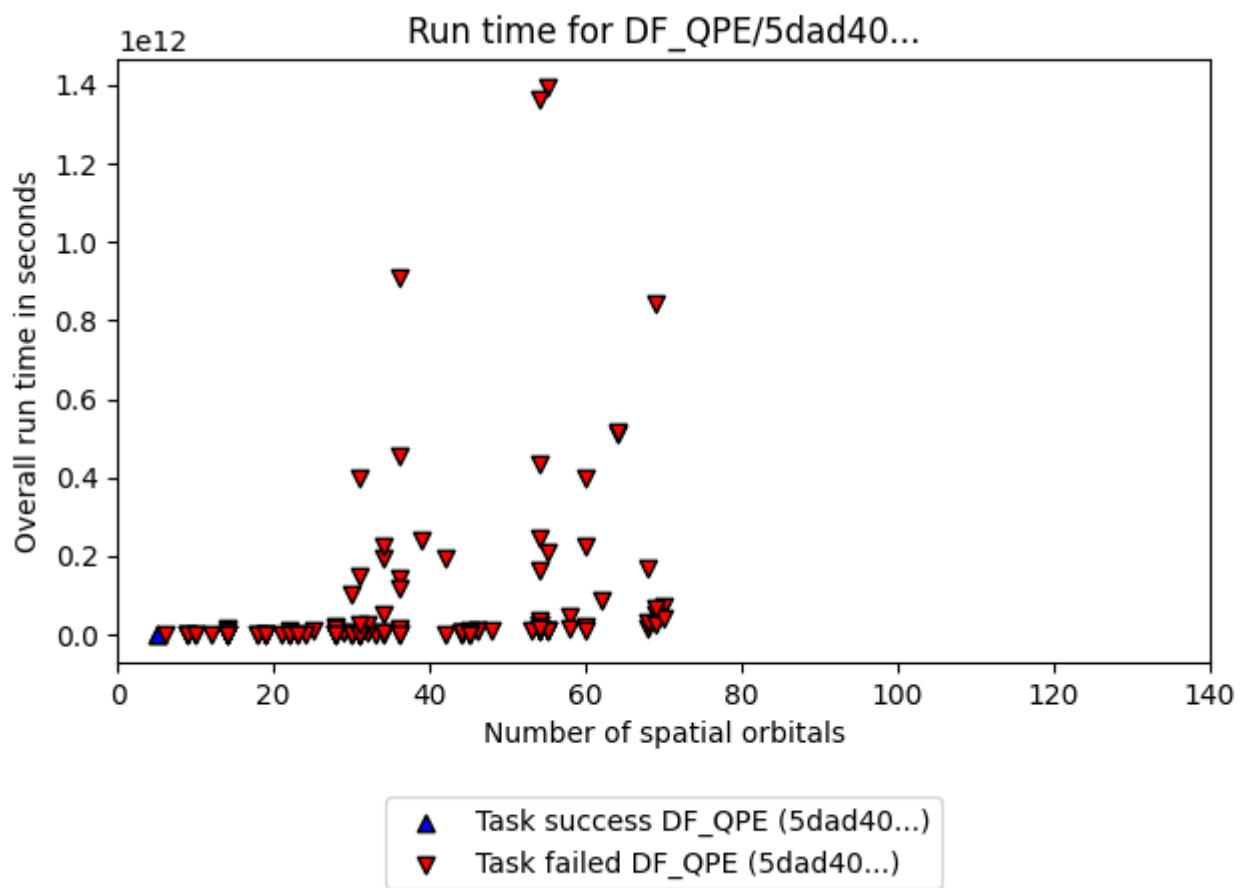
sum\_of\_run\_time\_of\_attempted\_tasks: 10701894024019.273

solvability\_ratio: 0.0394

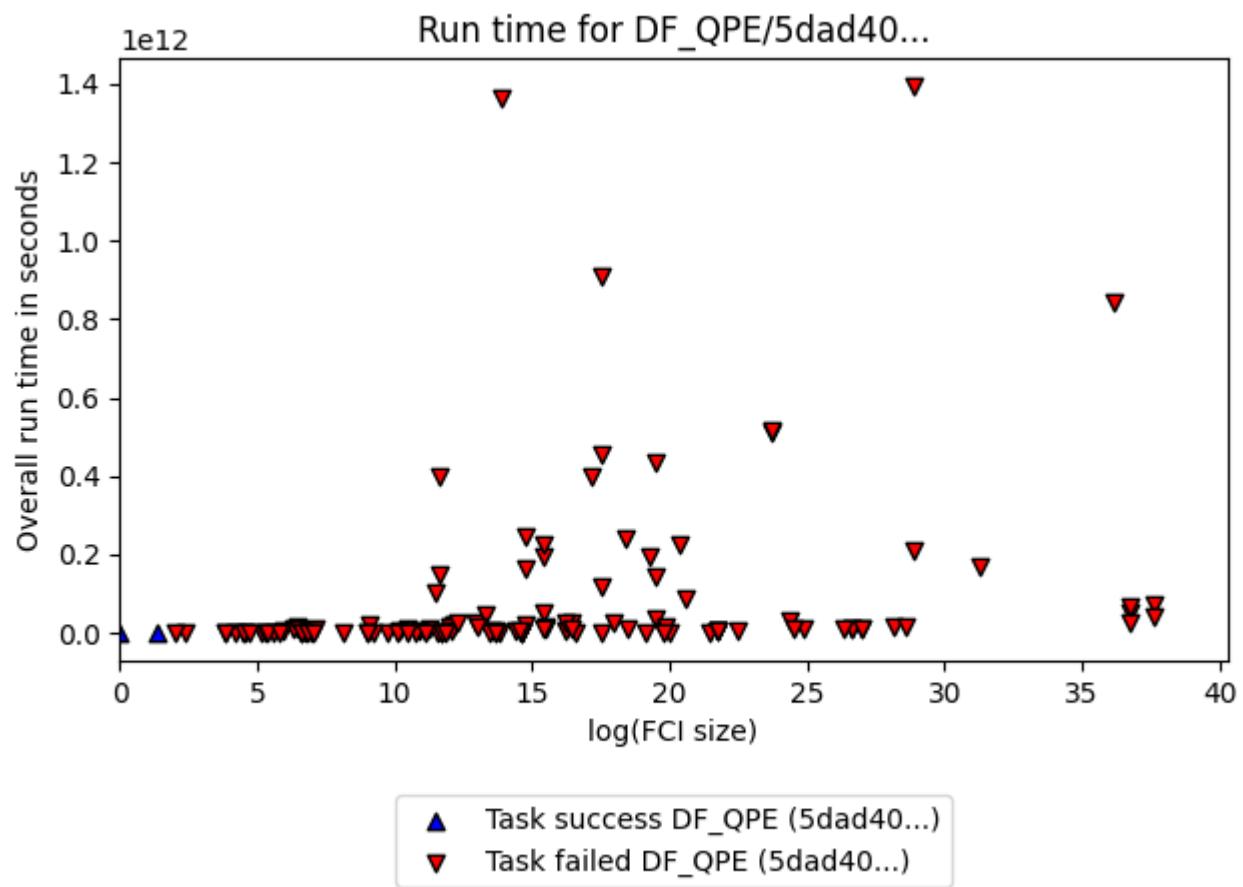
comments: solvability ratio based on PCA embedding.

f1\_score: [1.0, 1.0]

ml\_metrics\_calculator\_version: 1



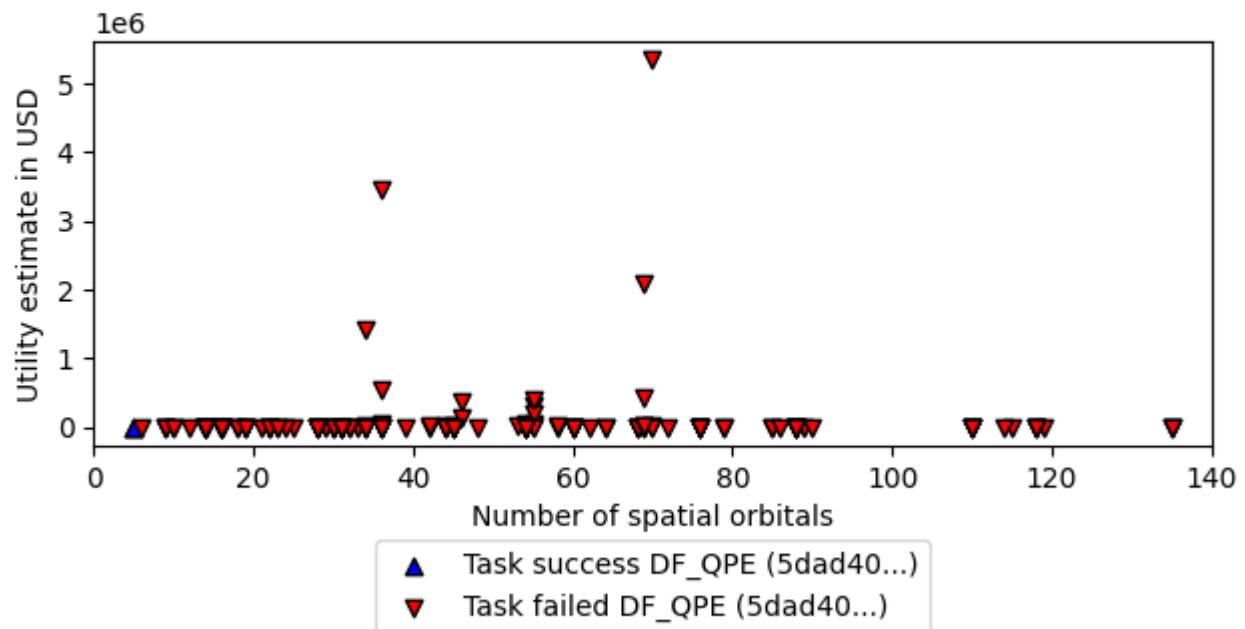
Note: plot only contains attempted tasks.



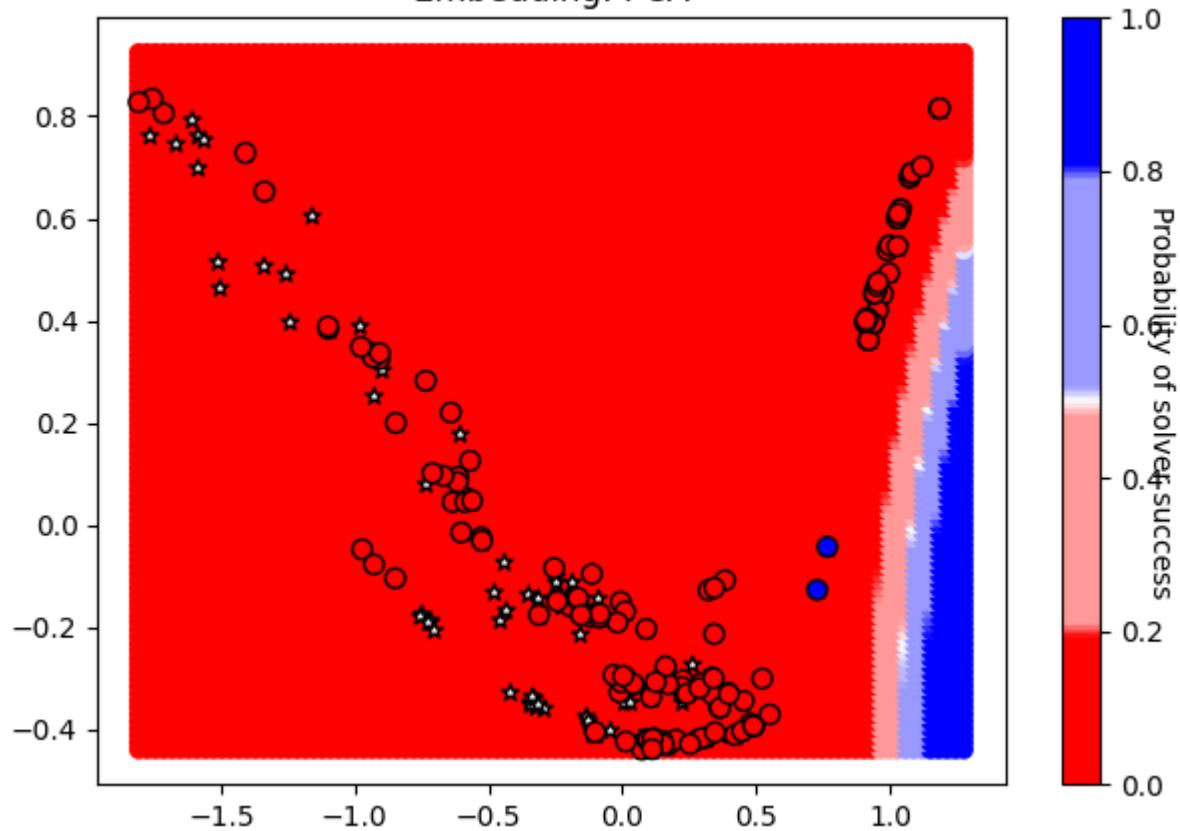
Note: plot only contains attempted tasks.

## Utility capture from DF\_QPE/5dad40...

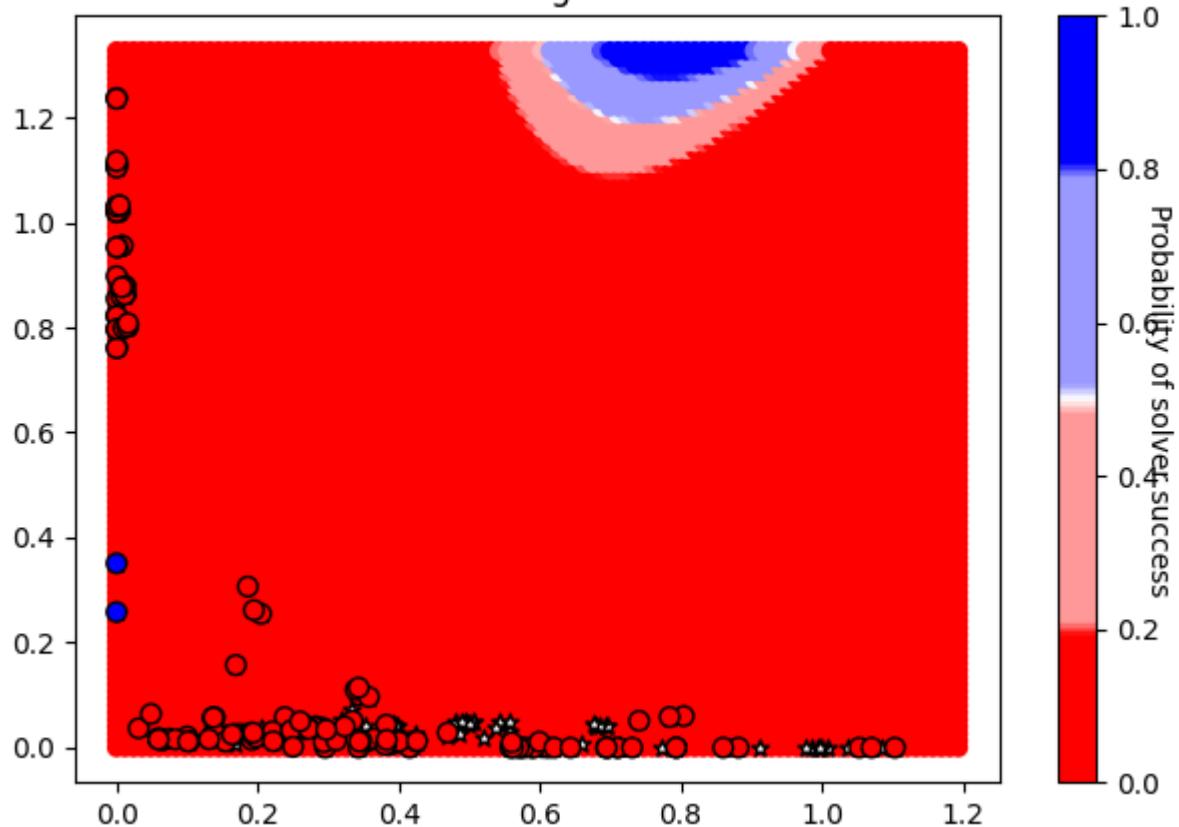
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



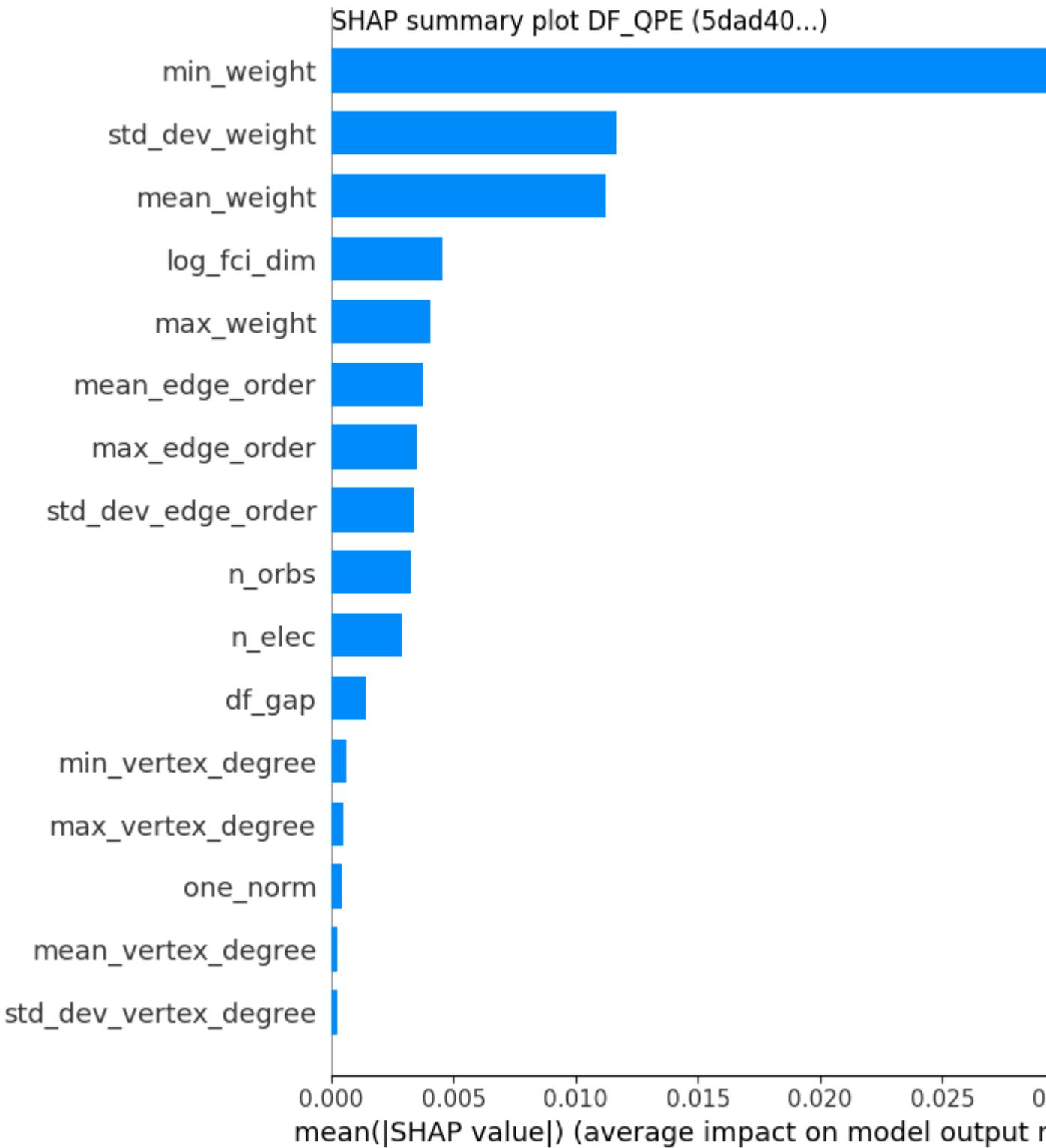
Solver DF\_QPE (5dad40...)  
Embedding: PCA



Solver DF\_QPE (5dad40...)  
Embedding: NMF



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.



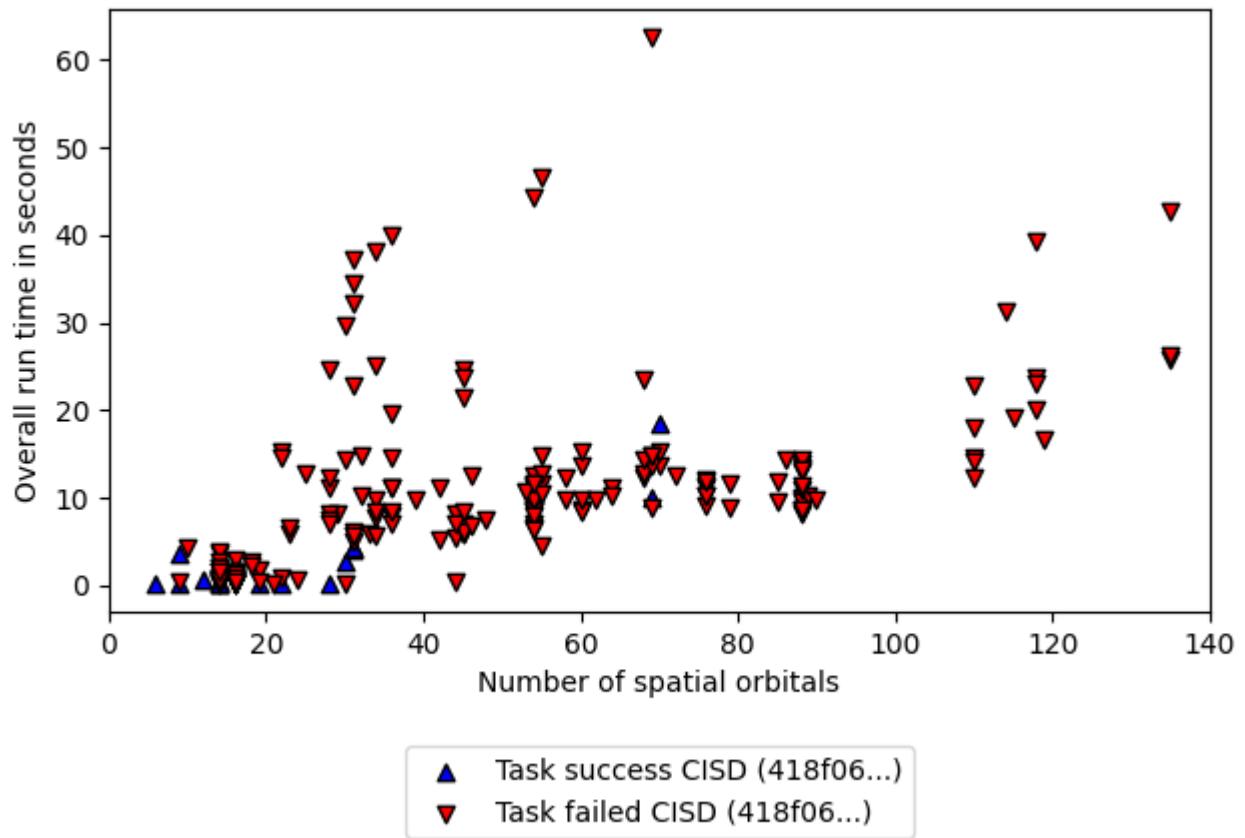
## Solver CISD, **418f060e-496b-4024-8d2d-9b1f8791e76d**

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

solver\_short\_name:CISD

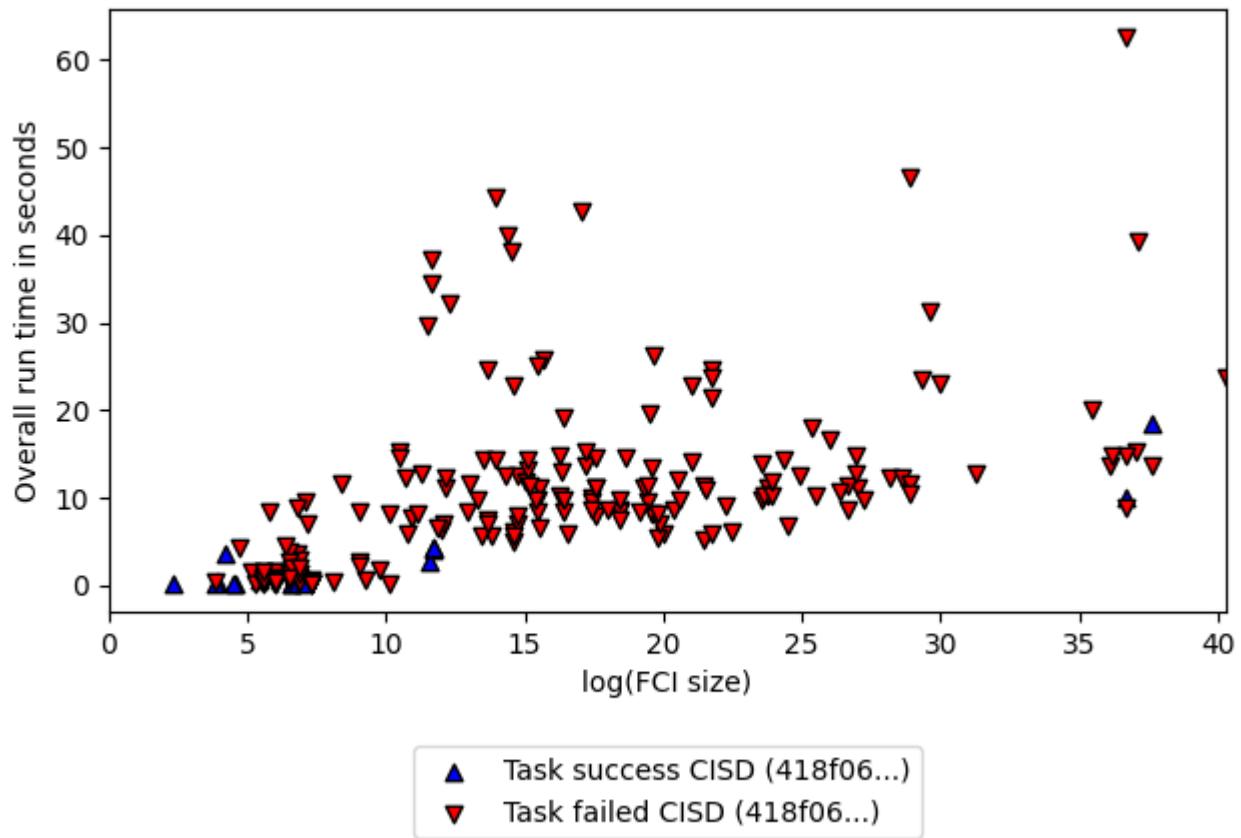
compute.hardware\_type:classical\_computer  
classical.hardware\_details:{'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}  
algorithm\_details:CISD  
software\_details:pyscf (<https://github.com/pyscf/pyscf>).  
performance\_metrics\_uuid: 17e72a9c-9b7b-4949-a192-366d01fe53ec  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 9  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 17  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 224  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 17  
max\_run\_time\_of\_attempted\_tasks: 62.58296537399292  
sum\_of\_run\_time\_of\_attempted\_tasks: 2141.729572057724  
solvability\_ratio: 0.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9774436090225563, 0.85]  
ml\_metrics\_calculator\_version: 1

### Run time for CISD/418f06...



Note: plot only contains attempted tasks.

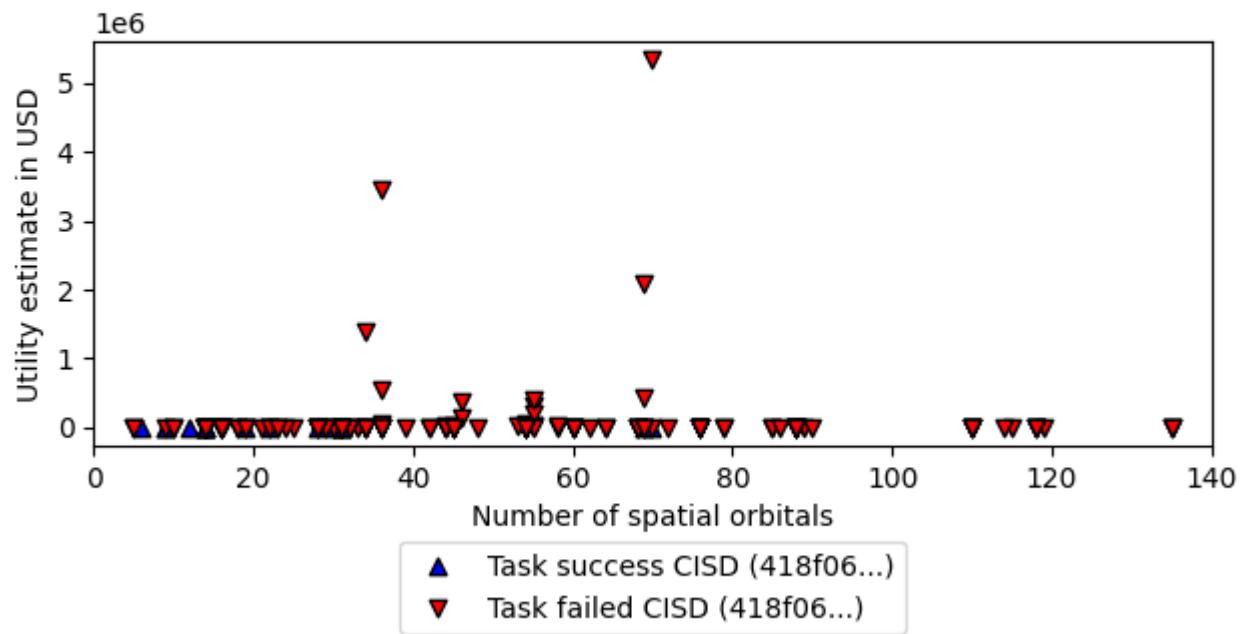
### Run time for CISD/418f06...



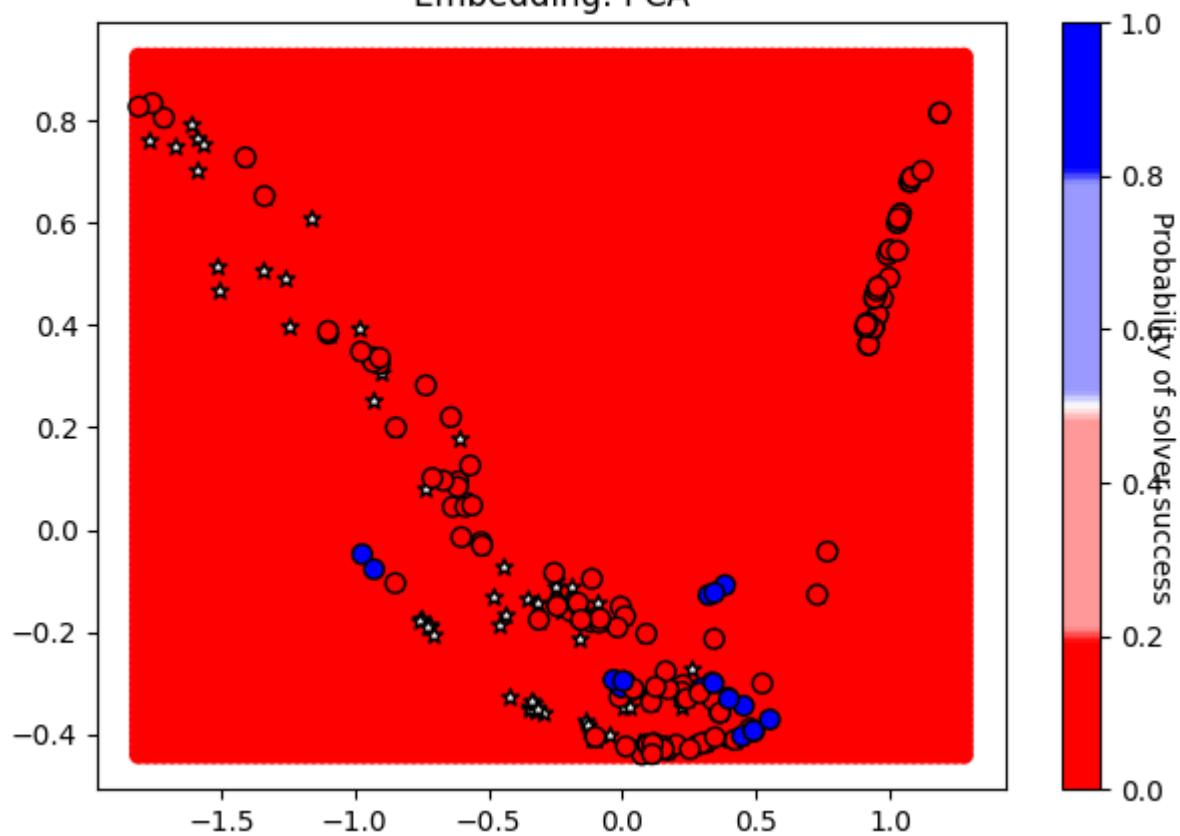
Note: plot only contains attempted tasks.

## Utility capture from CISD/418f06...

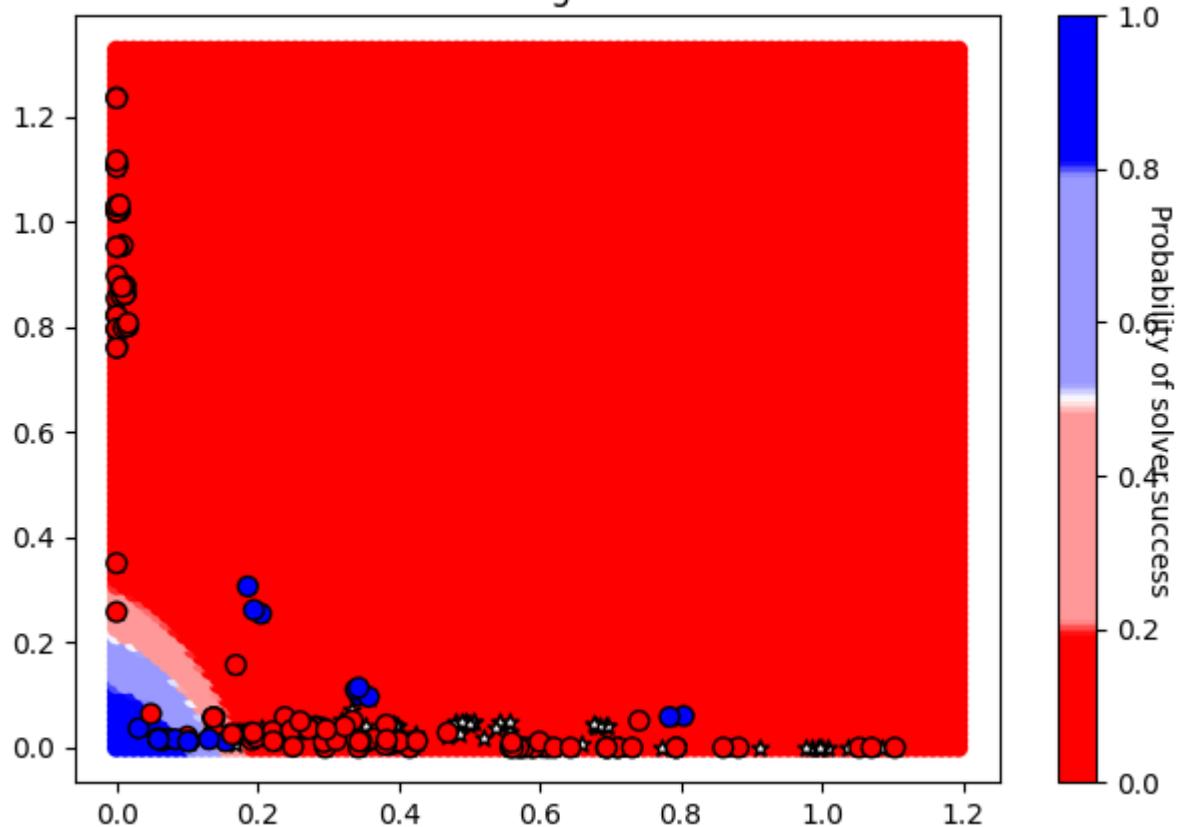
(captured: \$4.8e-03/1.5e+07, approximately 3.2e-08%)



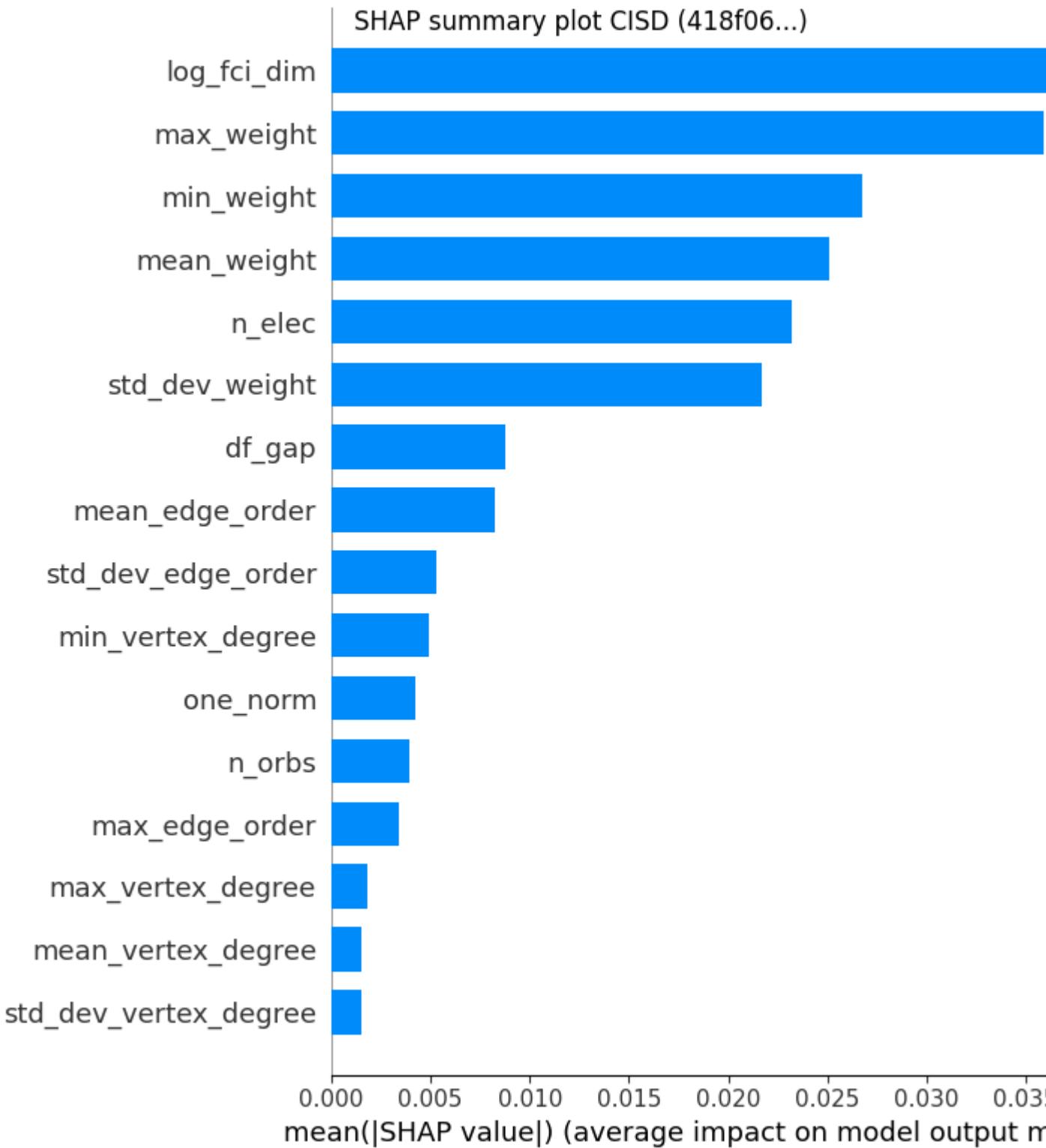
Solver CISD (418f06...)  
Embedding: PCA



Solver CISD (418f06...)  
Embedding: NNMF



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.



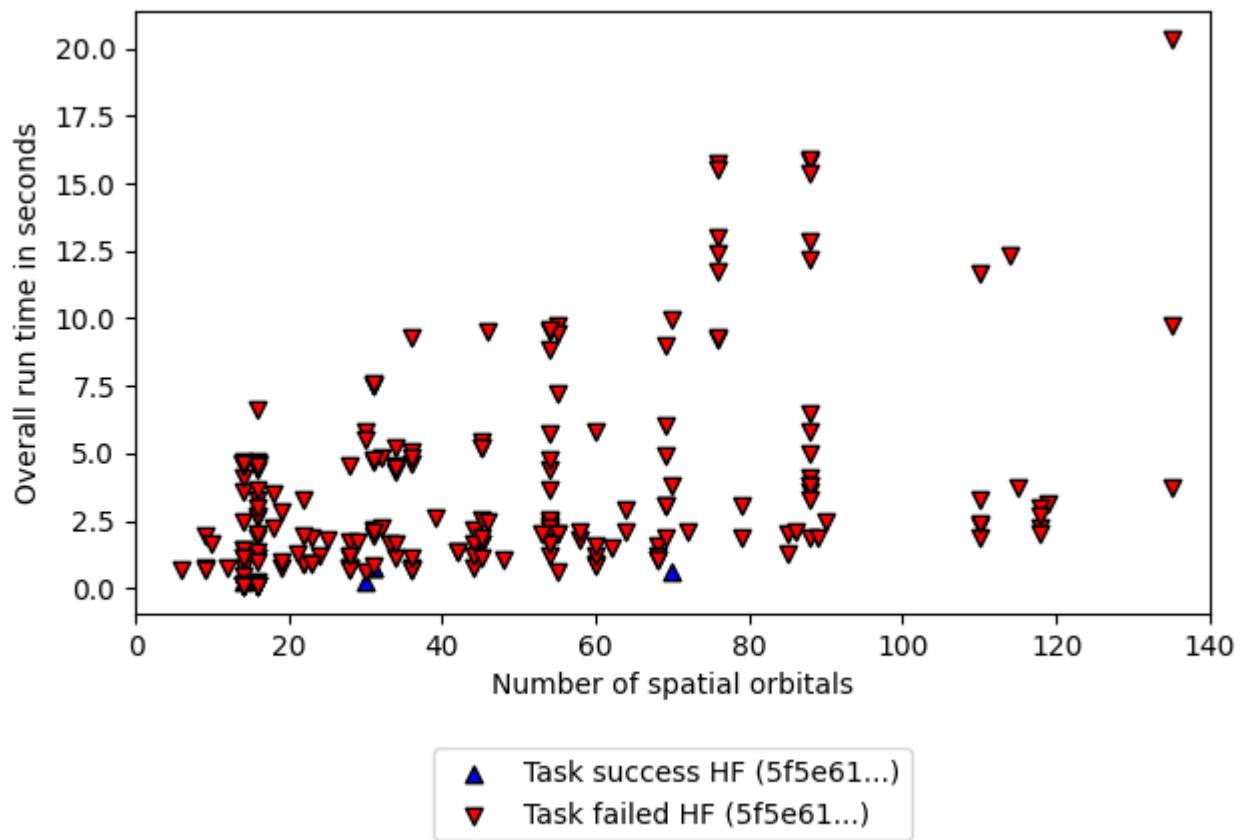
## Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

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

solver\_short\_name:HF

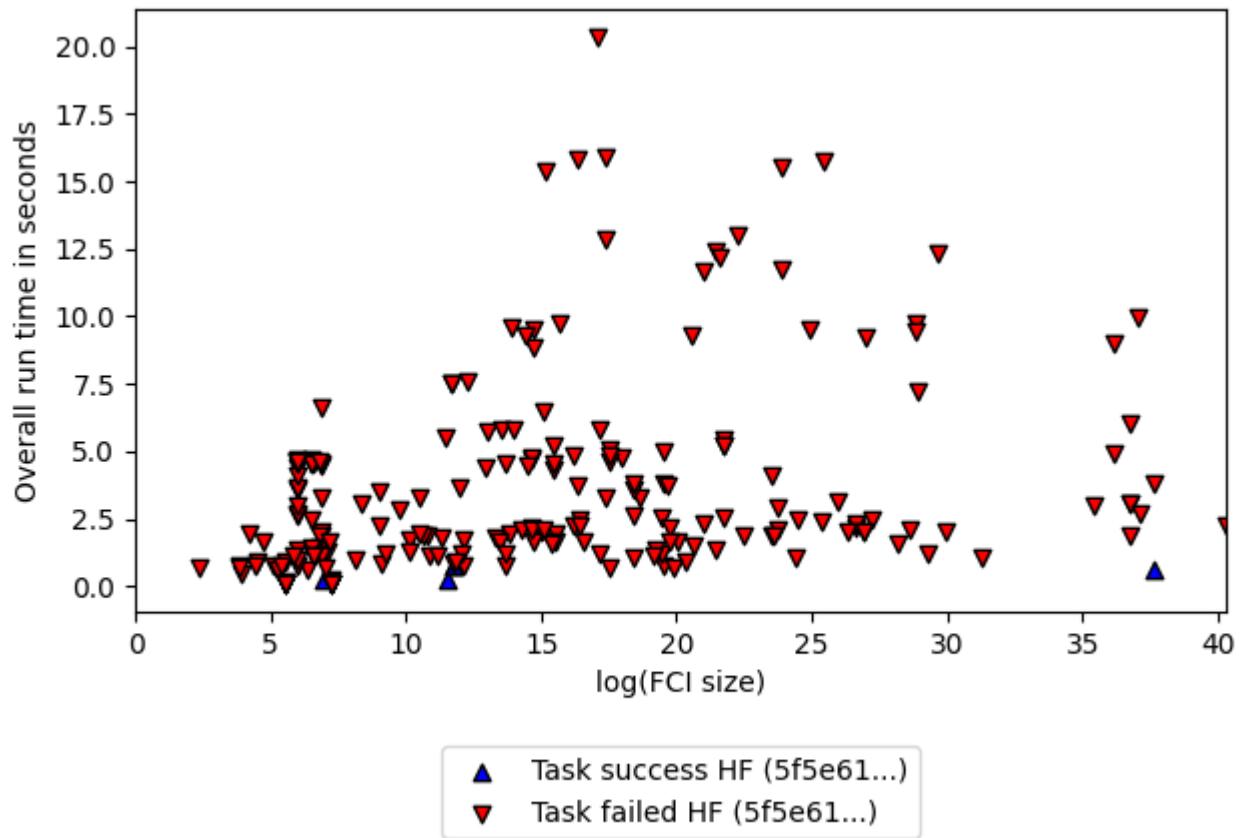
compute.hardware\_type:classical\_computer  
classical.hardware\_details:{'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}  
algorithm\_details:Hartree Fock  
software\_details:pyscf (<https://github.com/pyscf/pyscf>).  
performance\_metrics\_uuid: c6b8511e-663d-4b2f-b896-72bbf747b553  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 64  
number\_of\_problem\_instances\_solved: 5  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 224  
number\_of\_tasks\_solved: 5  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 224  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 5  
max\_run\_time\_of\_attempted\_tasks: 20.338801622390747  
sum\_of\_run\_time\_of\_attempted\_tasks: 798.9929344654083  
solvability\_ratio: 0.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9863013698630136, 0.7142857142857143]  
ml\_metrics\_calculator\_version: 1

### Run time for HF/5f5e61...



Note: plot only contains attempted tasks.

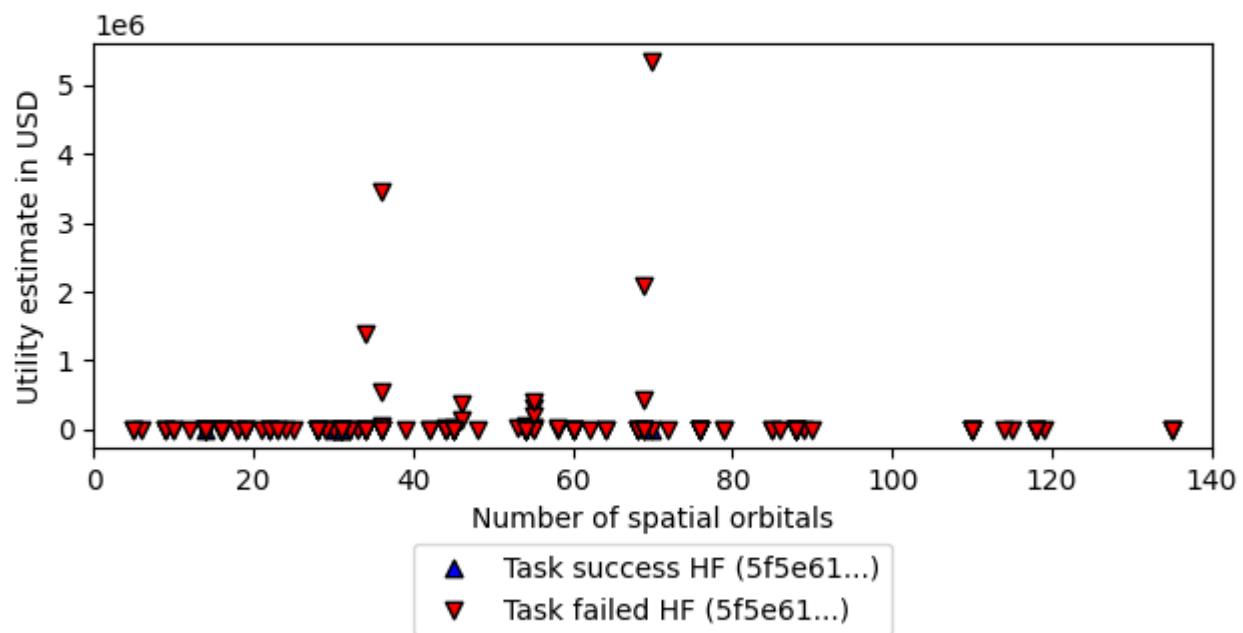
### Run time for HF/5f5e61...



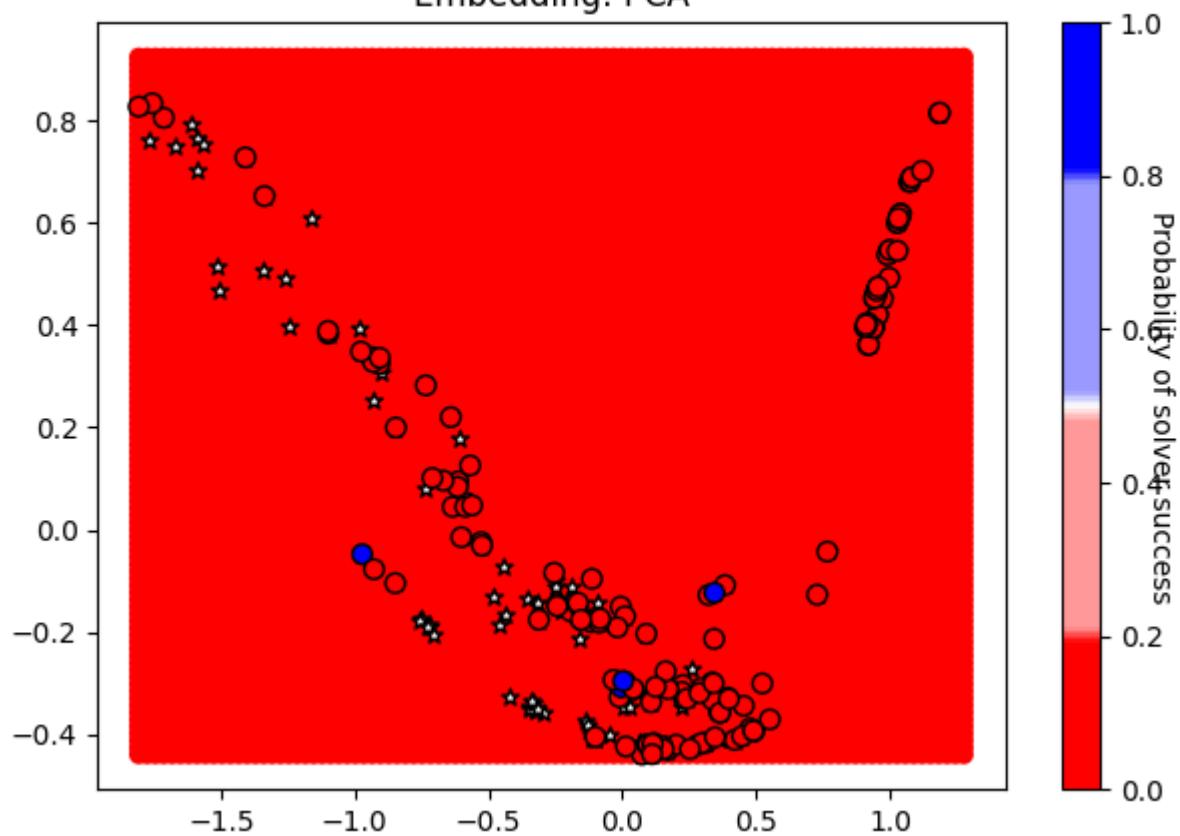
Note: plot only contains attempted tasks.

## Utility capture from HF/5f5e61...

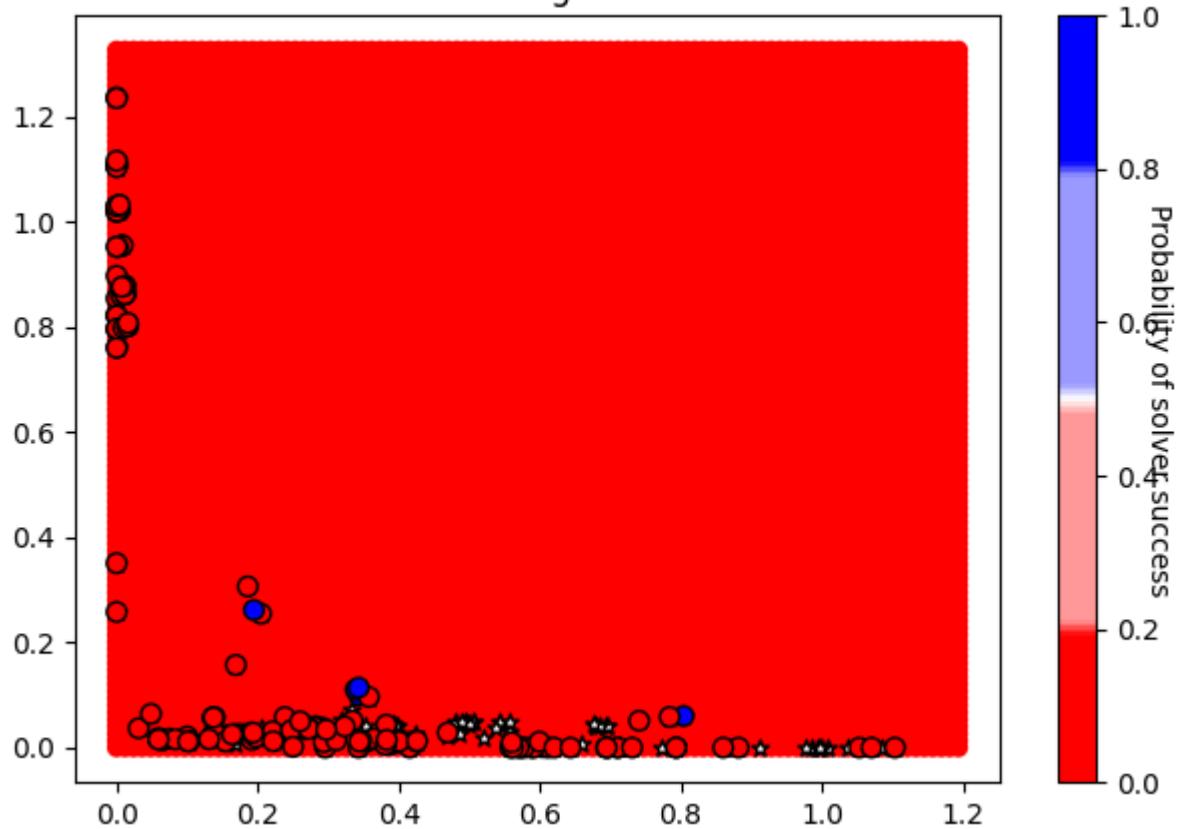
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



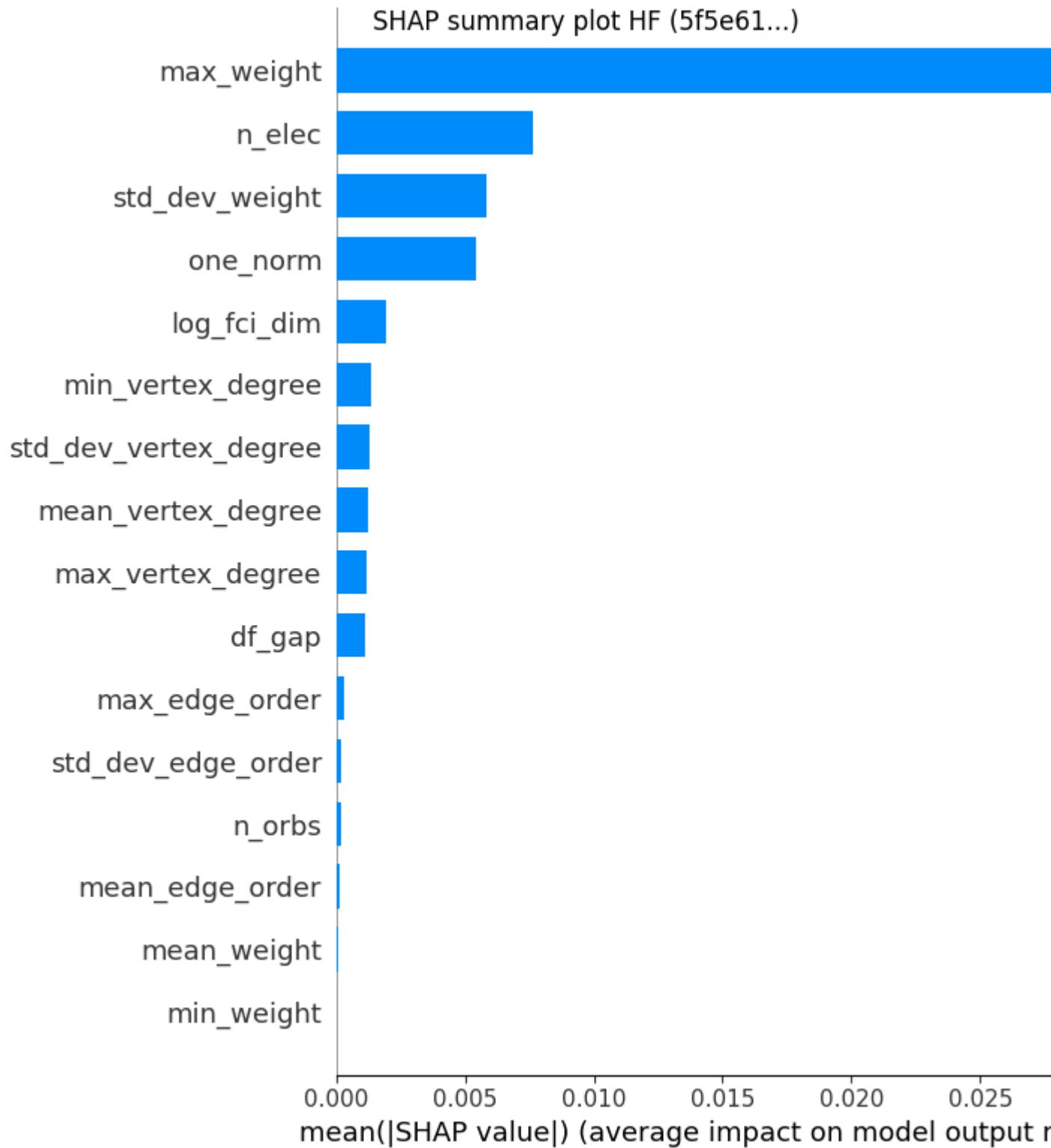
Solver HF (5f5e61...)  
Embedding: PCA



Solver HF (5f5e61...)  
Embedding: NNMF



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.



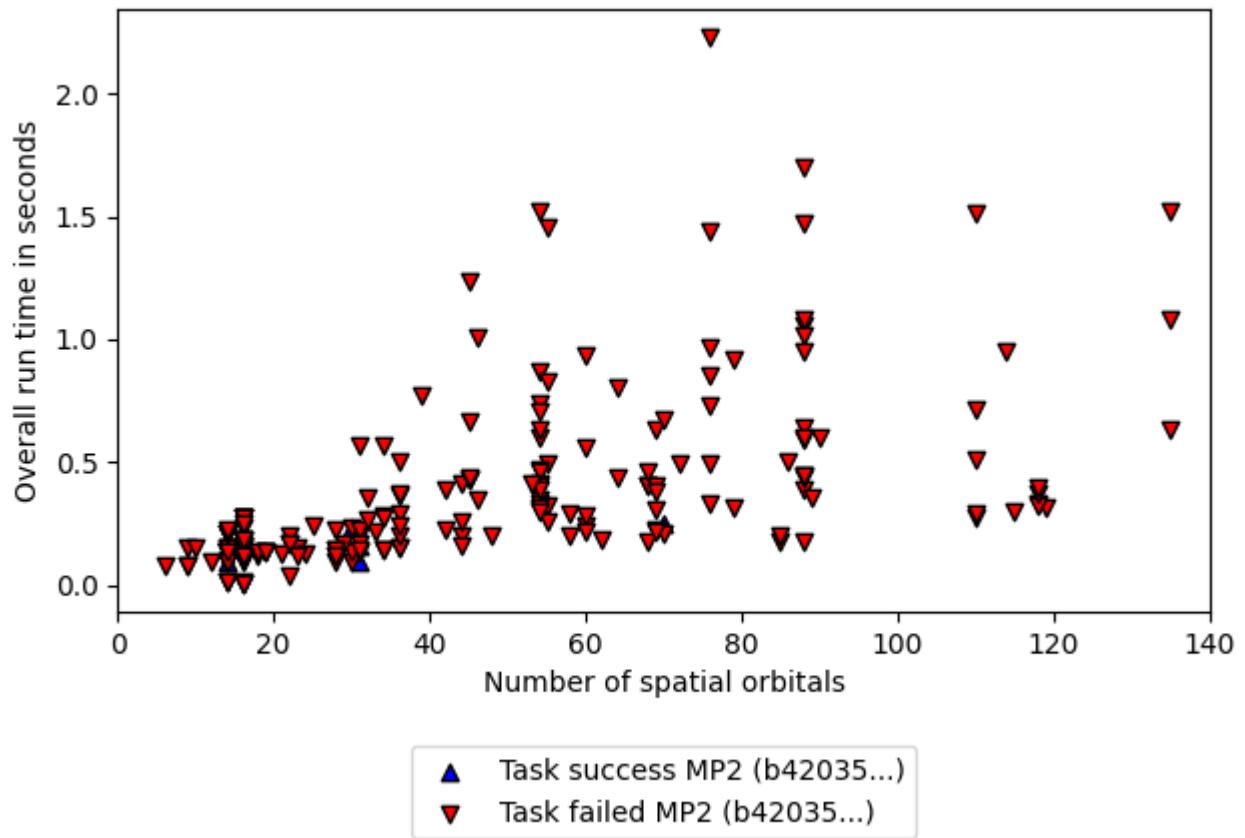
## Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aecd2

solver\_uuid:b420358b-5def-41e6-8c5d-b9d93b6aecd2

solver\_short\_name:MP2

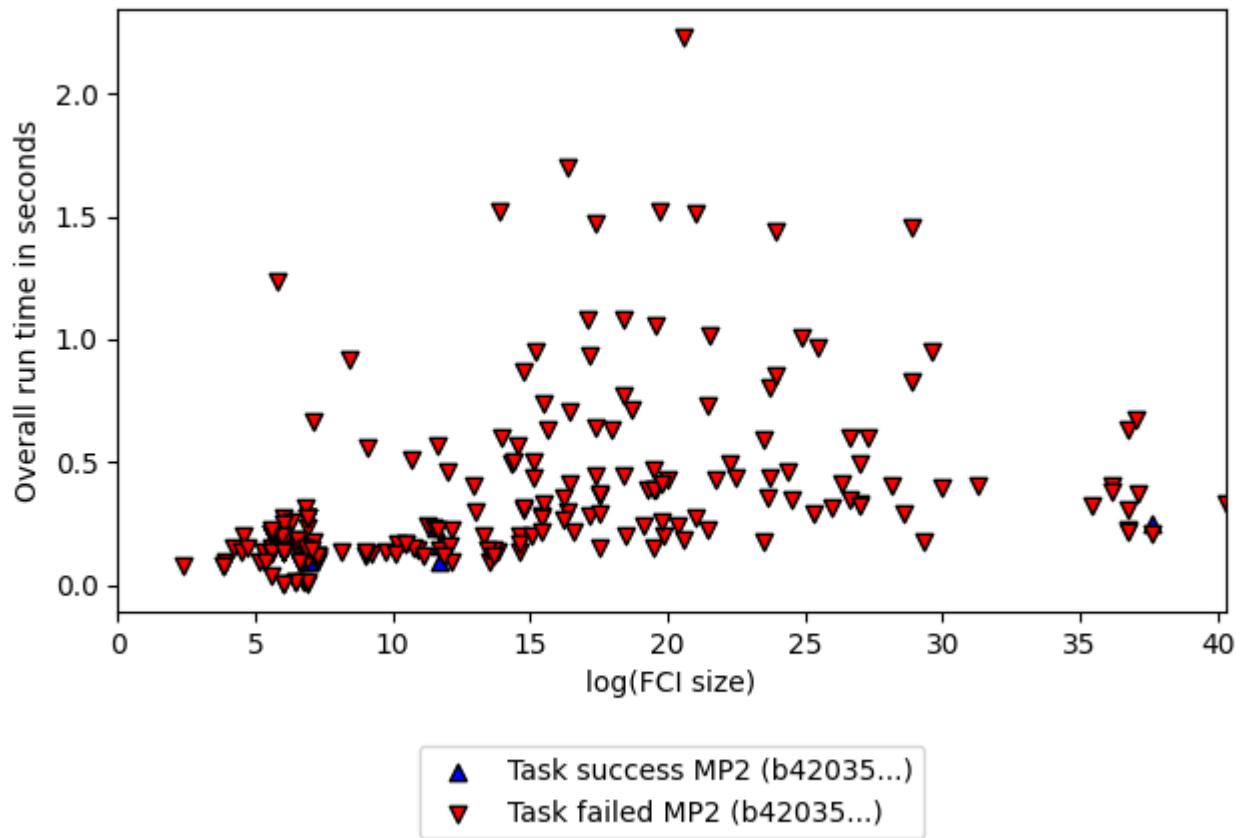
compute.hardware\_type:classical\_computer  
classical.hardware\_details:{'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}  
algorithm\_details:MP2  
software\_details:pyscf (<https://github.com/pyscf/pyscf>).  
performance\_metrics\_uuid: e06c981e-7e3b-449f-a9a9-e8f335e5f803  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 61  
number\_of\_problem\_instances\_solved: 5  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 216  
number\_of\_tasks\_solved: 5  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 216  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 5  
max\_run\_time\_of\_attempted\_tasks: 2.230440139770508  
sum\_of\_run\_time\_of\_attempted\_tasks: 78.34016704559326  
solvability\_ratio: 0.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9863013698630136, 0.7142857142857143]  
ml\_metrics\_calculator\_version: 1

### Run time for MP2/b42035...



Note: plot only contains attempted tasks.

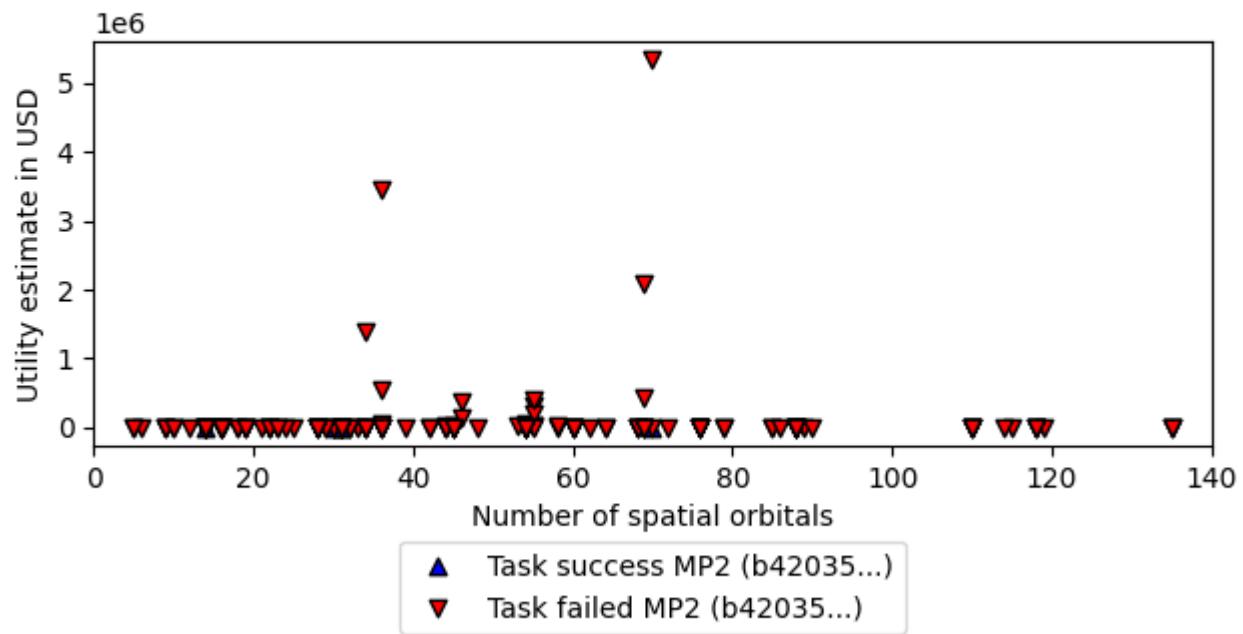
### Run time for MP2/b42035...



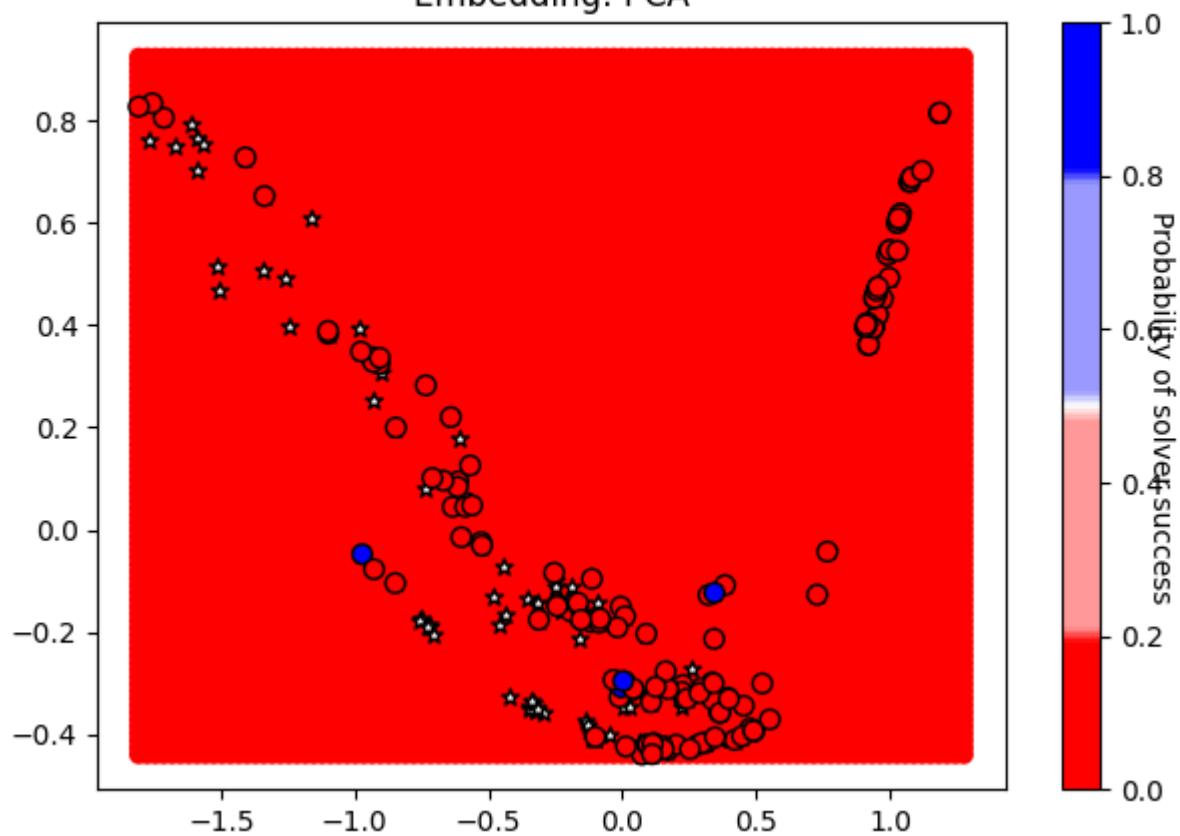
Note: plot only contains attempted tasks.

## Utility capture from MP2/b42035...

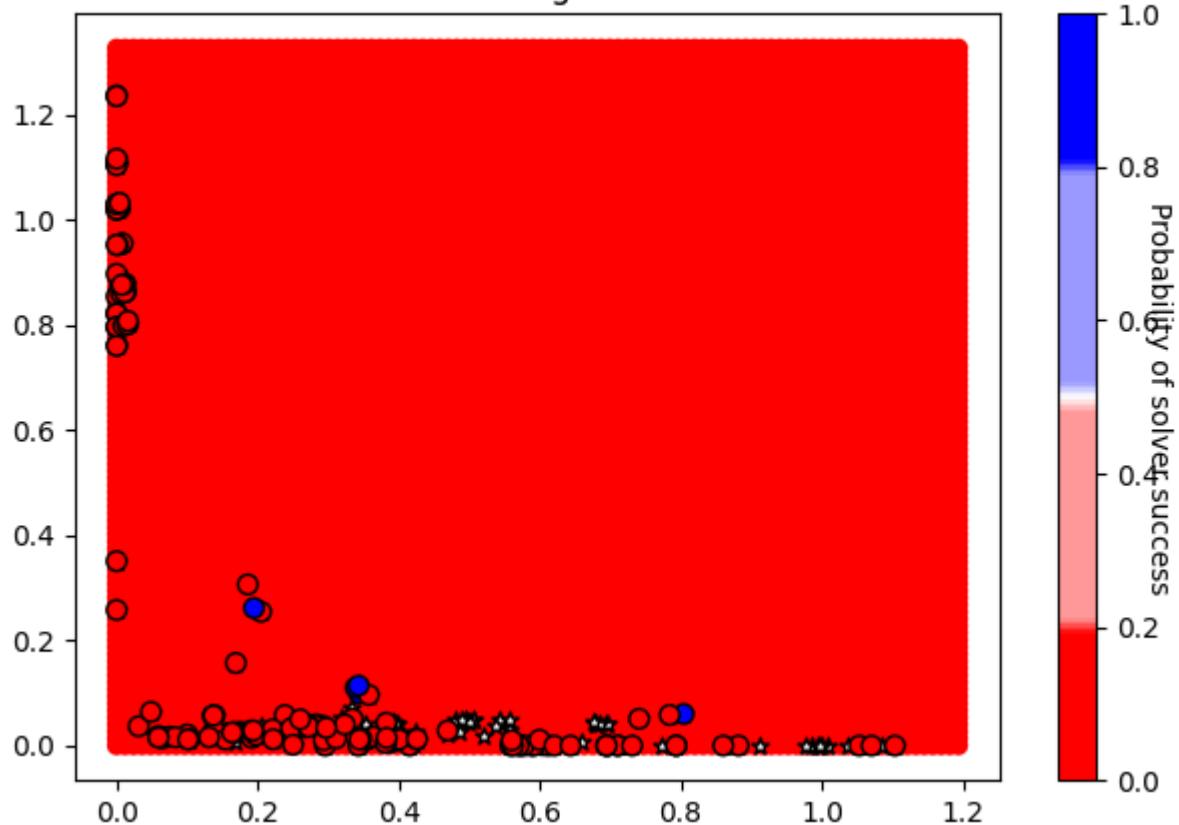
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



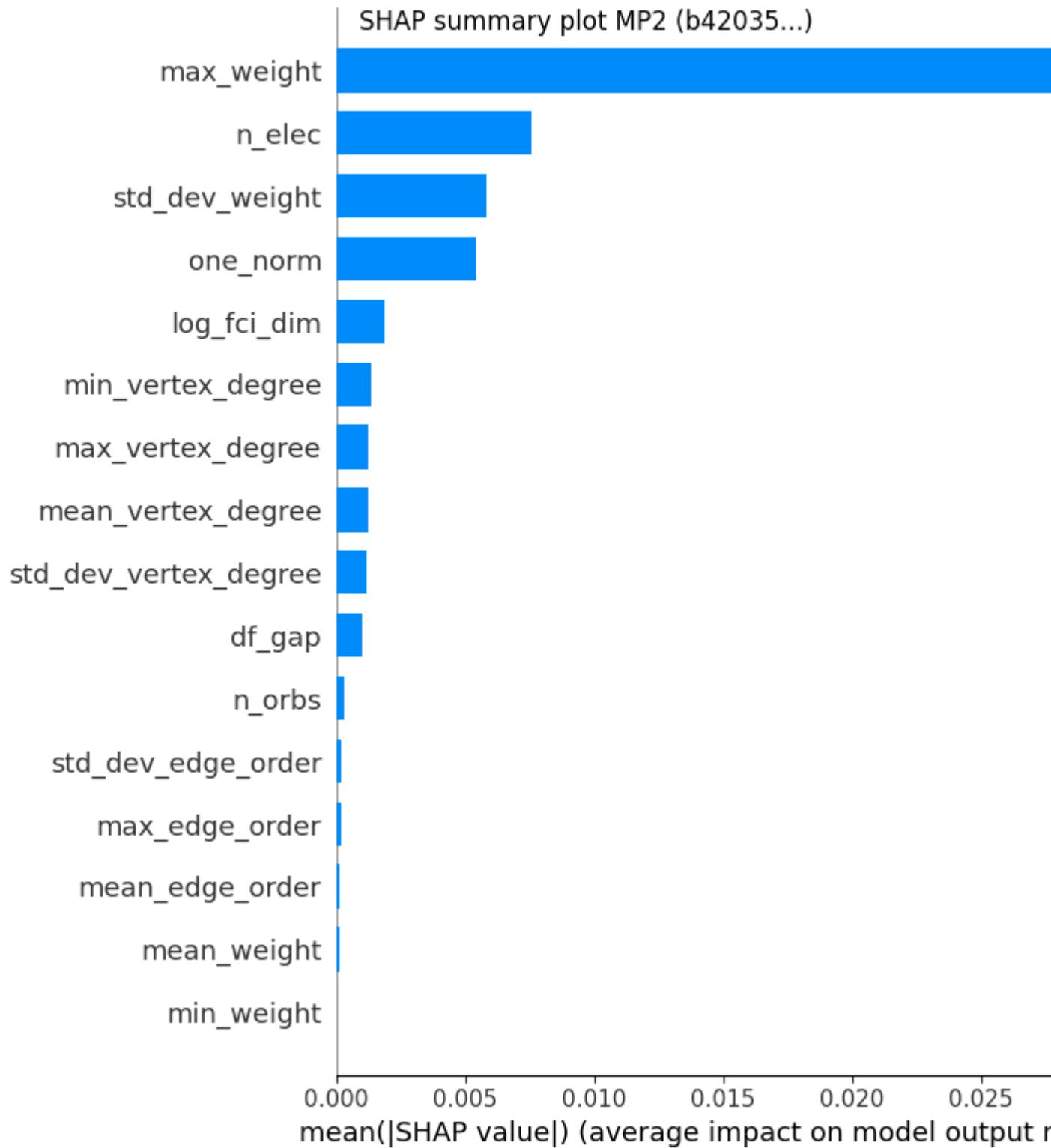
Solver MP2 (b42035...)  
Embedding: PCA



Solver MP2 (b42035...)  
Embedding: NNMF



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.



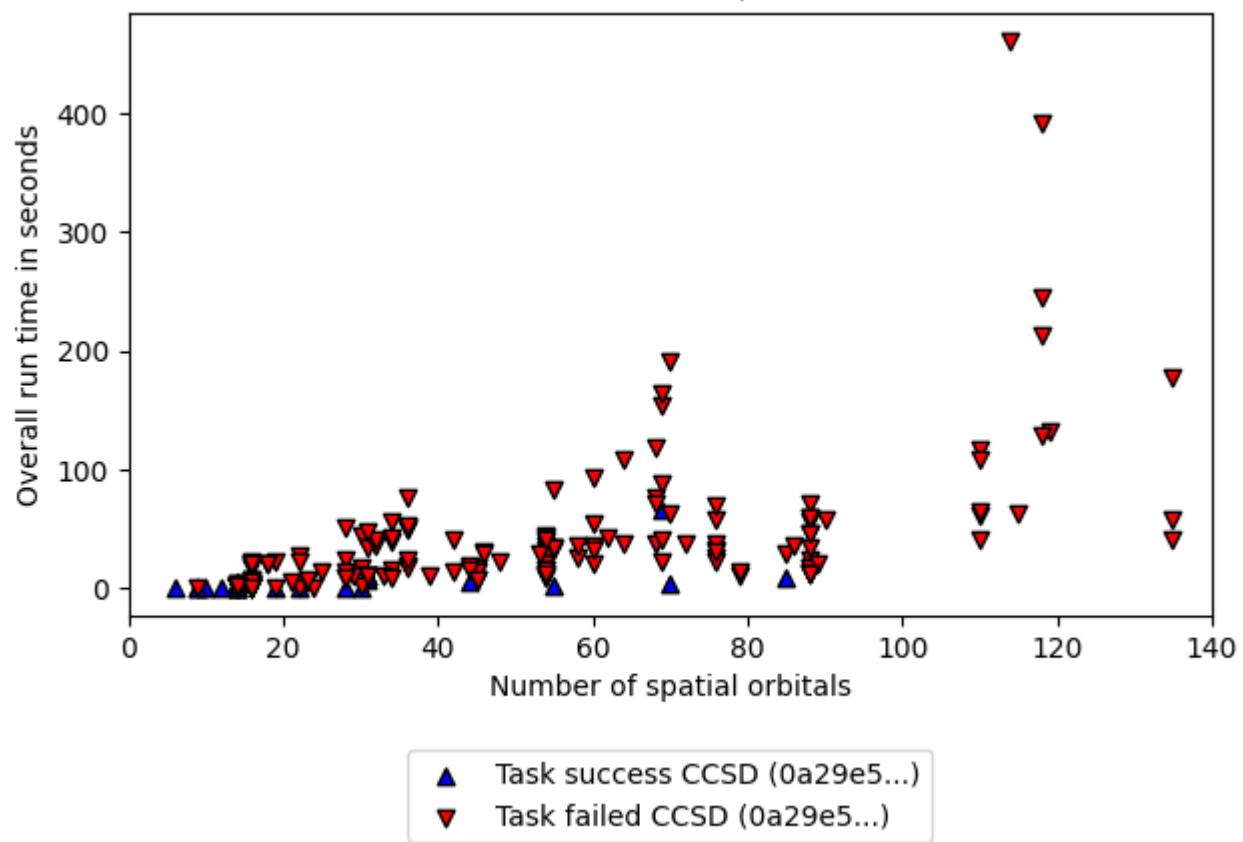
## Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

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

solver\_short\_name:CCSD

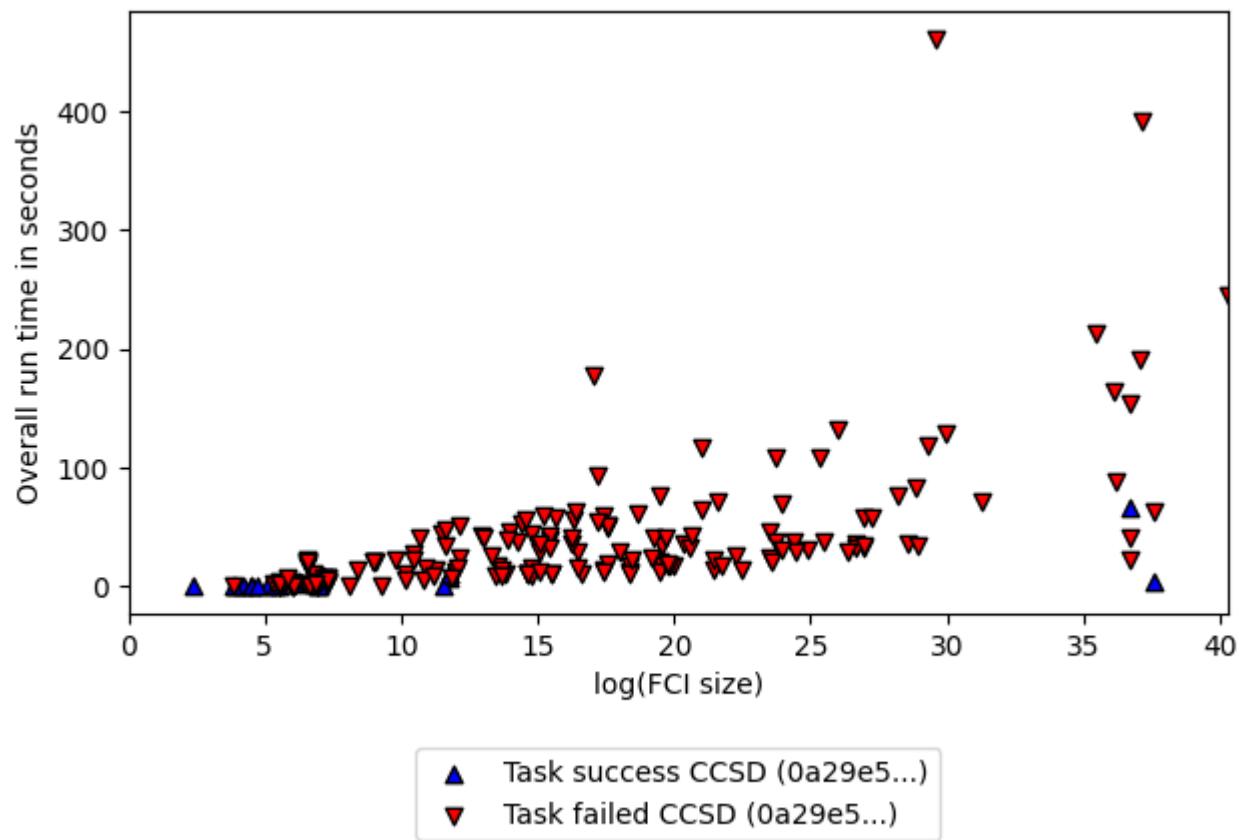
compute.hardware\_type:classical\_computer  
classical.hardware\_details:{'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}  
algorithm\_details:CCSD  
software\_details:pyscf (<https://github.com/pyscf/pyscf>).  
performance\_metrics\_uuid: 106963a0-169c-4fa7-ab23-5e8b9752cead  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 60  
number\_of\_problem\_instances\_solved: 10  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 213  
number\_of\_tasks\_solved: 23  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 213  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 23  
max\_run\_time\_of\_attempted\_tasks: 460.71552085876465  
sum\_of\_run\_time\_of\_attempted\_tasks: 7092.587965488434  
solvability\_ratio: 0.0  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9763779527559056, 0.8846153846153846]  
ml\_metrics\_calculator\_version: 1

### Run time for CCSD/0a29e5...



Note: plot only contains attempted tasks.

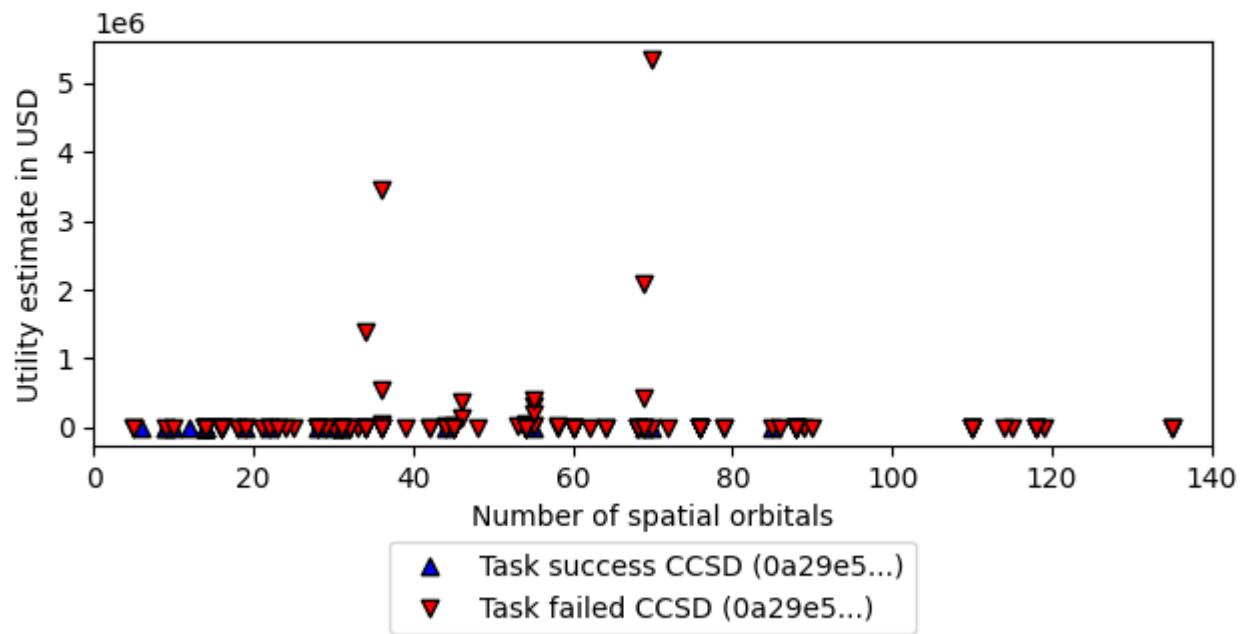
Run time for CCSD/0a29e5...



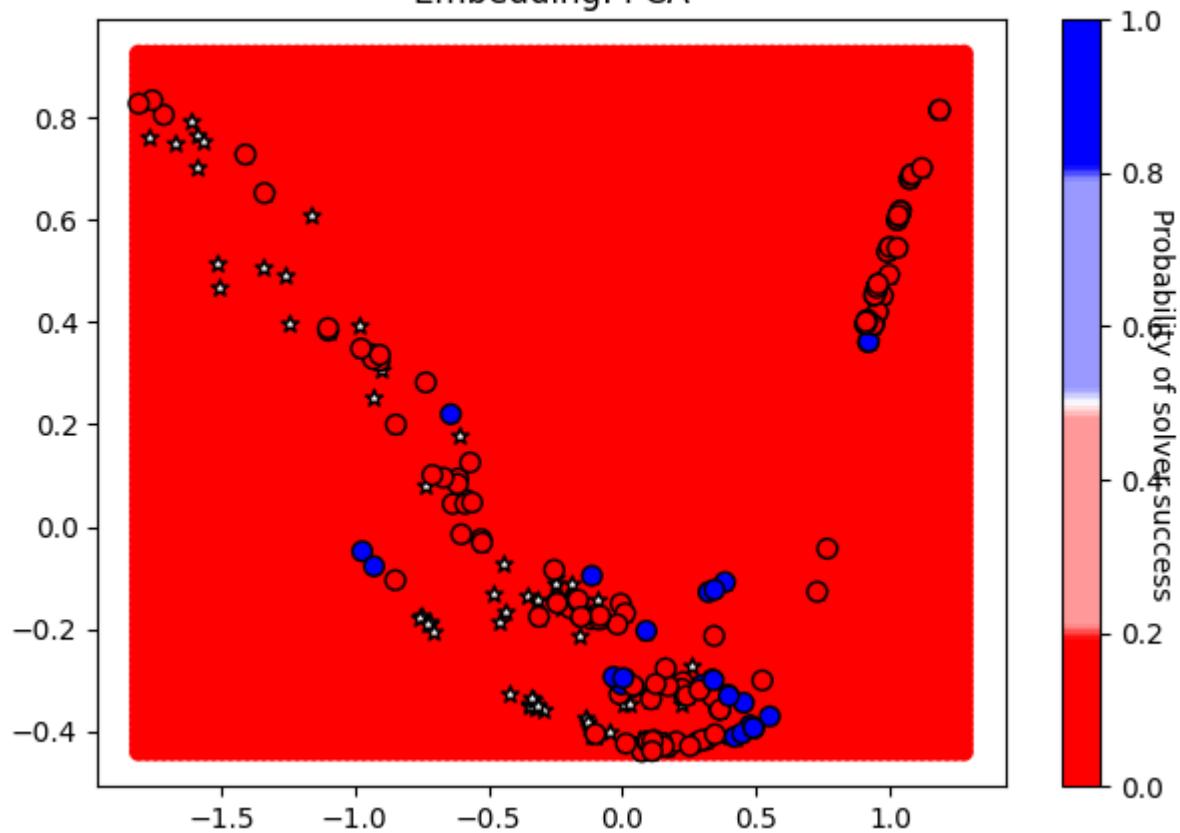
Note: plot only contains attempted tasks.

## Utility capture from CCSD/0a29e5...

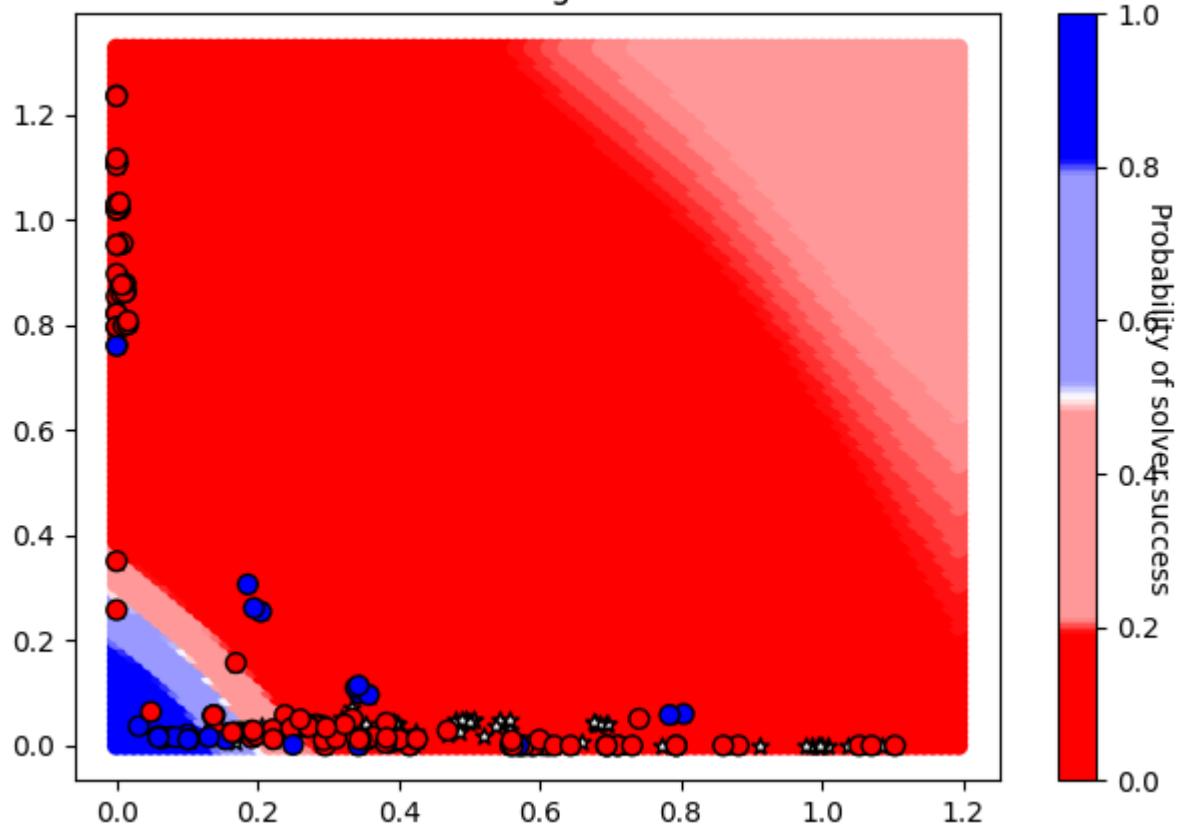
(captured: \$2.1e-02/1.5e+07, approximately 1.4e-07%)



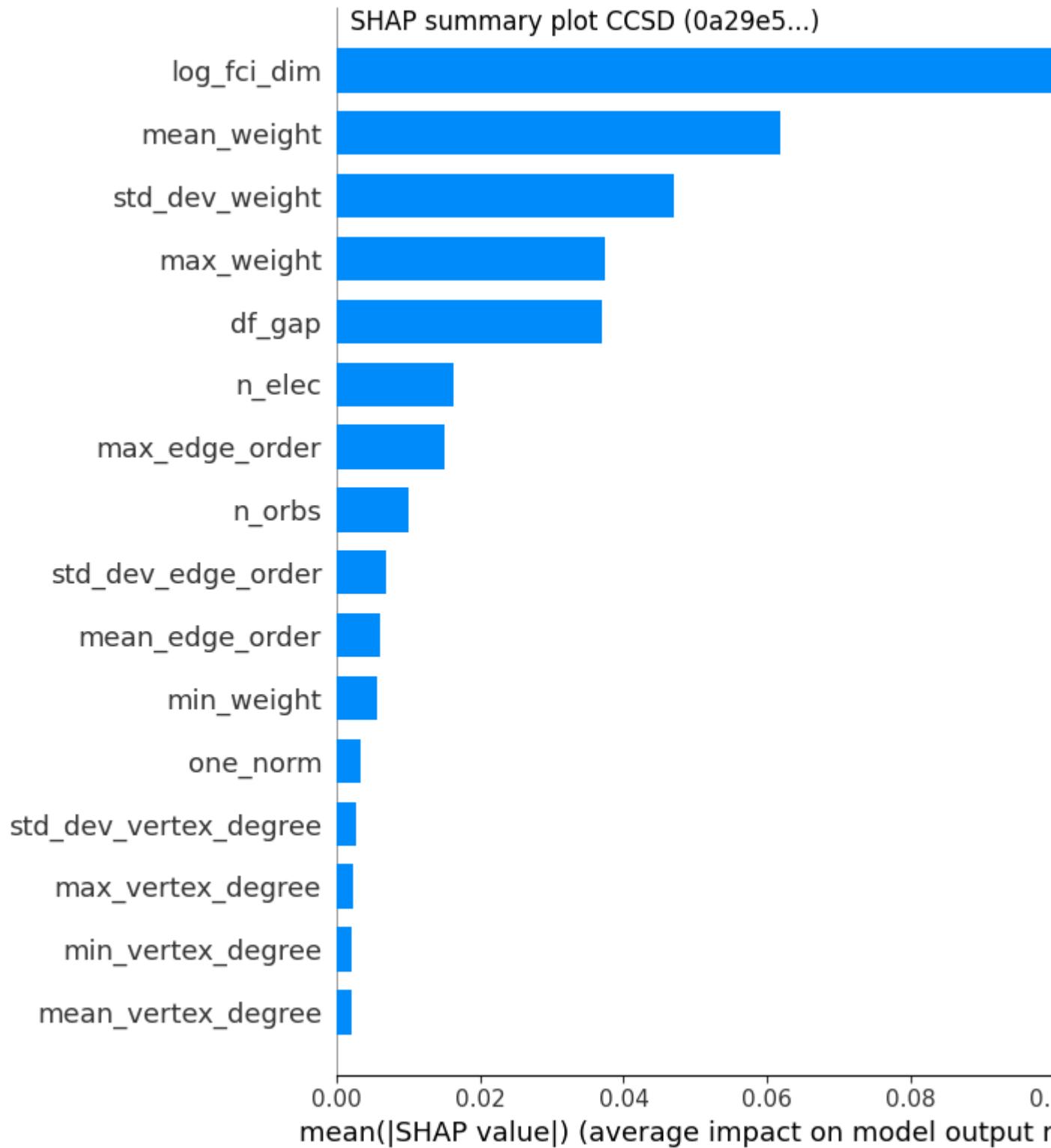
Solver CCSD (0a29e5...)  
Embedding: PCA



Solver CCSD (0a29e5...)  
Embedding: NMF



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.



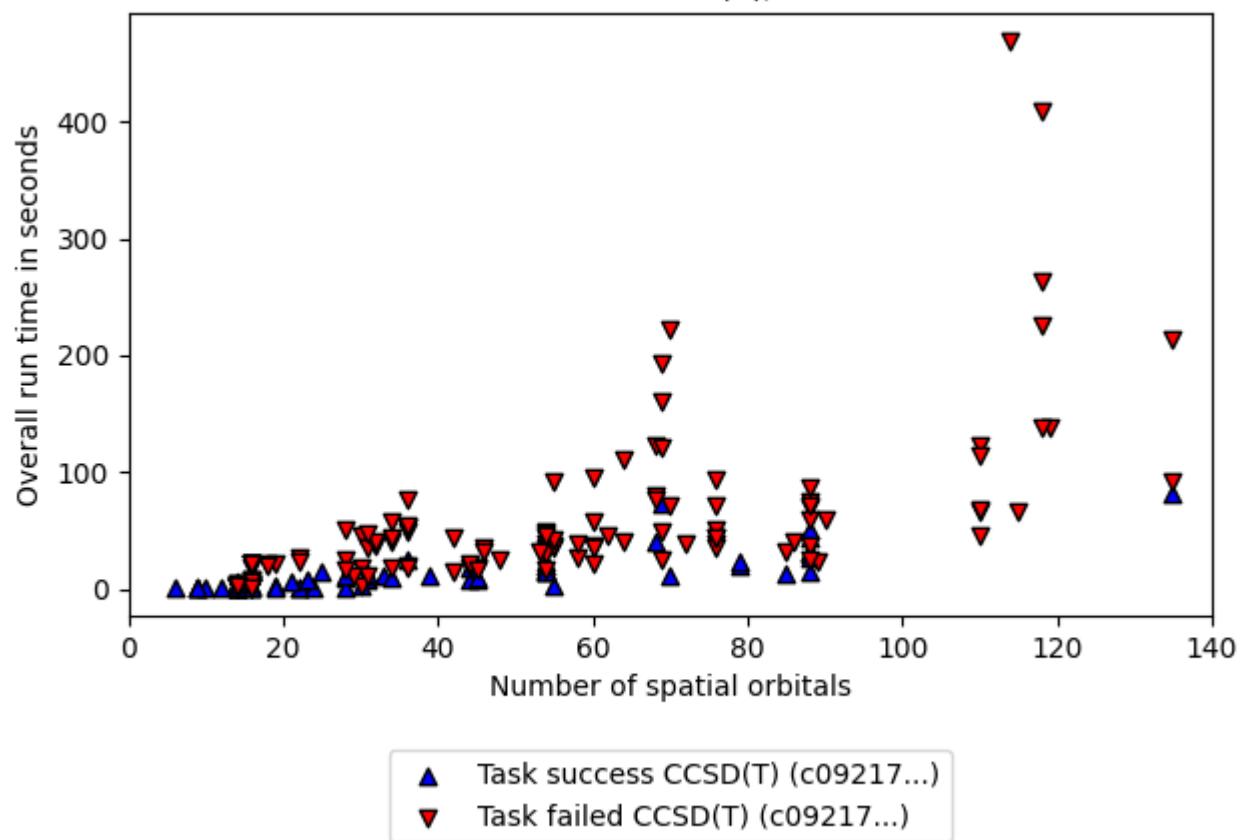
## Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878

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

solver\_short\_name:CCSD(T)

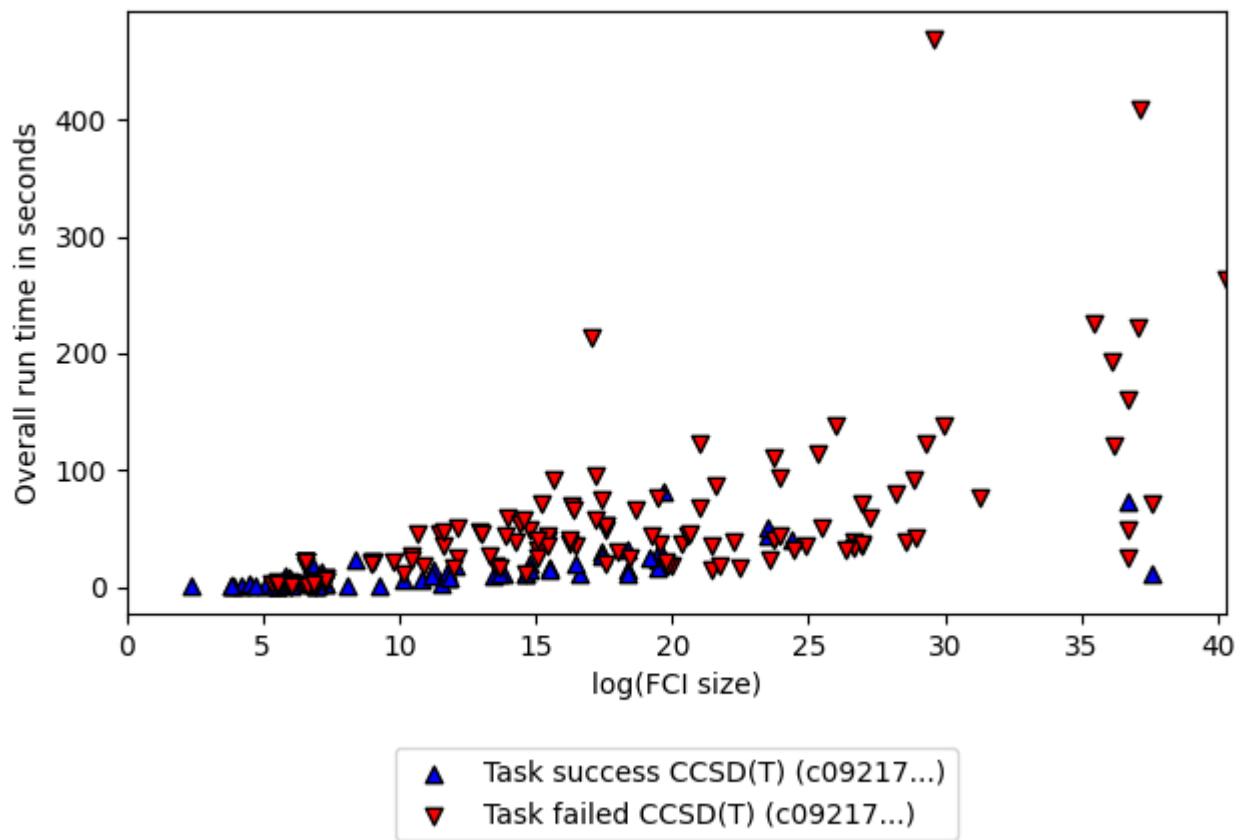
compute.hardware\_type:classical\_computer  
classical.hardware\_details:{'computing\_environment\_name': 'LCRC Improv (per node)', 'cpu\_description': '2x AMD EPYC 7713 64C', 'ram\_available\_gb': '256GB', 'clock\_speed': '2 GHz', 'total\_num\_cores': 128}  
algorithm\_details:CCSD(T)  
software\_details:pyscf (<https://github.com/pyscf/pyscf>).  
performance\_metrics\_uuid: b4fb23af-ea1f-410f-93a2-88b714ddaa4c  
creation\_timestamp: 2025-03-12T17:03:13.578128+00:00  
number\_of\_problem\_instances: 68  
number\_of\_problem\_instances\_attempted: 60  
number\_of\_problem\_instances\_solved: 19  
number\_of\_tasks: 228  
number\_of\_tasks\_attempted: 213  
number\_of\_tasks\_solved: 67  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 213  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 67  
max\_run\_time\_of\_attempted\_tasks: 469.1432478427887  
sum\_of\_run\_time\_of\_attempted\_tasks: 7912.881755828857  
solvability\_ratio: 0.305  
comments: solvability ratio based on PCA embedding.  
f1\_score: [0.9512195121951219, 0.9436619718309859]  
ml\_metrics\_calculator\_version: 1

### Run time for CCSD(T)/c09217...



Note: plot only contains attempted tasks.

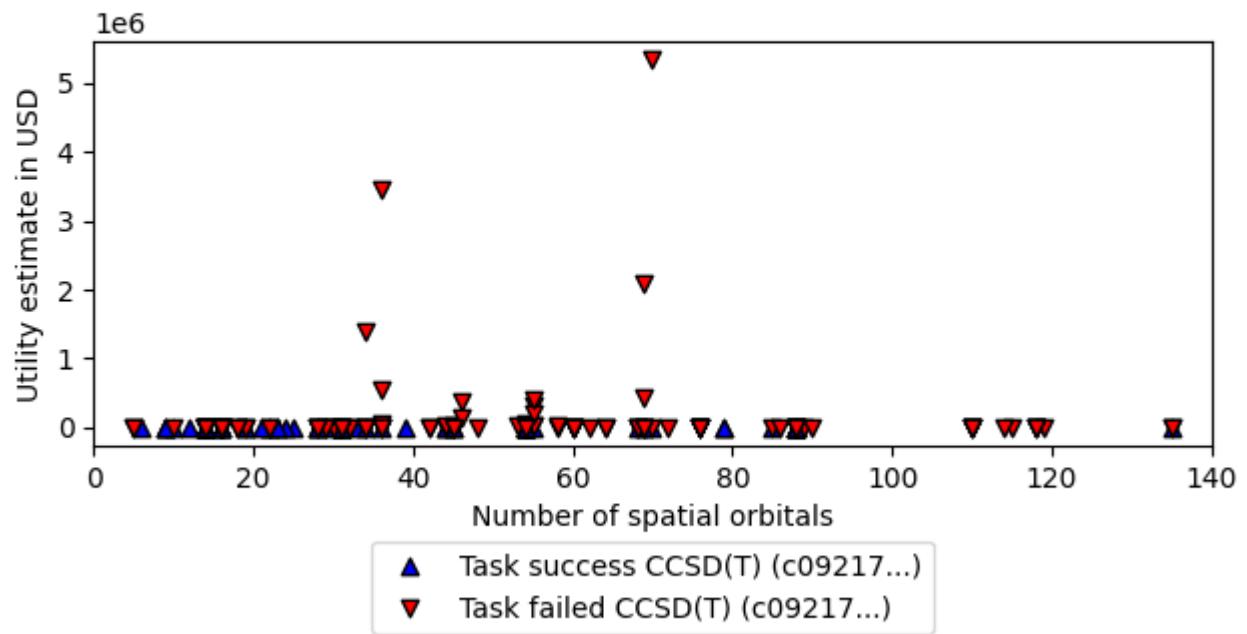
### Run time for CCSD(T)/c09217...



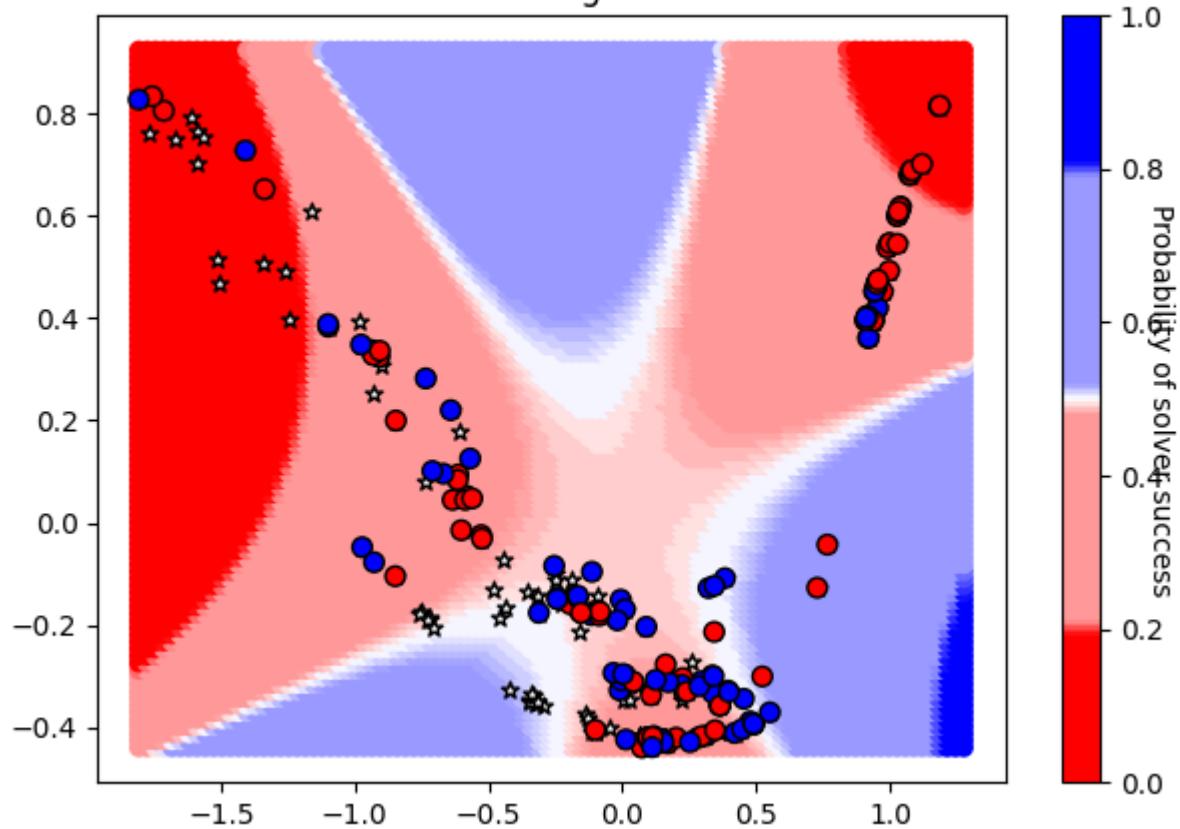
Note: plot only contains attempted tasks.

Utility capture from CCSD(T)/c09217...

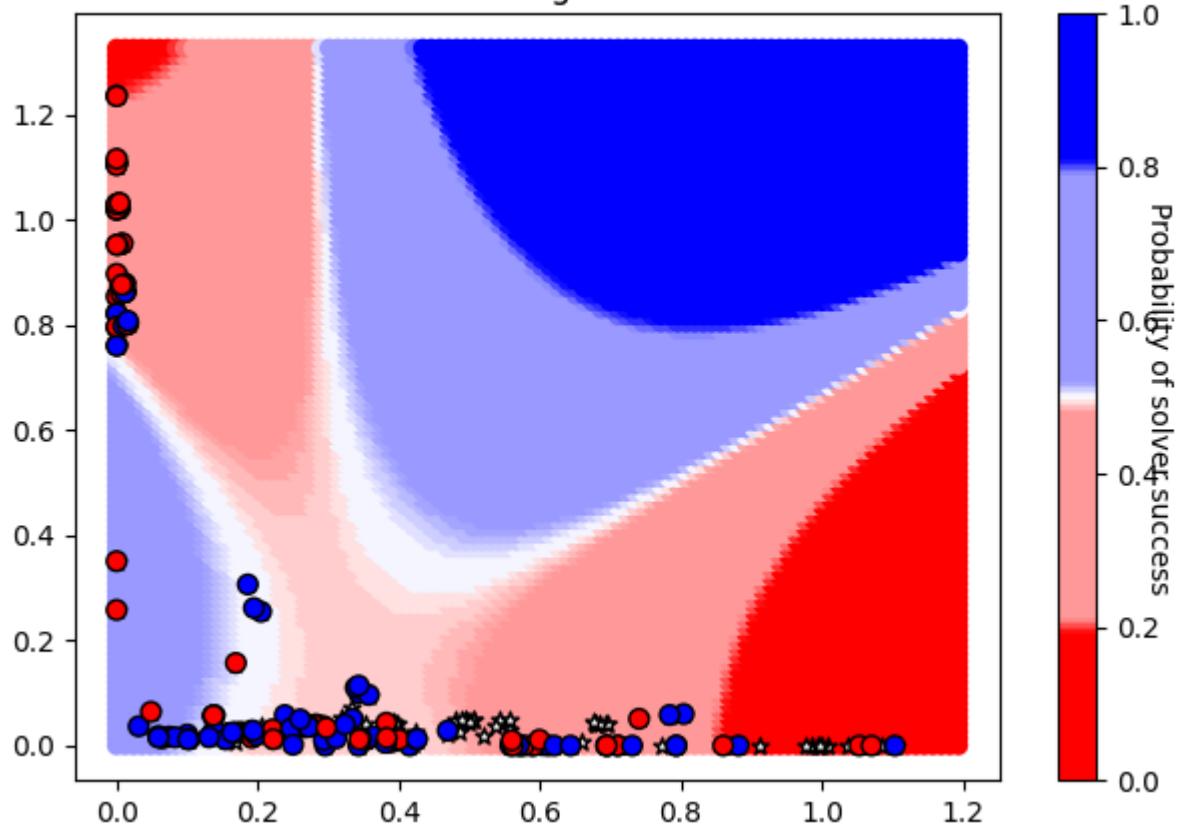
(captured:  $\$1.8e+02/1.5e+07$ , approximately  $1.2e-03\%$ )



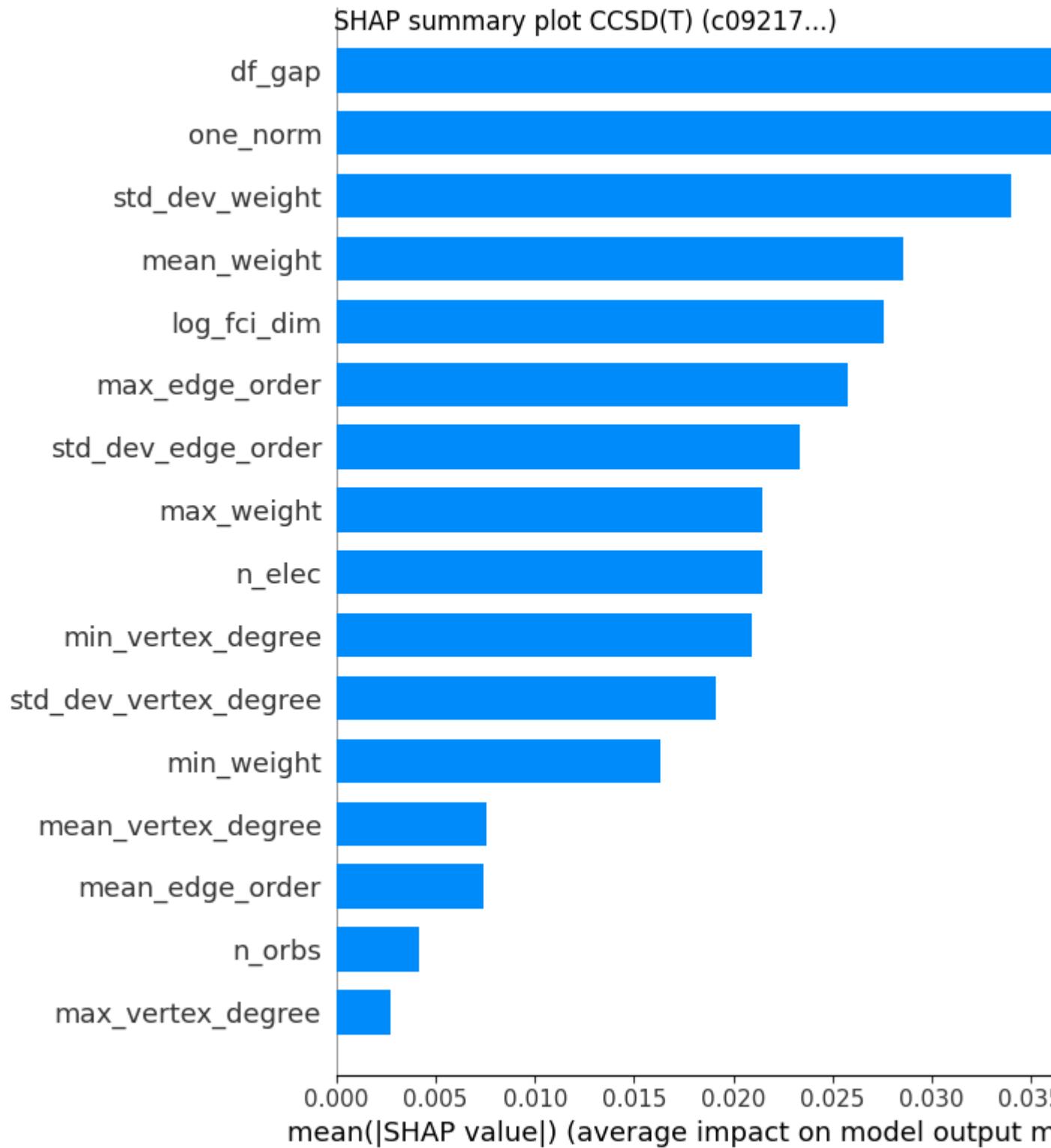
Solver CCSD(T) (c09217...)  
Embedding: PCA



Solver CCSD(T) (c09217...)  
Embedding: NMF



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, 7c8ef984-4d3a-4468-8900-e0da3bd8b22d

solver\_uuid:7c8ef984-4d3a-4468-8900-e0da3bd8b22d

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': 0.94868329805, 'sf\_threshold': 1e-12, 'df\_threshold': 0.001, 'max\_orbitals': 70}}

software\_details:[{'software\_name': 'benchq', 'software\_version': '0.7.1.dev10+g80b8279.d20250116'}, {'software\_name': 'openfermion', 'software\_version': '1.6.1'}, {'software\_name': 'Python', 'software\_version': '3.11.5 (main, Sep 11 2023, 08:31:25) [Clang 14.0.6]'}, {'software\_name': 'benchq', 'software\_version': '0.7.1.dev10+g80b8279.d20250116'}]

quantum\_hardware\_details:{'quantum\_hardware\_description': 'Superconducting hardware model based on the optimistic model 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:e135679c-e314-4808-9634-252bc376d295

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

performance\_metrics\_uuid: a0693bc5-3990-4c6e-b373-1fd0d40d1575

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 4

number\_of\_problem\_instances\_solved: 1

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 24

number\_of\_tasks\_solved: 1

number\_of\_tasks\_solved\_within\_run\_time\_limit: 1

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

max\_run\_time\_of\_attempted\_tasks: 451622221.769206

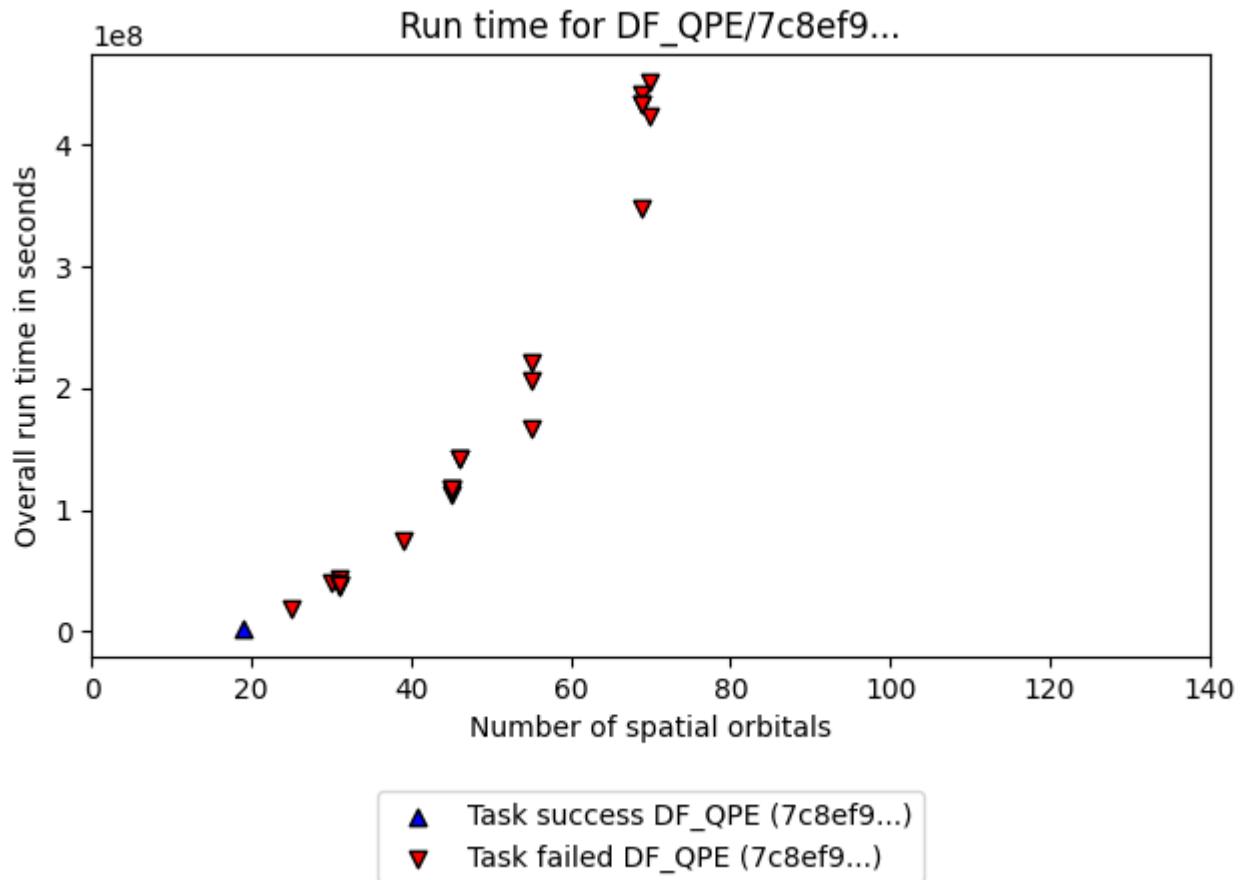
sum\_of\_run\_time\_of\_attempted\_tasks: 4206142119.5542016

solvability\_ratio: 0.0

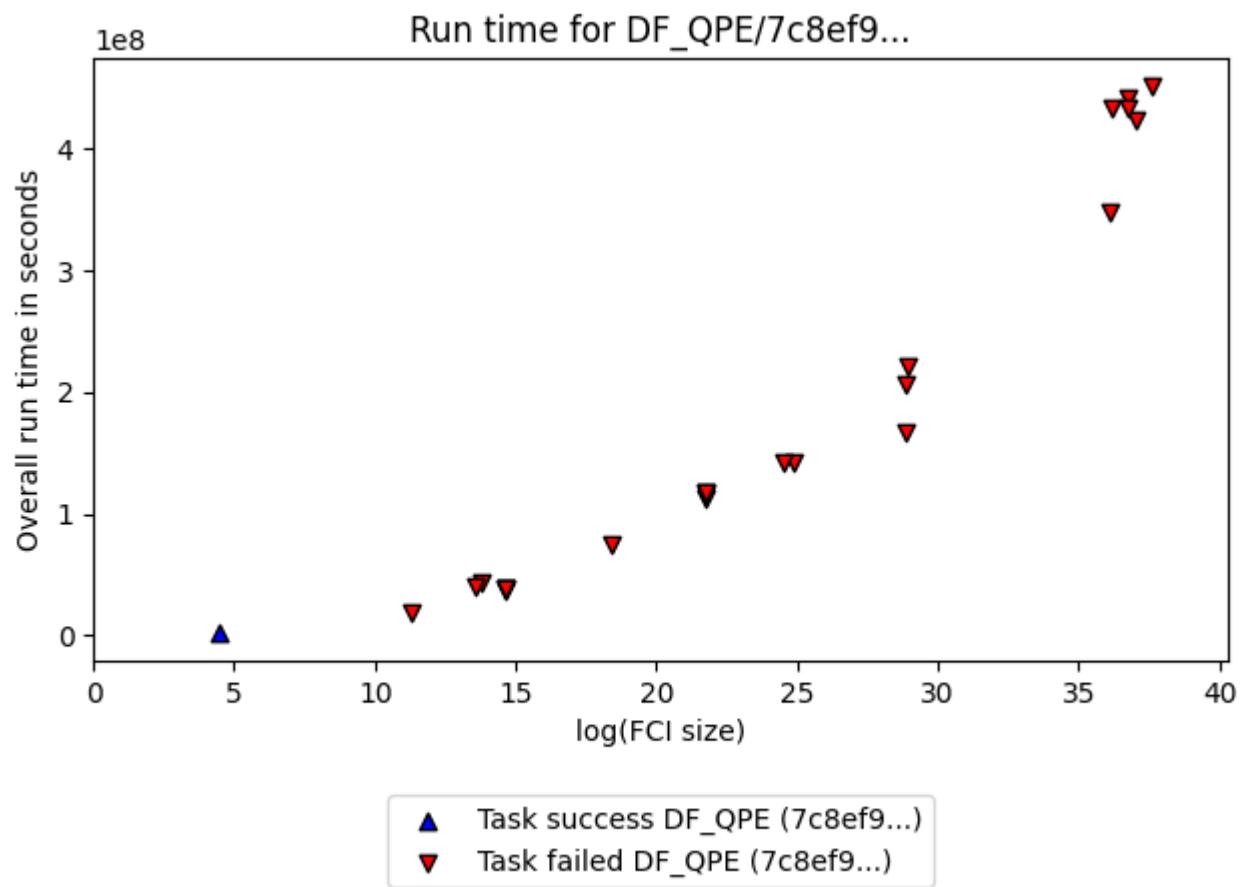
comments: solvability ratio based on PCA embedding., ML model calculated without GridSearchCV

f1\_score: [0.9370629370629371, 0.1]

ml\_metrics\_calculator\_version: 1



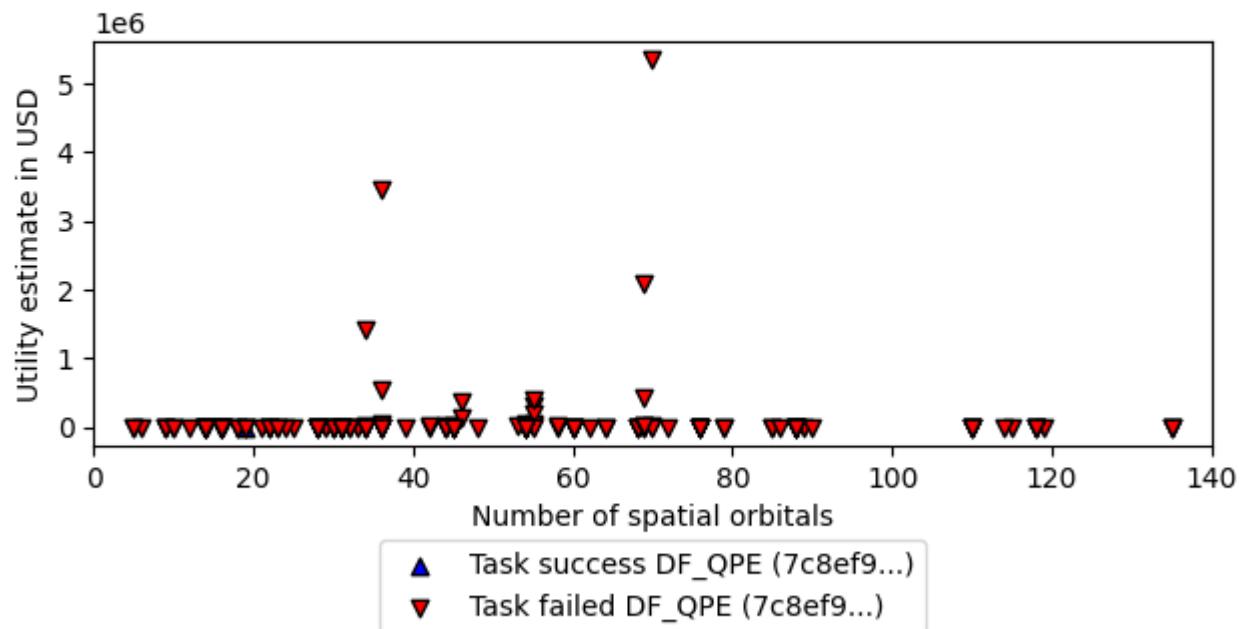
Note: plot only contains attempted tasks.



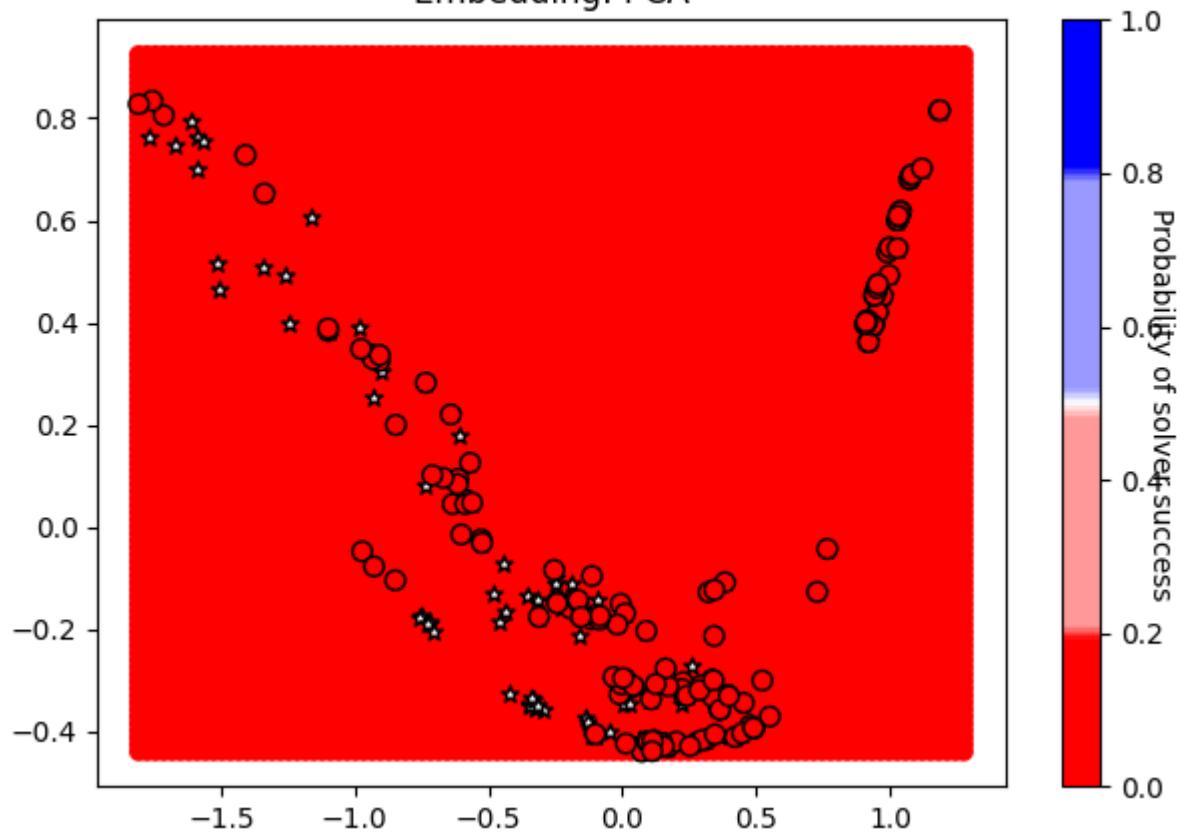
Note: plot only contains attempted tasks.

## Utility capture from DF\_QPE/7c8ef9...

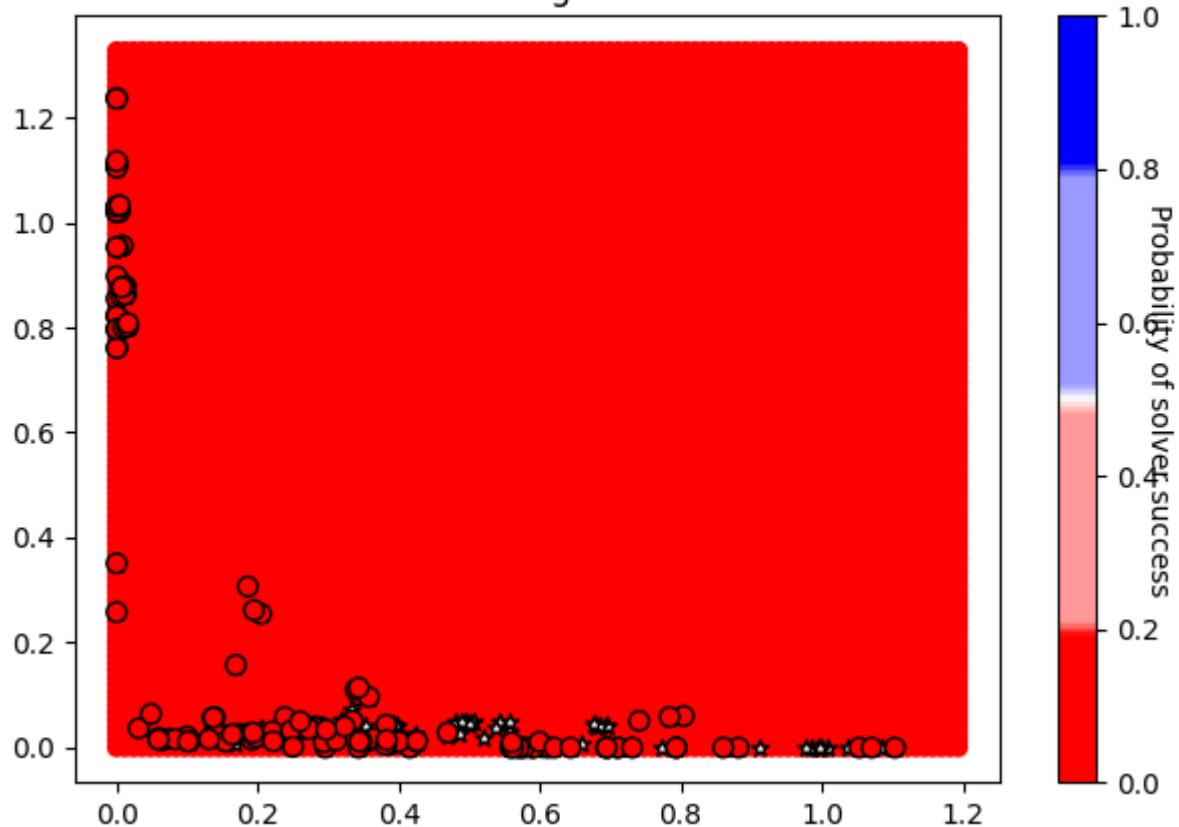
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



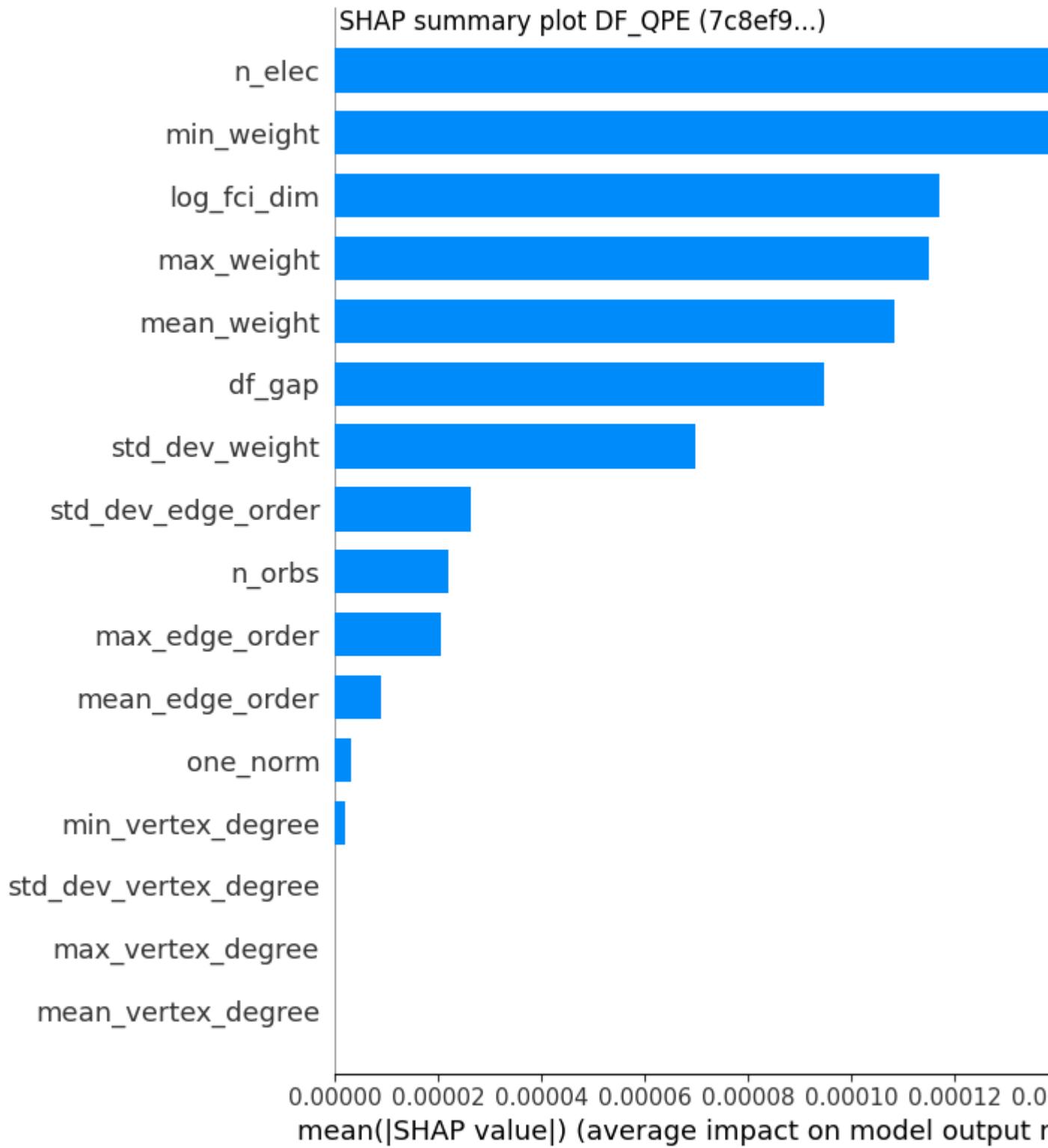
Solver DF\_QPE (7c8ef9...)  
Embedding: PCA



Solver DF\_QPE (7c8ef9...)  
Embedding: NNMF



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, 5d768520-b3d0-4292-bbb4-9776fa128107

solver\_uuid:5d768520-b3d0-4292-bbb4-9776fa128107

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': '1.3.6'}, {'software\_name': 'qb-gsee-benchmark', 'software\_version': '0.1.0a3.dev68+g2b90efd'}, {'software\_name': 'Python', 'software\_version': '3.10.12 (main, Feb 4 2025, 14:57:36) [GCC 11.4.0]'}, {'software\_name': 'qualtran', 'software\_version': '0.4.0'}]

quantum\_hardware\_details:{'quantum\_hardware\_description': 'Superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494 with an extremely optimistic physical error rate.', 'quantum\_hardware\_parameters': {'num\_factories': 4, 'physical\_error\_rate': 1e-06, 'cycle\_time\_microseconds': 1, 'parallelize\_shots': False}}

logical\_resource\_estimate\_solution\_uuid:608bffed-be36-4414-ab5c-fd3ee6838530

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

performance\_metrics\_uuid: c6cf4628-7e59-4220-89b5-432cd3114055

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 24

number\_of\_problem\_instances\_solved: 2

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 137

number\_of\_tasks\_solved: 2

number\_of\_tasks\_solved\_within\_run\_time\_limit: 2

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

max\_run\_time\_of\_attempted\_tasks: 71881480309947.6

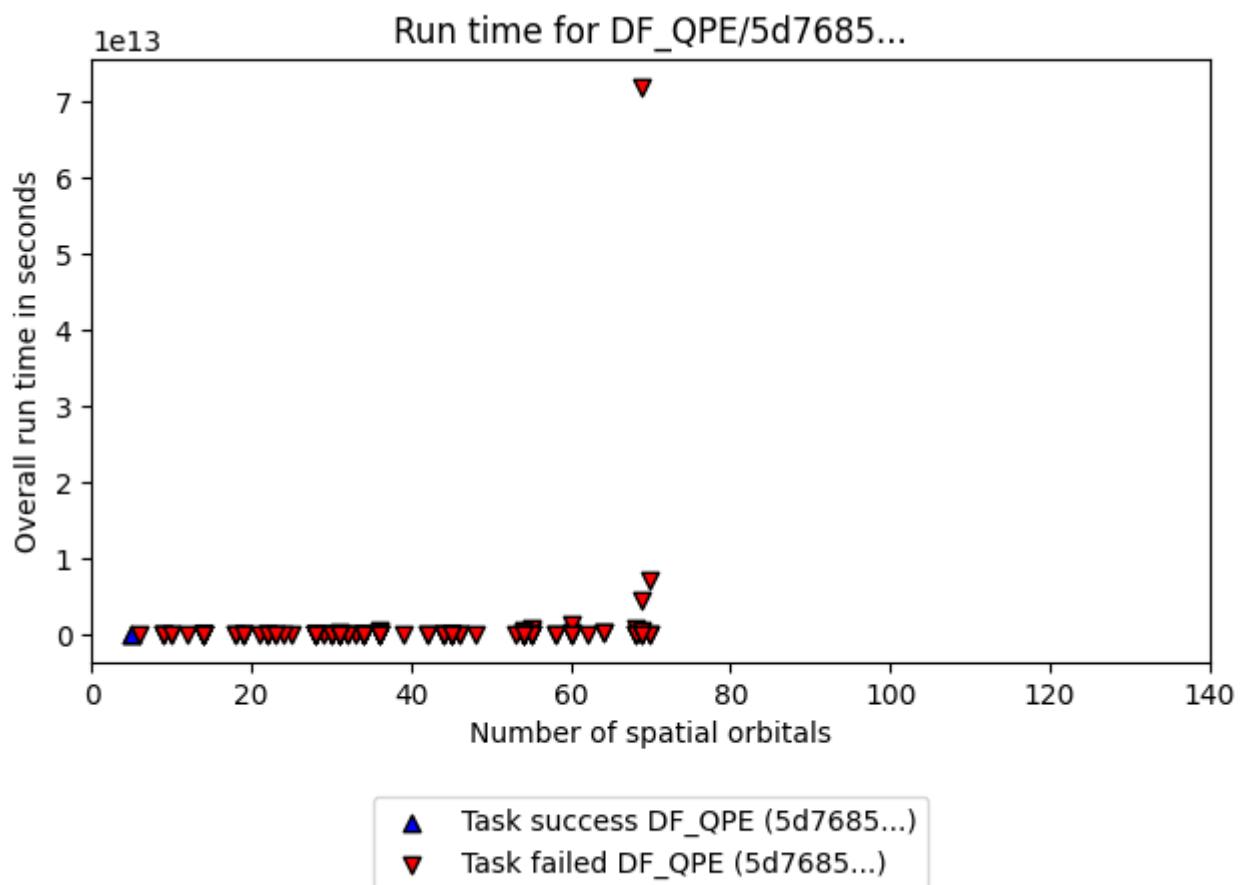
sum\_of\_run\_time\_of\_attempted\_tasks: 92303779447162.08

solvability\_ratio: 0.0394

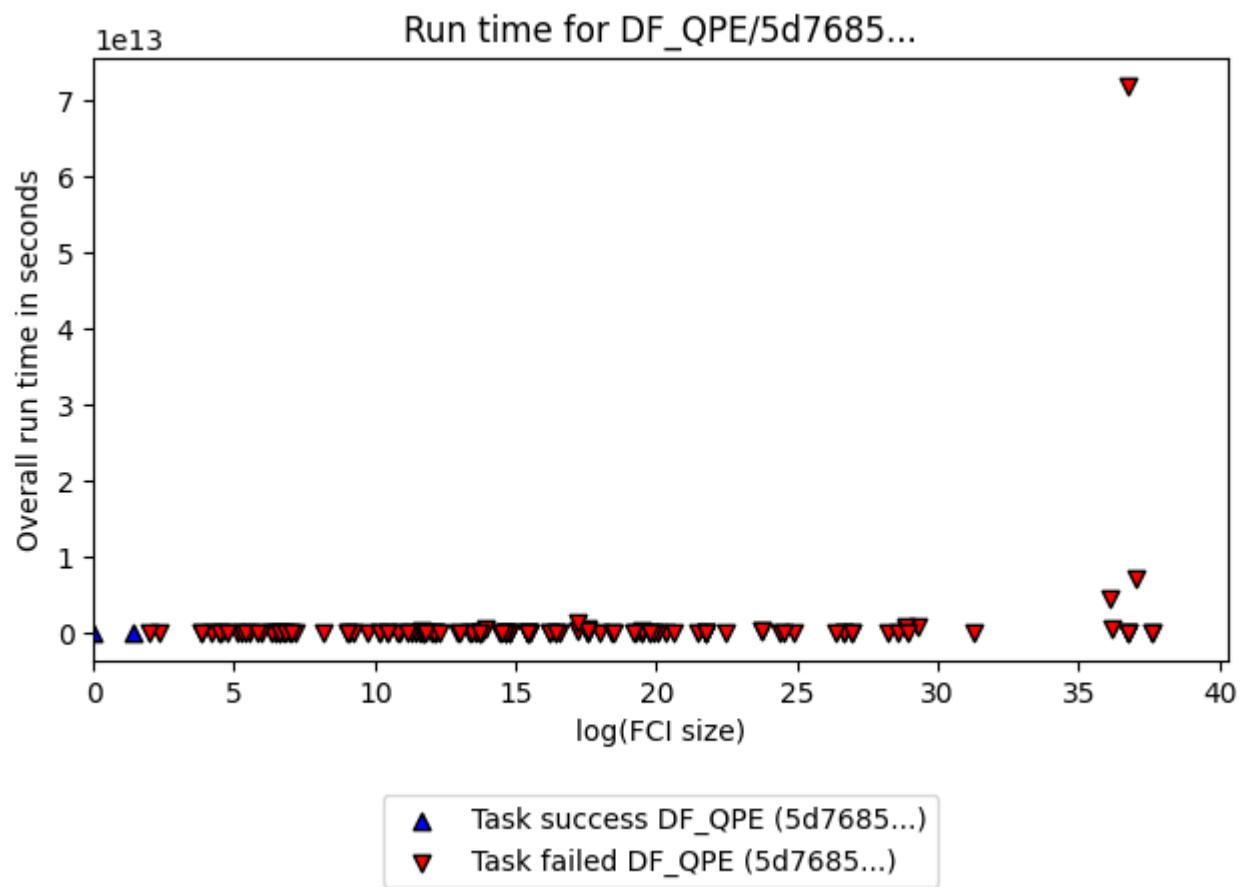
comments: solvability ratio based on PCA embedding.

f1\_score: [1.0, 1.0]

ml\_metrics\_calculator\_version: 1



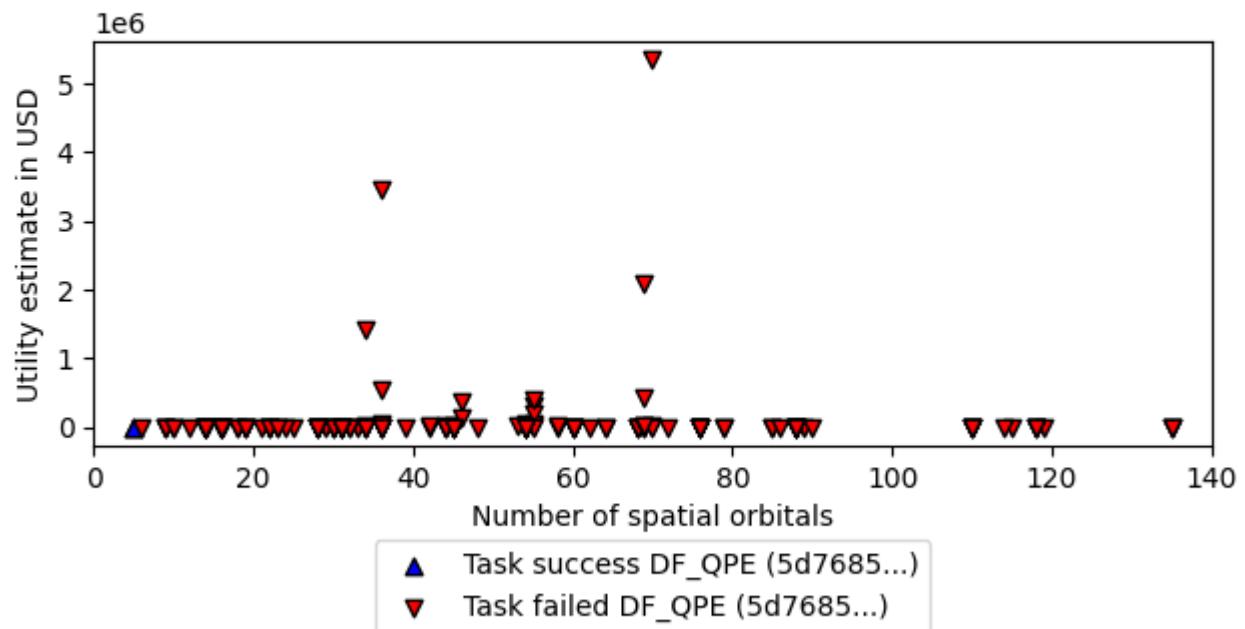
Note: plot only contains attempted tasks.



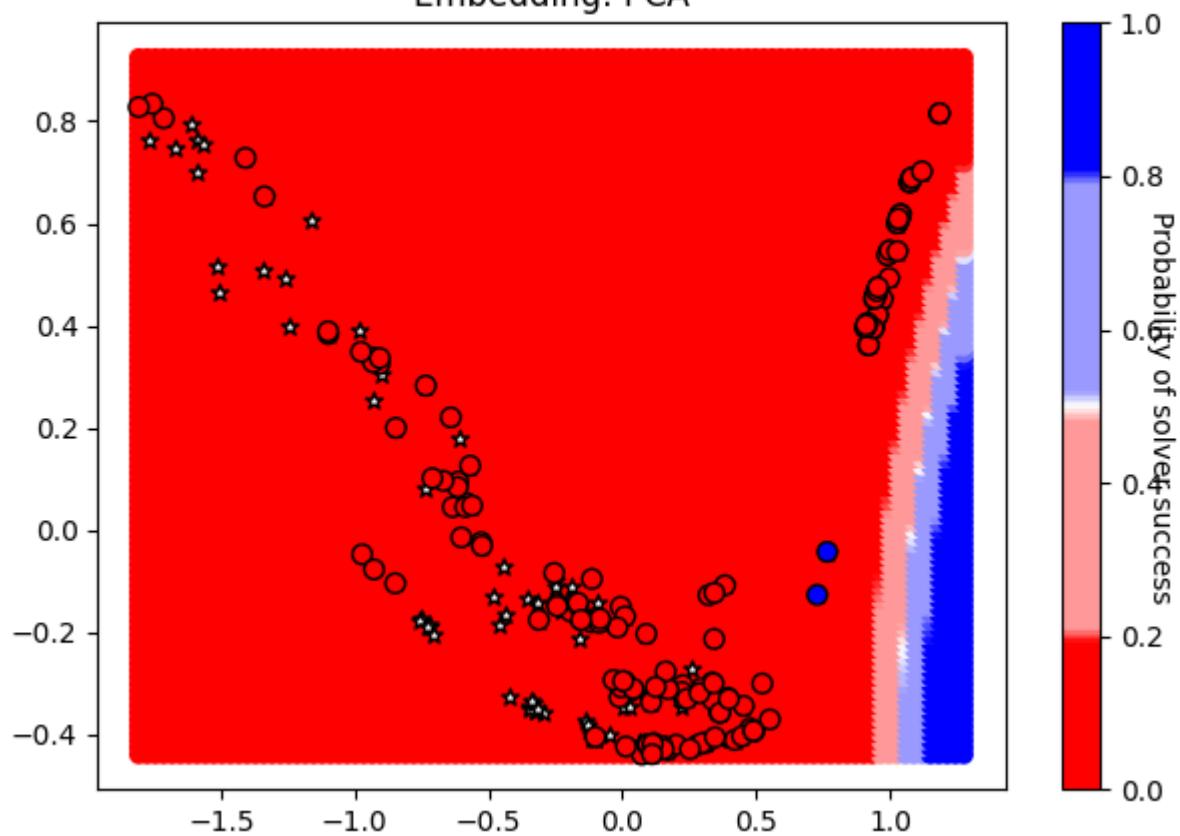
Note: plot only contains attempted tasks.

## Utility capture from DF\_QPE/5d7685...

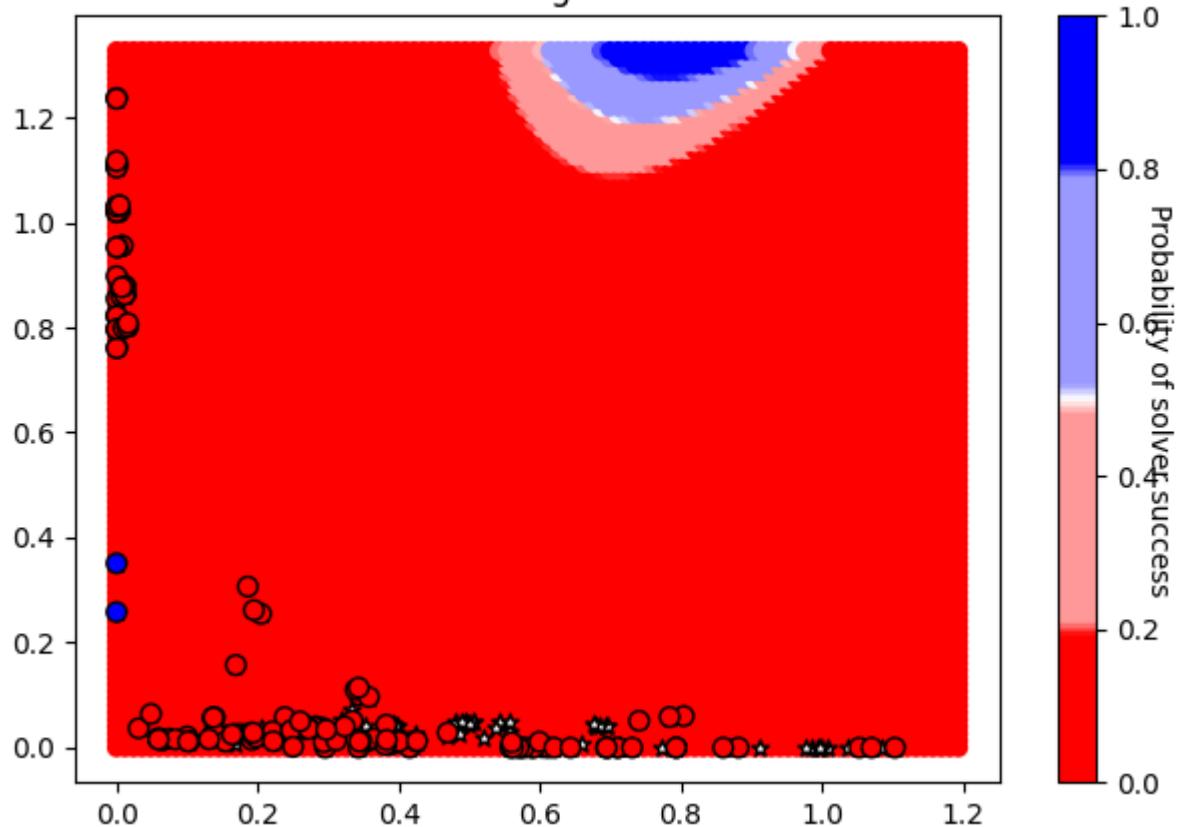
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



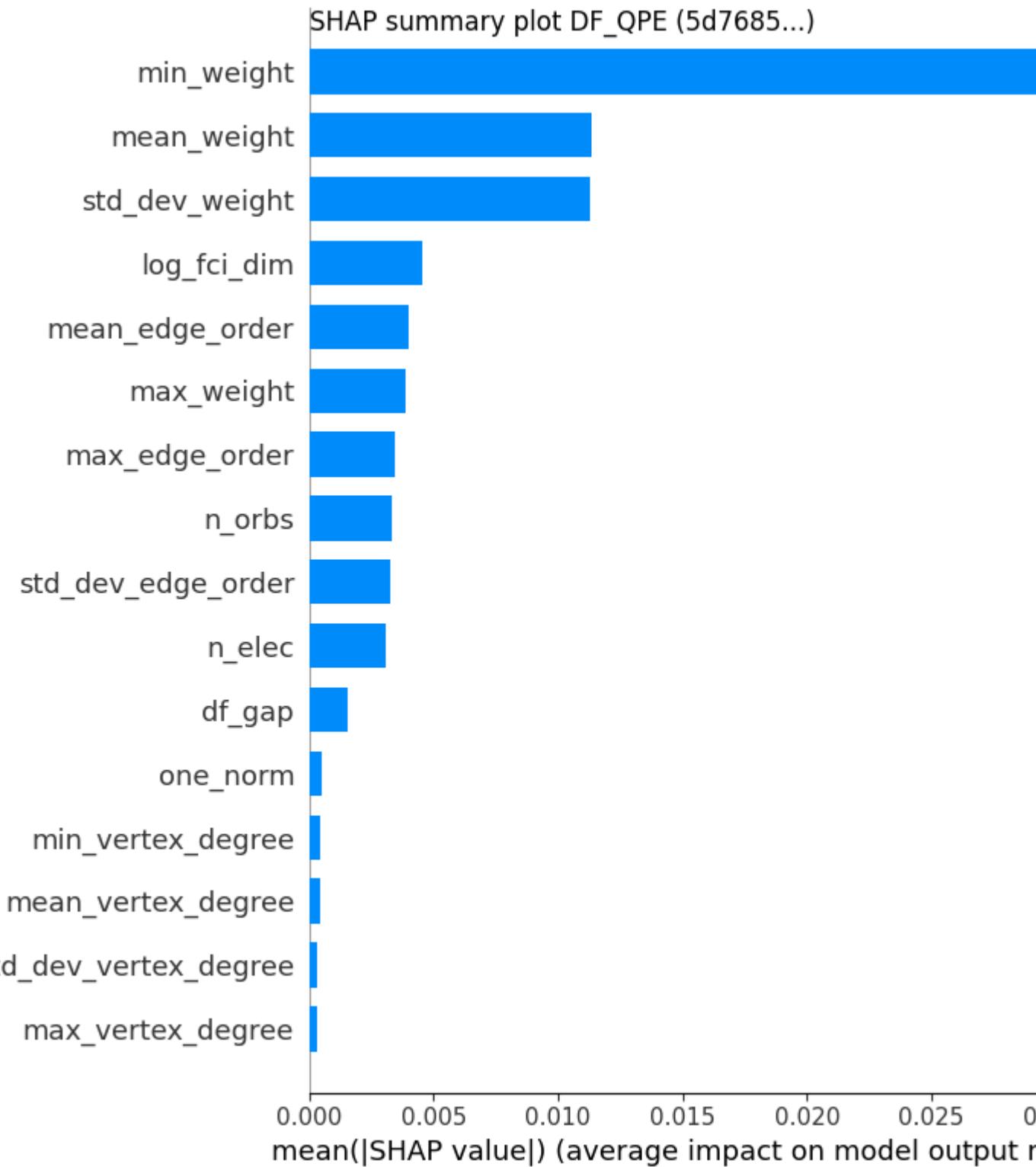
Solver DF\_QPE (5d7685...)  
Embedding: PCA



Solver DF\_QPE (5d7685...)  
Embedding: NMF



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: 431d3701-def8-49ff-8f1b-f7cb9e8986f7

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 68

number\_of\_problem\_instances\_solved: 13

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 228

number\_of\_tasks\_solved: 107

number\_of\_tasks\_solved\_within\_run\_time\_limit: 228

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 107

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

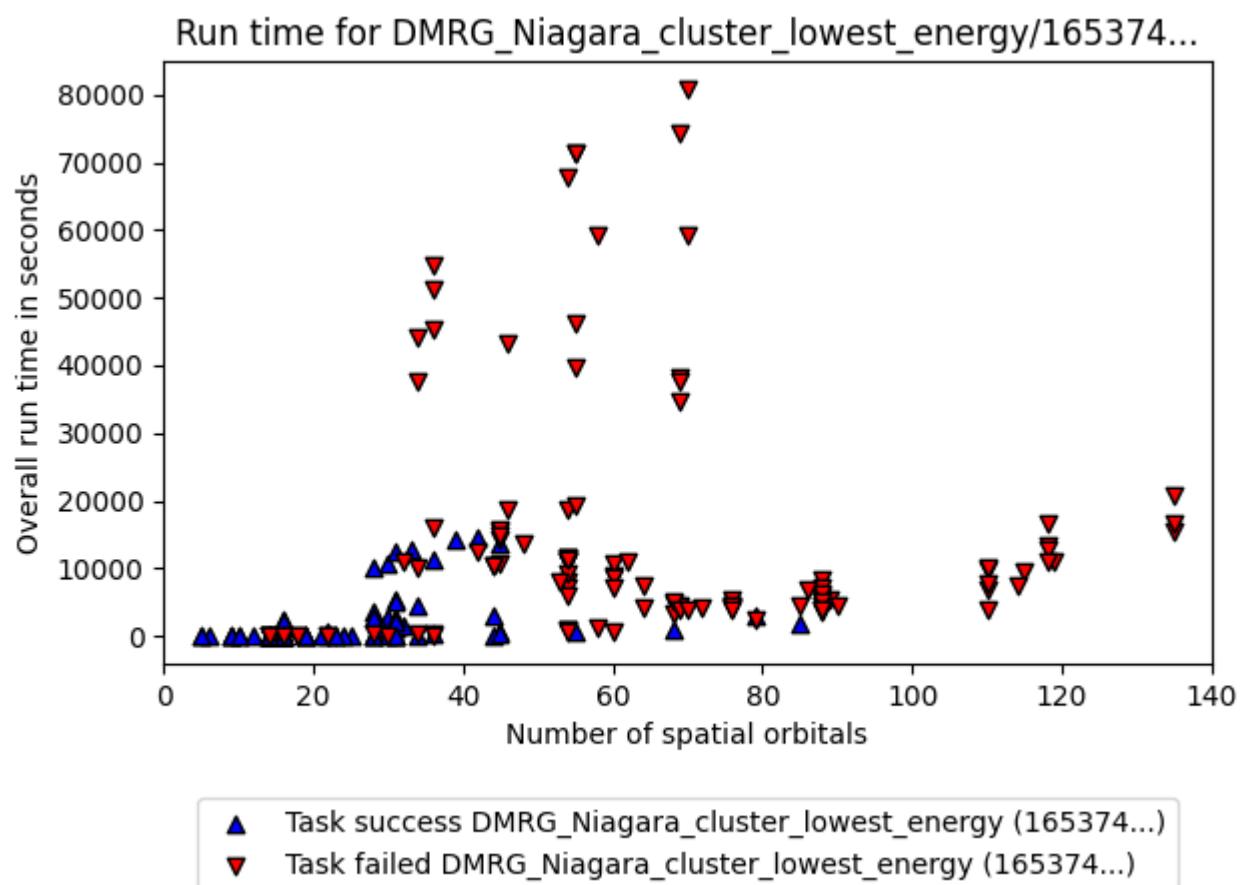
sum\_of\_run\_time\_of\_attempted\_tasks: 1841774.710900084

solvability\_ratio: 0.4126

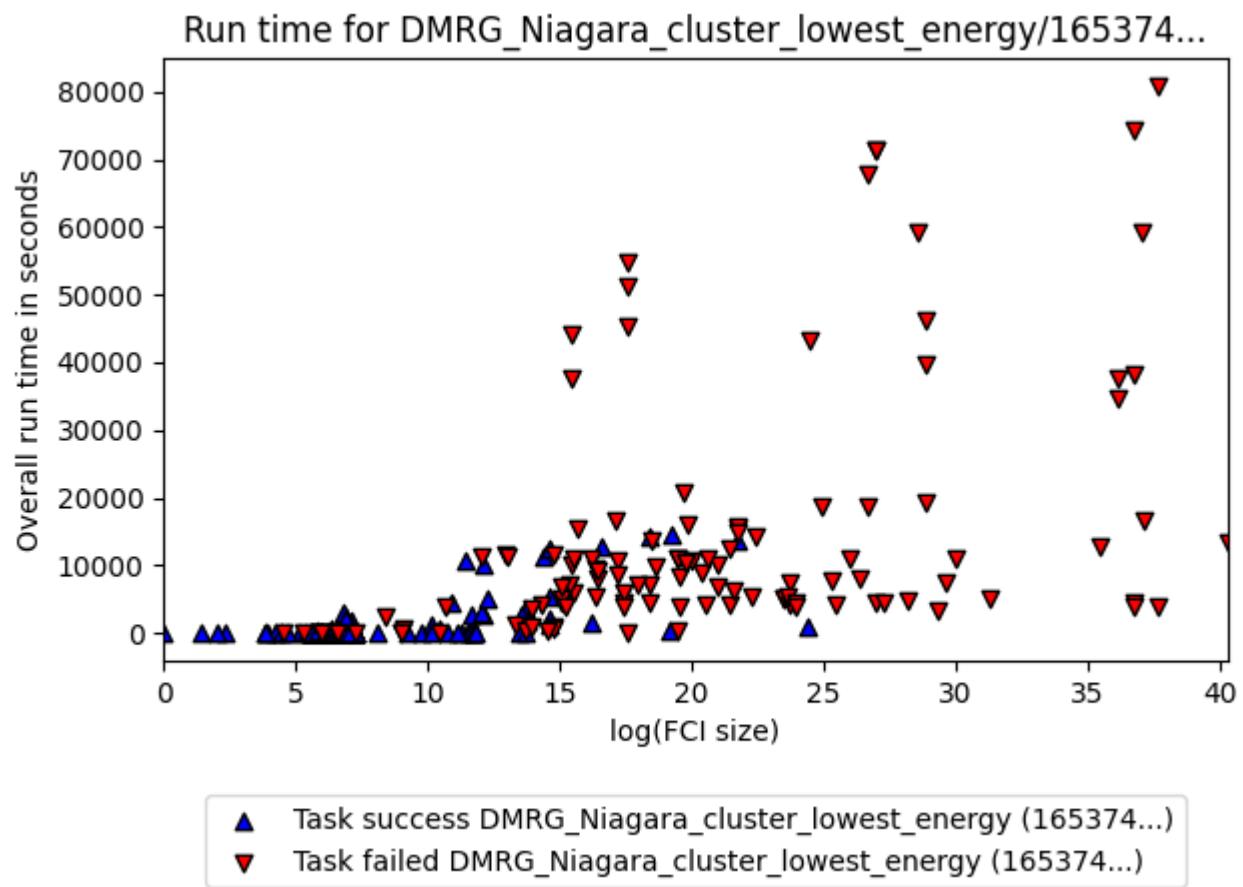
comments: solvability ratio based on PCA embedding.

f1\_score: [0.9130434782608695, 0.9626168224299065]

ml\_metrics\_calculator\_version: 1



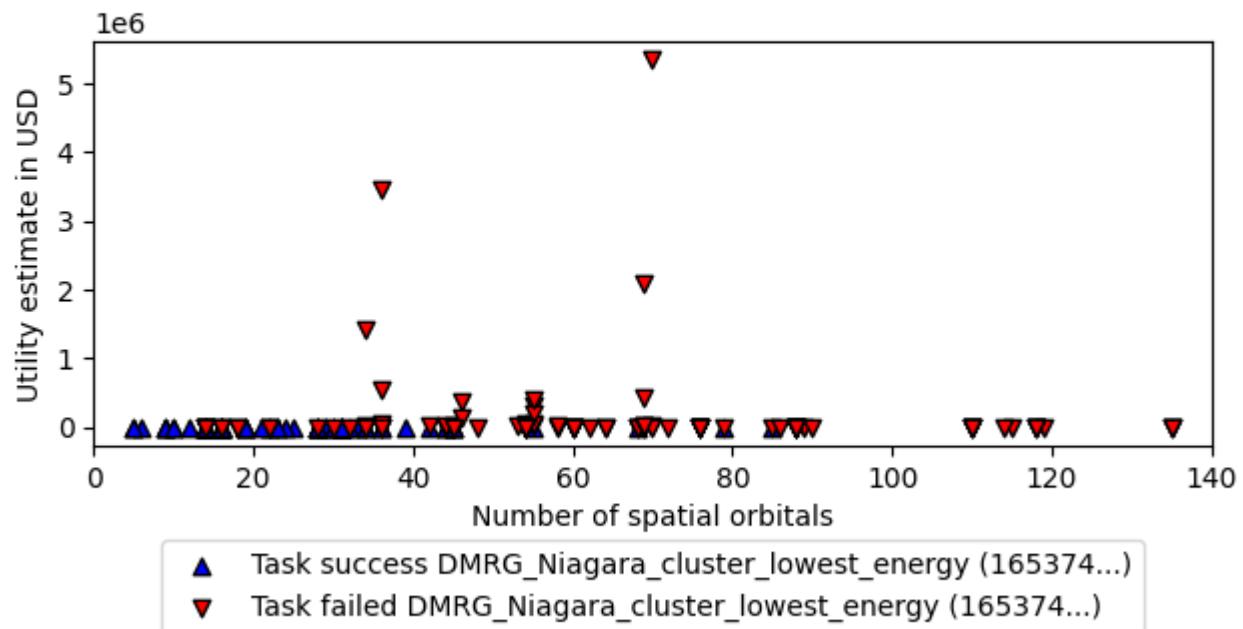
Note: plot only contains attempted tasks.



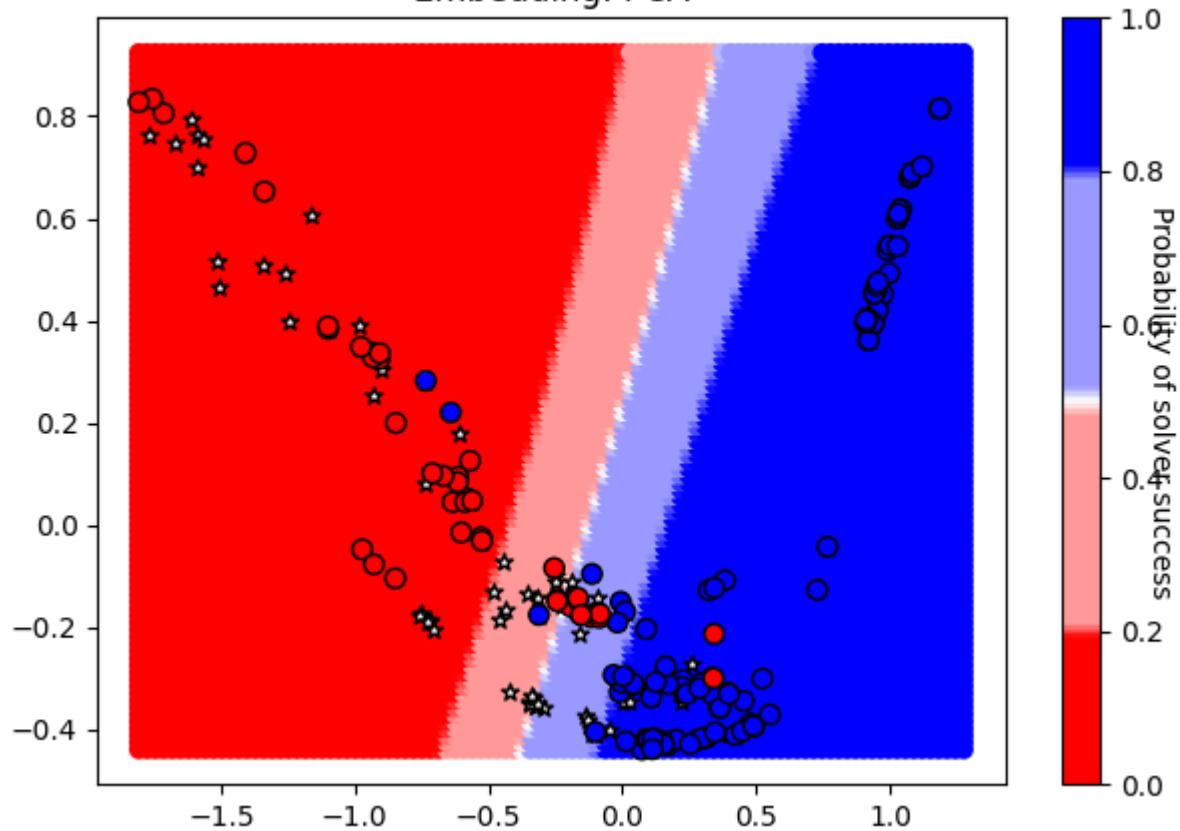
Note: plot only contains attempted tasks.

# Utility capture from DMRG\_Niagara\_cluster\_lowest\_energy/165374

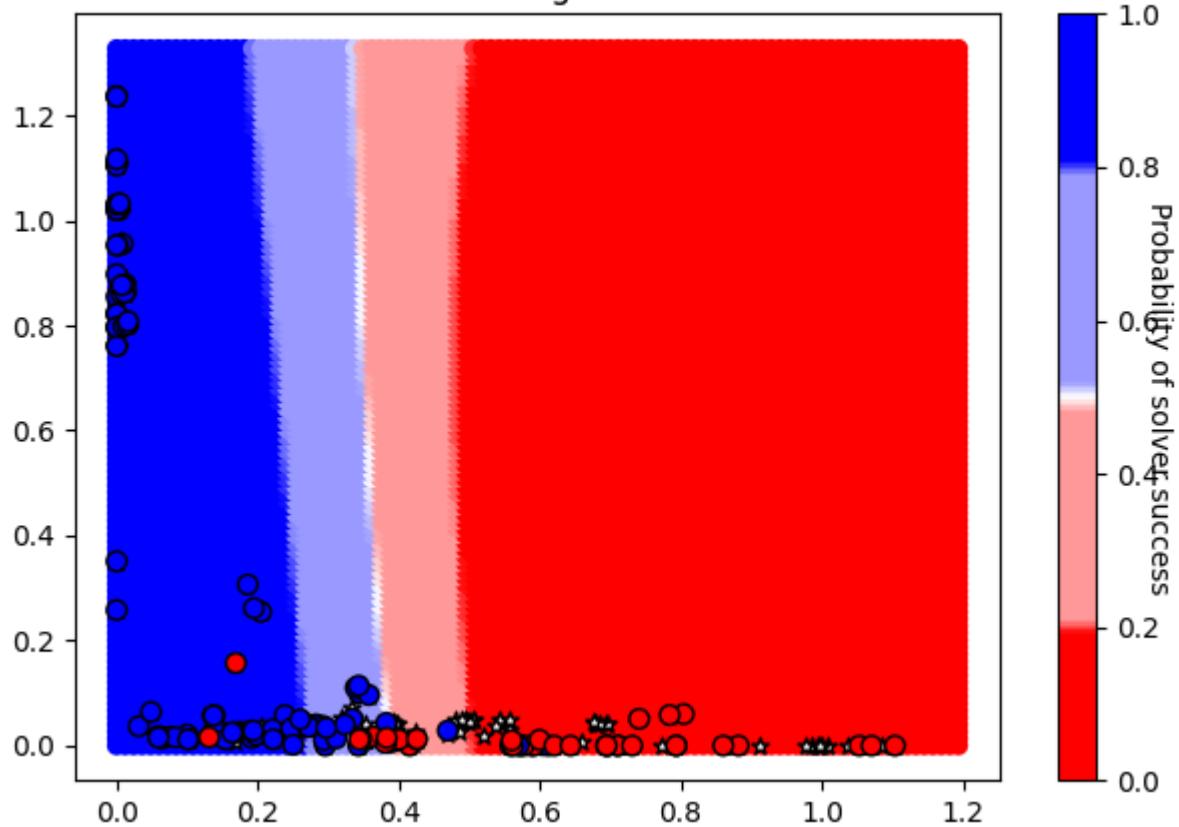
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



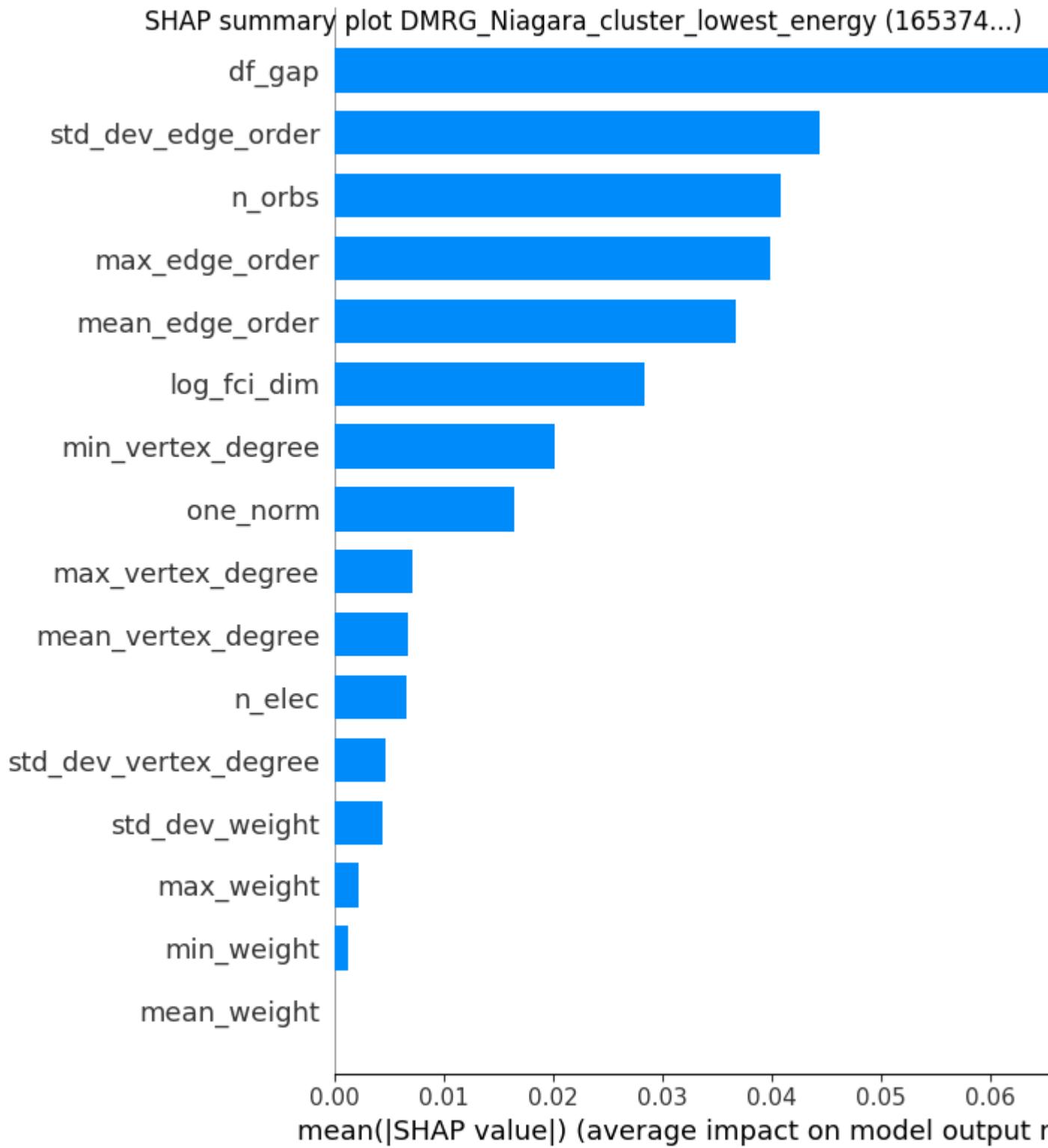
Solver DMRG\_Niagara\_cluster\_lowest\_energy (165374...)  
Embedding: PCA



Solver DMRG\_Niagara\_cluster\_lowest\_energy (165374...)  
Embedding: NNMF



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, 2610d8de-bd3a-469e-9a80-473e8988755f

solver\_uuid:2610d8de-bd3a-469e-9a80-473e8988755f

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': '1.3.6'}, {'software\_name': 'qb-gsee-benchmark', 'software\_version': '0.1.0a3.dev68+g2b90efd'}, {'software\_name': 'Python', 'software\_version': '3.10.12 (main, Feb 4 2025, 14:57:36) [GCC 11.4.0]'}, {'software\_name': 'qualtran', 'software\_version': '0.4.0'}]

quantum\_hardware\_details:{'quantum\_hardware\_description': 'Ultra-optimistic hardware model based on the superconducting architecture described in https://arxiv.org/abs/2011.03494.'}, 'quantum\_hardware\_parameters': {'num\_factories': 4, 'physical\_error\_rate': 0.0001, 'cycle\_time\_microseconds': 0.1, 'parallelize\_shots': False}}

logical\_resource\_estimate\_solution\_uuid:ce296b29-5026-4b14-ba76-c131ef6d354e

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

performance\_metrics\_uuid: 8ef7625d-cf56-456e-ac69-9e13cc01f7b8

creation\_timestamp: 2025-03-12T17:03:13.578128+00:00

number\_of\_problem\_instances: 68

number\_of\_problem\_instances\_attempted: 22

number\_of\_problem\_instances\_solved: 3

number\_of\_tasks: 228

number\_of\_tasks\_attempted: 131

number\_of\_tasks\_solved: 4

number\_of\_tasks\_solved\_within\_run\_time\_limit: 4

number\_of\_tasks\_solved\_within\_accuracy\_threshold: 131

max\_run\_time\_of\_attempted\_tasks: 139405710024.59732

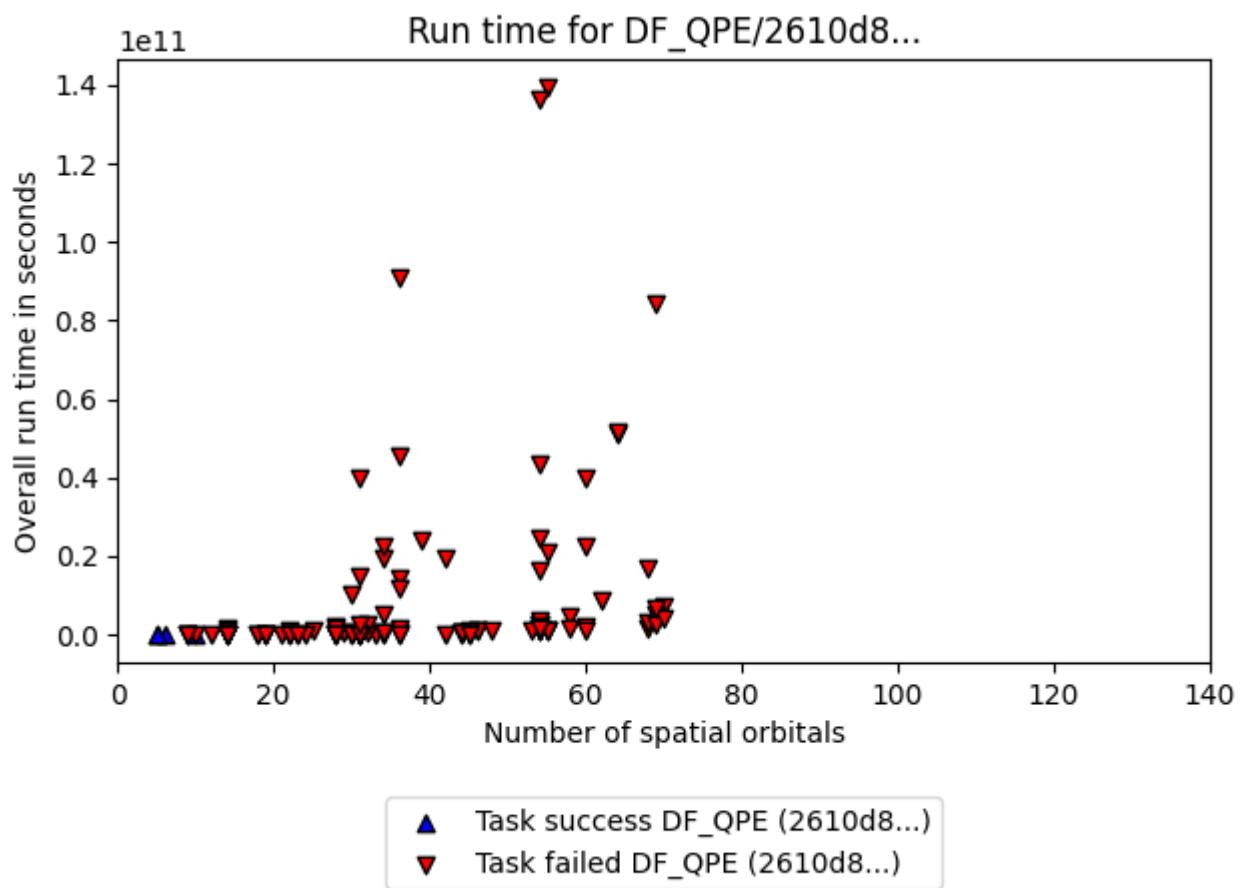
sum\_of\_run\_time\_of\_attempted\_tasks: 1070189510131.8345

solvability\_ratio: 0.0716

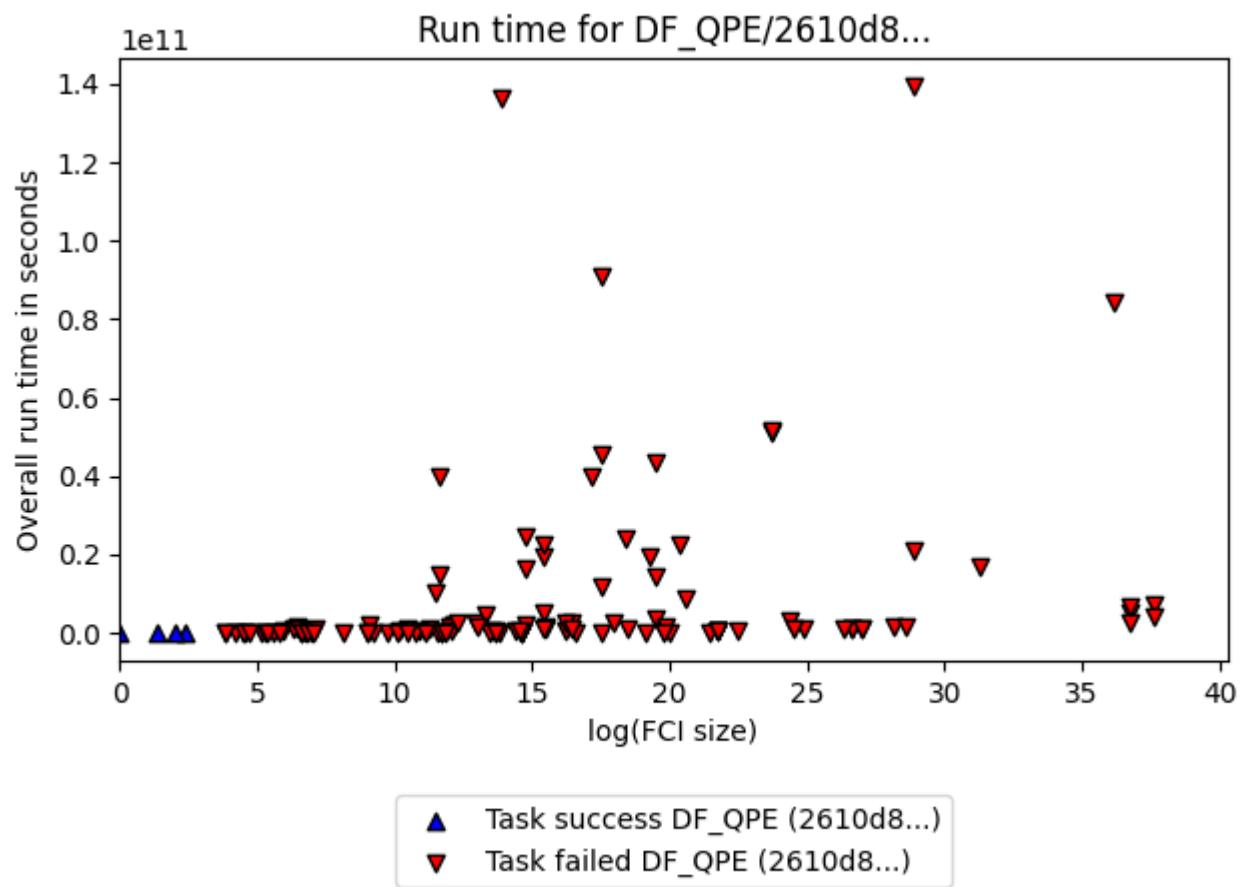
comments: solvability ratio based on PCA embedding.

f1\_score: [1.0, 1.0]

ml\_metrics\_calculator\_version: 1



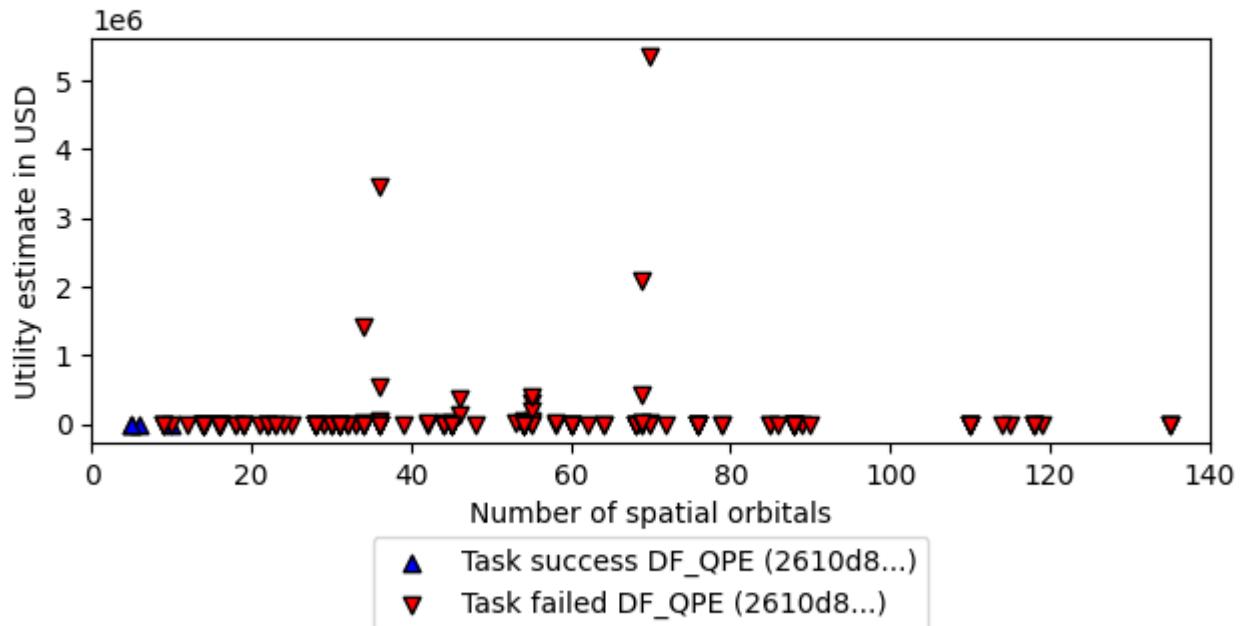
Note: plot only contains attempted tasks.



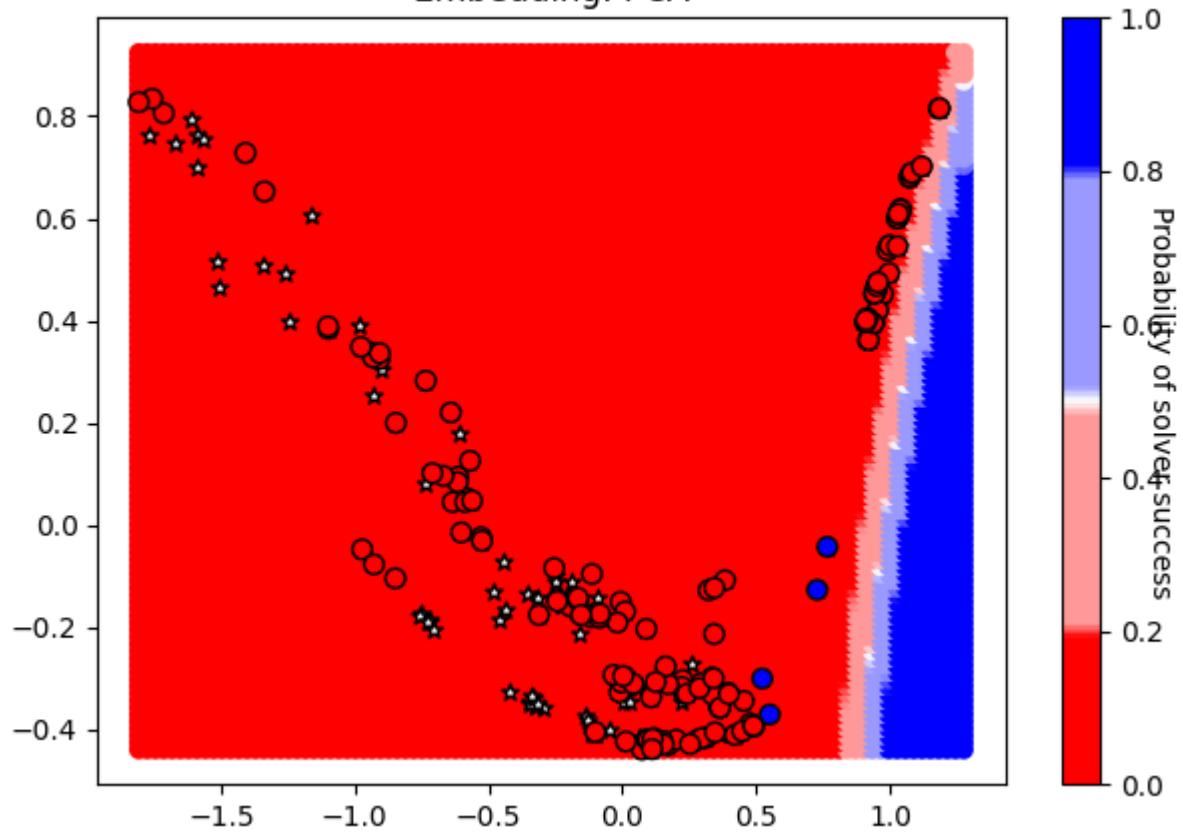
Note: plot only contains attempted tasks.

## Utility capture from DF\_QPE/2610d8...

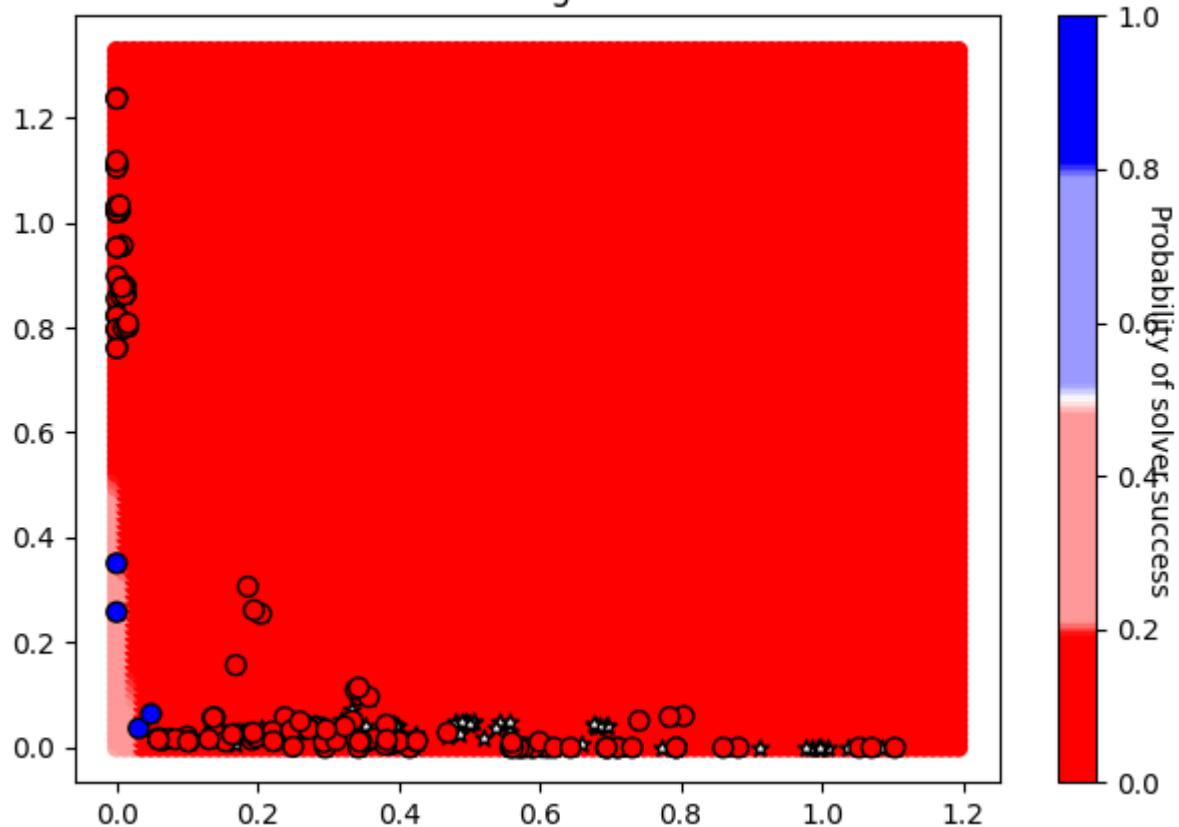
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



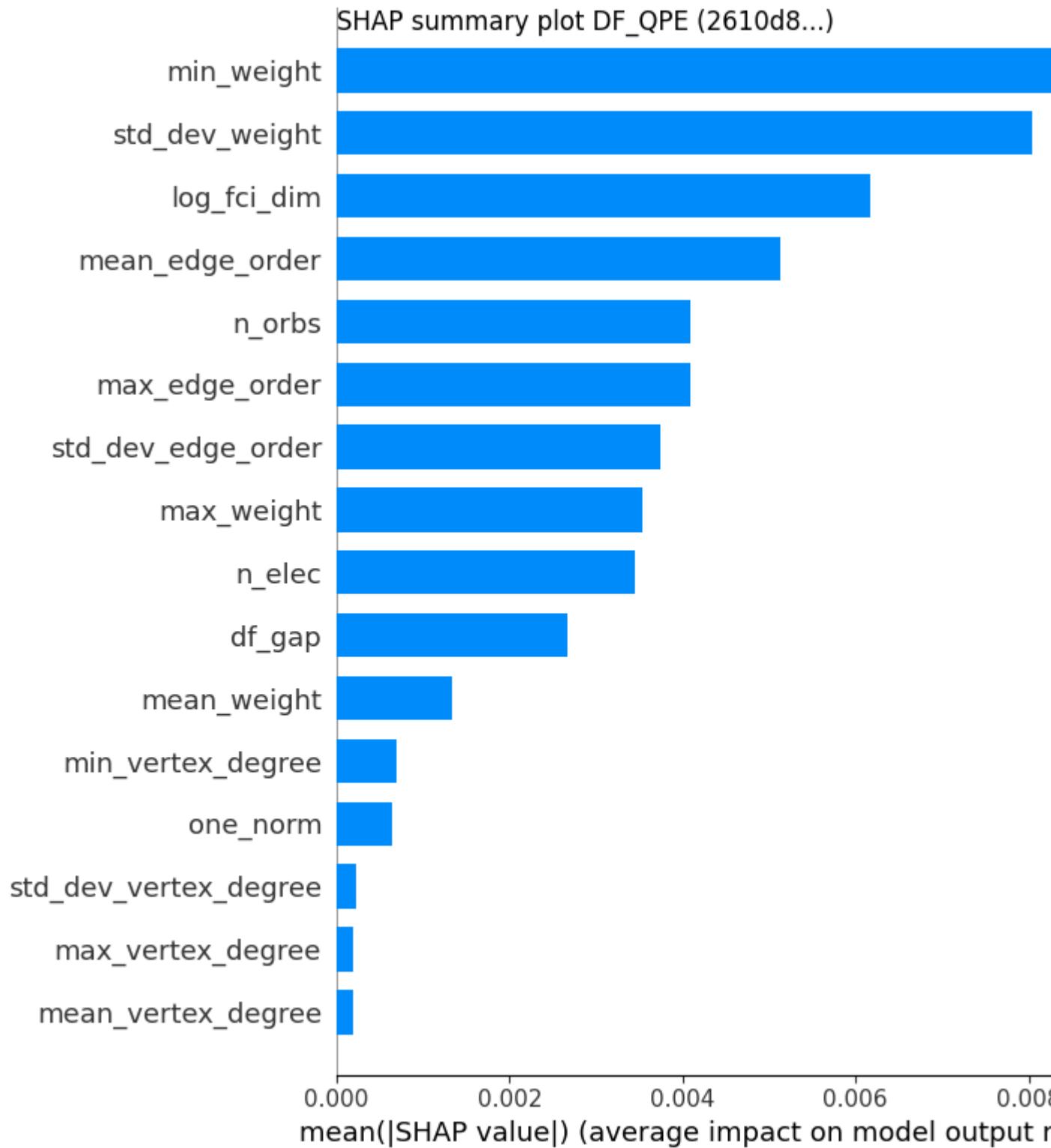
Solver DF\_QPE (2610d8...)  
Embedding: PCA



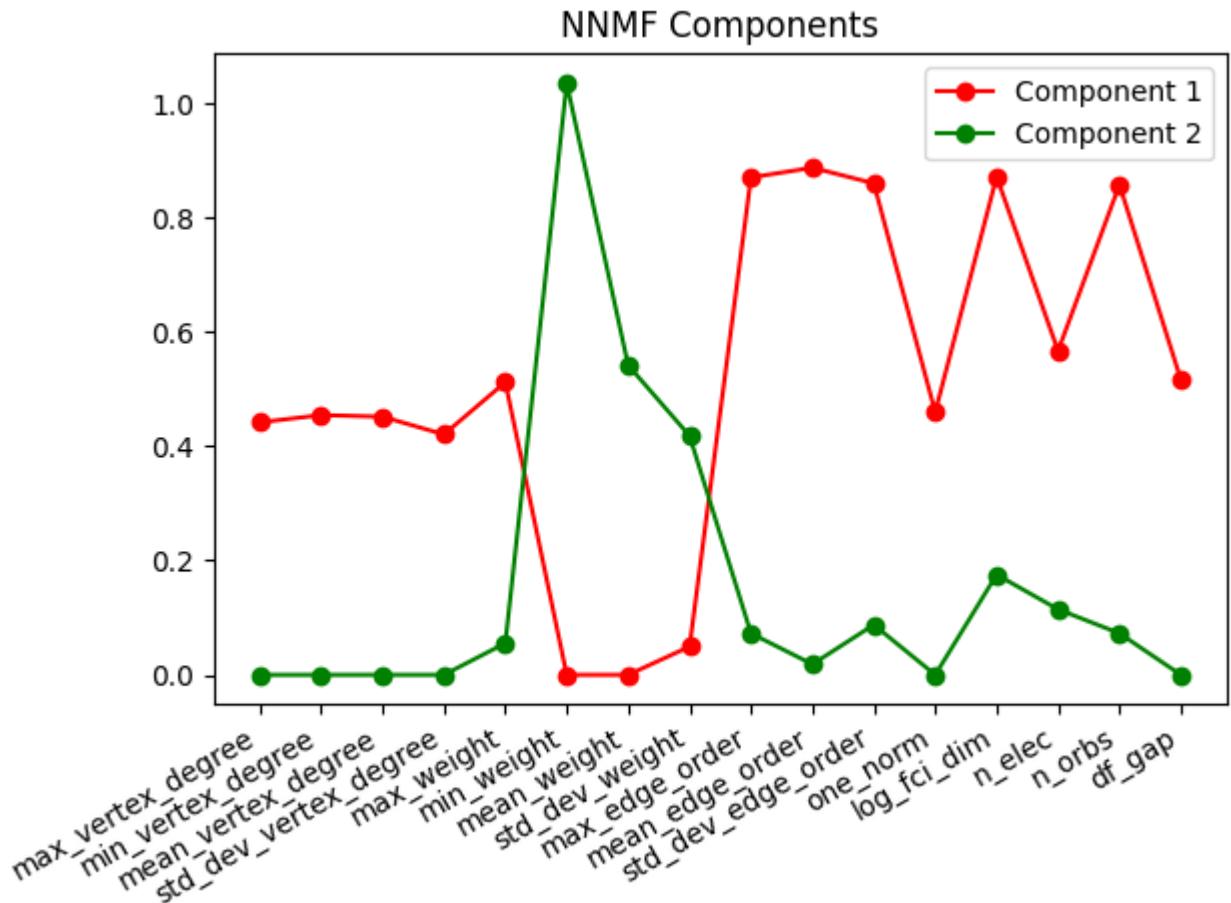
Solver DF\_QPE (2610d8...)  
Embedding: NMF



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.



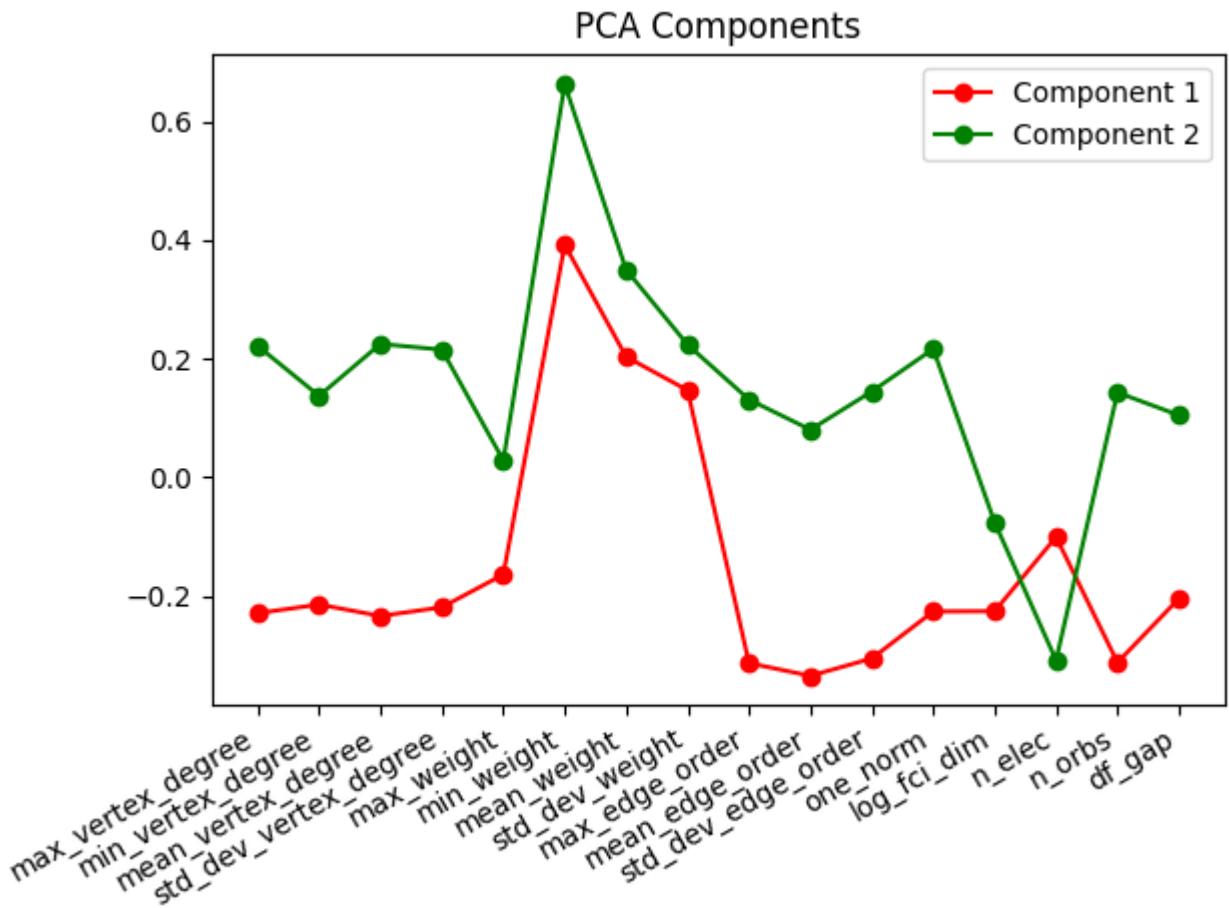
# ML Feature Analysis



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']

NNMF Component 1: [0.44176701 0.45449395 0.45163263 0.4206377  
0.51199883 0. 0. 0.04944855 0.87023998 0.88722992 0.85986962  
0.45957332 0.87154483 0.56686512 0.8574673 0.51617008]

NNMF Component 2: [0. 0. 0. 0. 0.05545233 1.03487444 0.54168445  
0.41821312 0.07259491 0.01856936 0.0876162 0. 0.1752886 0.11462803  
0.07264437 0. ]

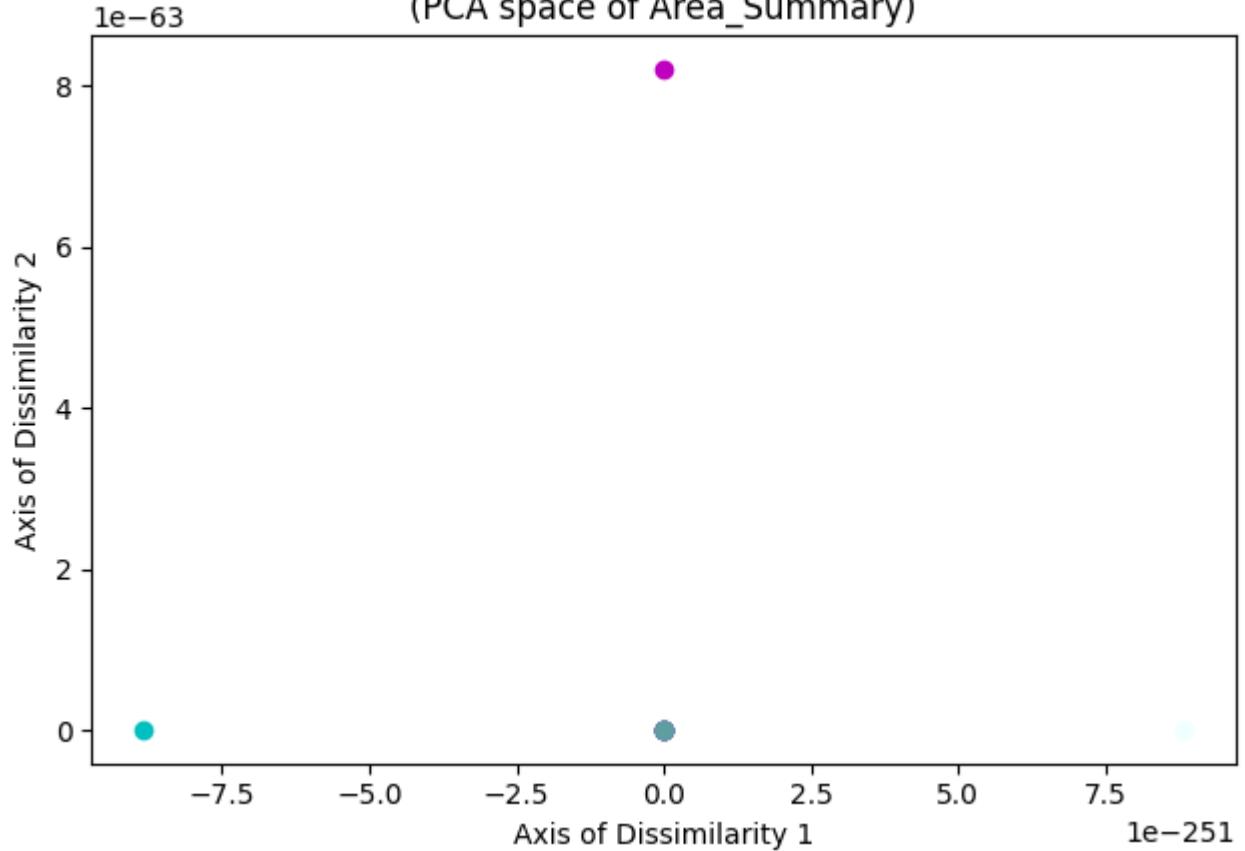


Features: ['max\_vertex\_degree', 'min\_vertex\_degree', 'mean\_vertex\_degree', 'std\_dev\_vertex\_degree', 'max\_weight', 'min\_weight', 'mean\_weight', 'std\_dev\_weight', 'max\_edge\_order', 'mean\_edge\_order', 'std\_dev\_edge\_order', 'one\_norm', 'log\_fci\_dim', 'n\_elec', 'n\_orbs', 'df\_gap']

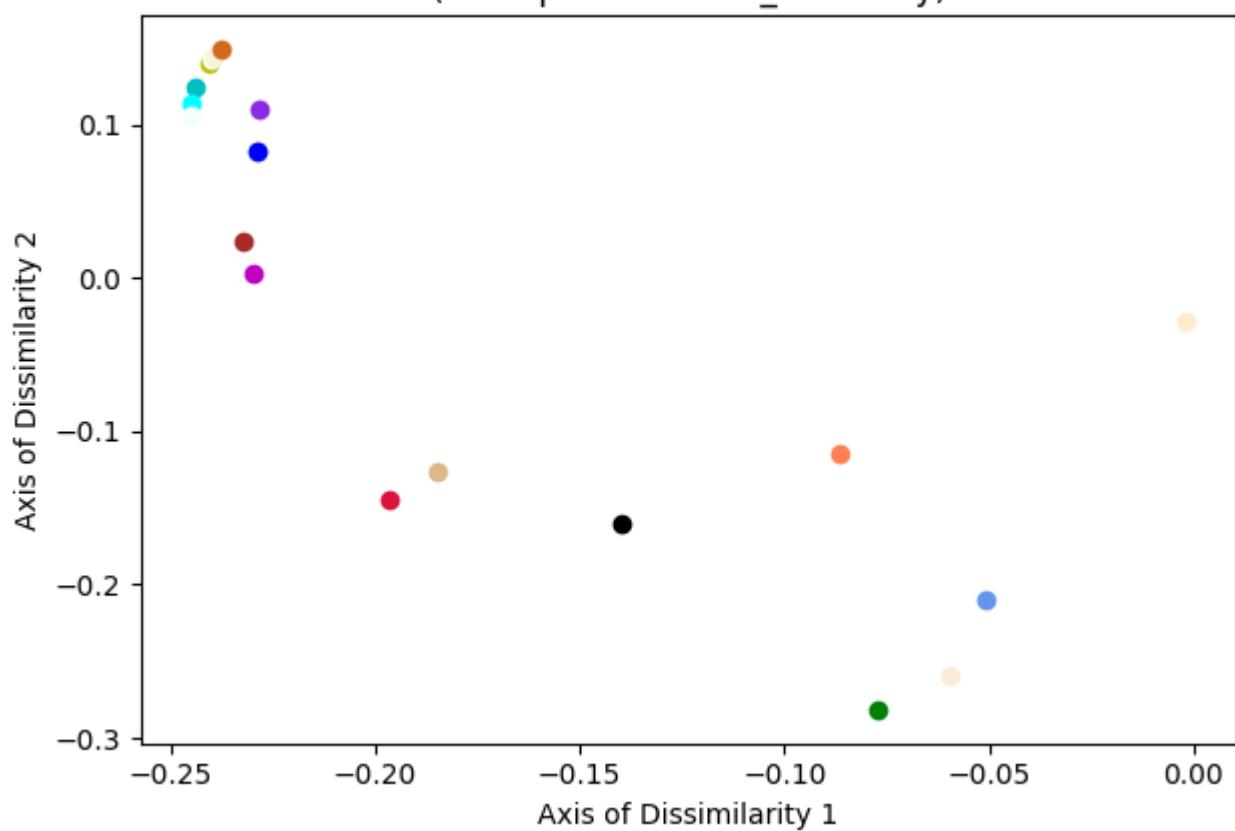
PCA Component 1: [-0.22922229 -0.21461603 -0.23398401 -0.21923522  
 -0.16402432 0.39183587 0.20302013 0.14659357 -0.3134204 -0.33485059  
 -0.30553226 -0.22630863 -0.2258685 -0.10070305 -0.31226268  
 -0.20457232]

PCA Component 2: [ 0.22146419 0.13713247 0.22479465 0.21502049  
 0.02836024 0.66237732 0.34970611 0.22348305 0.1309698 0.08010198  
 0.14460543 0.21623573 -0.07605394 -0.30861836 0.14283042 0.10453104]

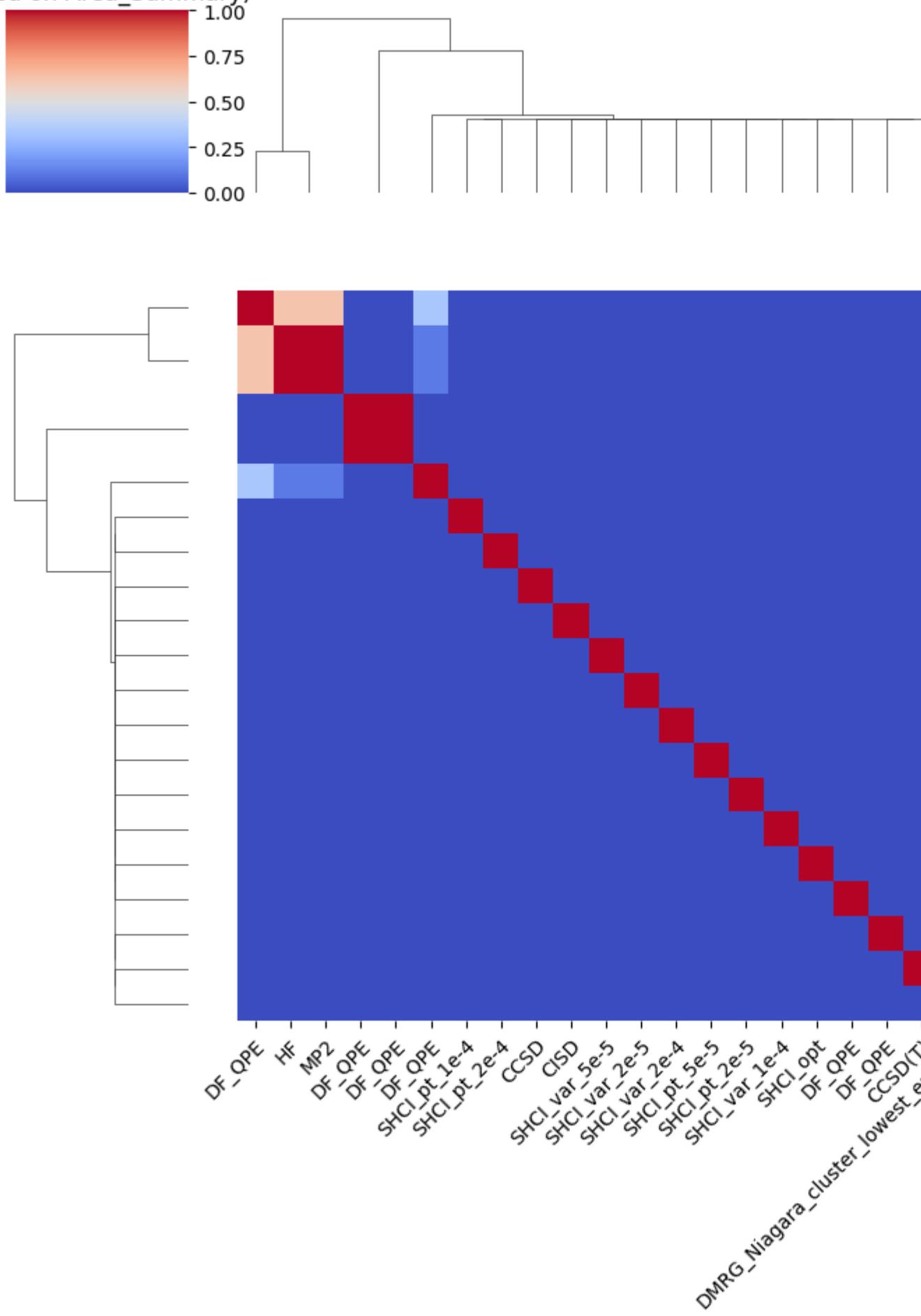
Solver points in PCA space  
(PCA space of Area\_Summary)



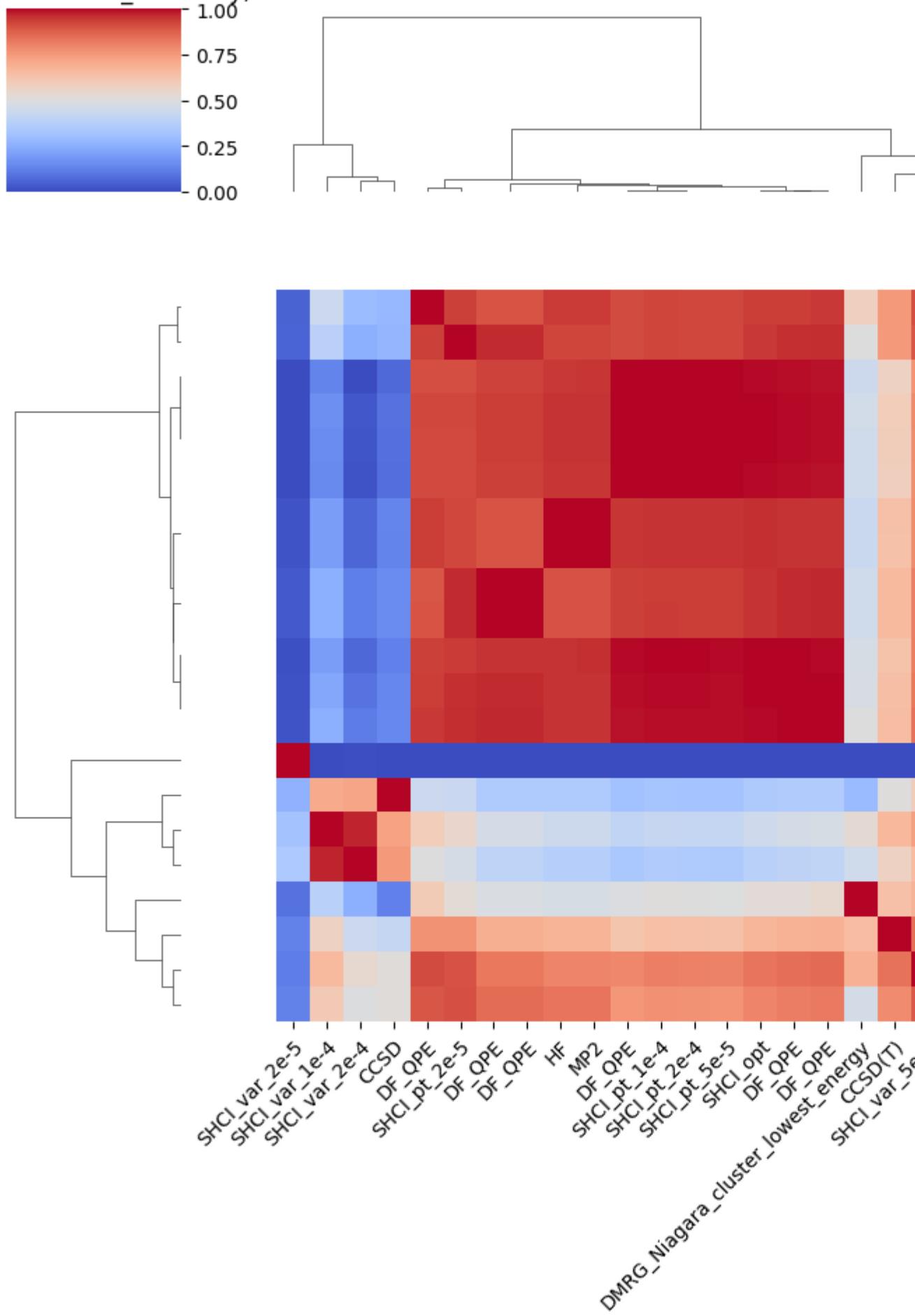
Solver points in PCA space  
(PCA space of SHAP\_summary)

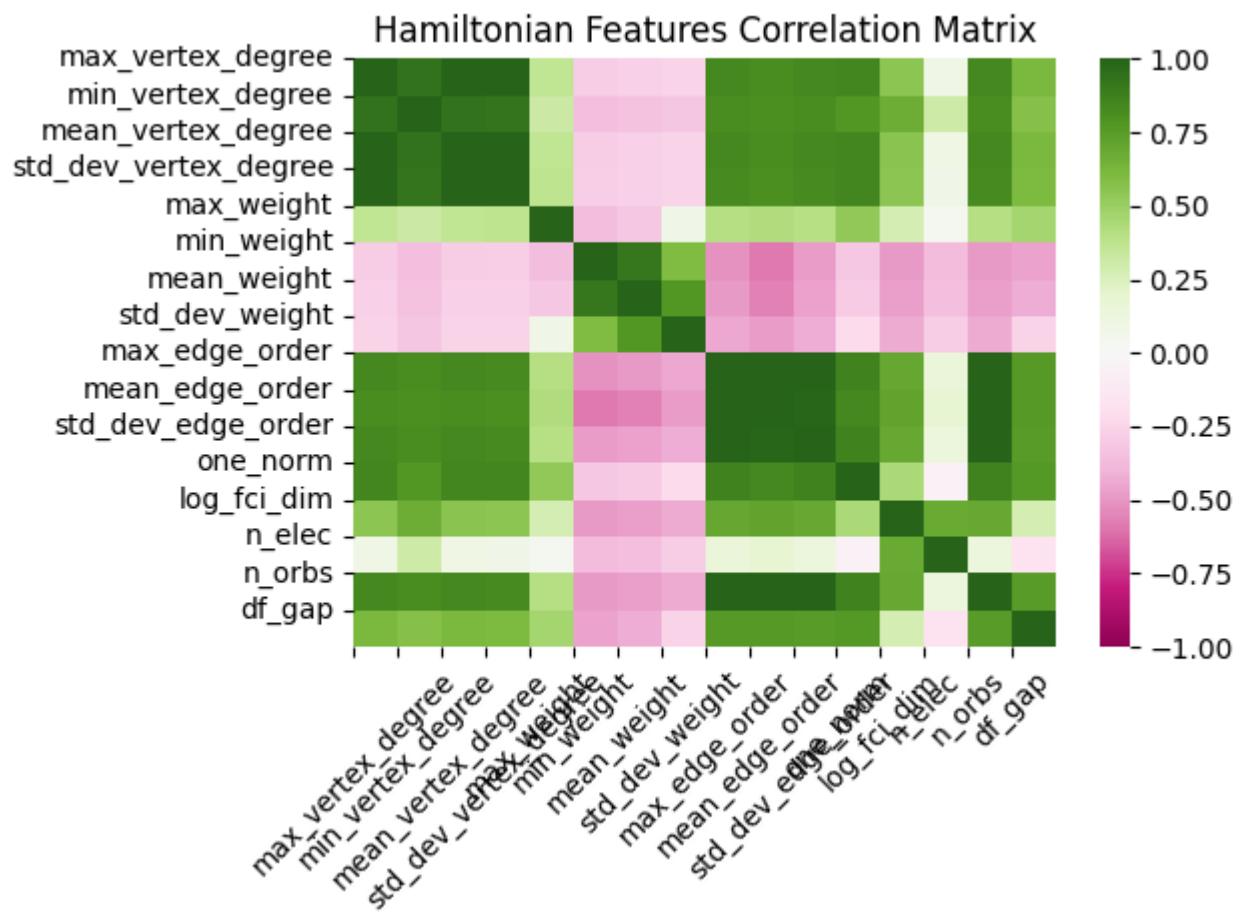


Solver similarity matrix  
(based on Area\_Summary)

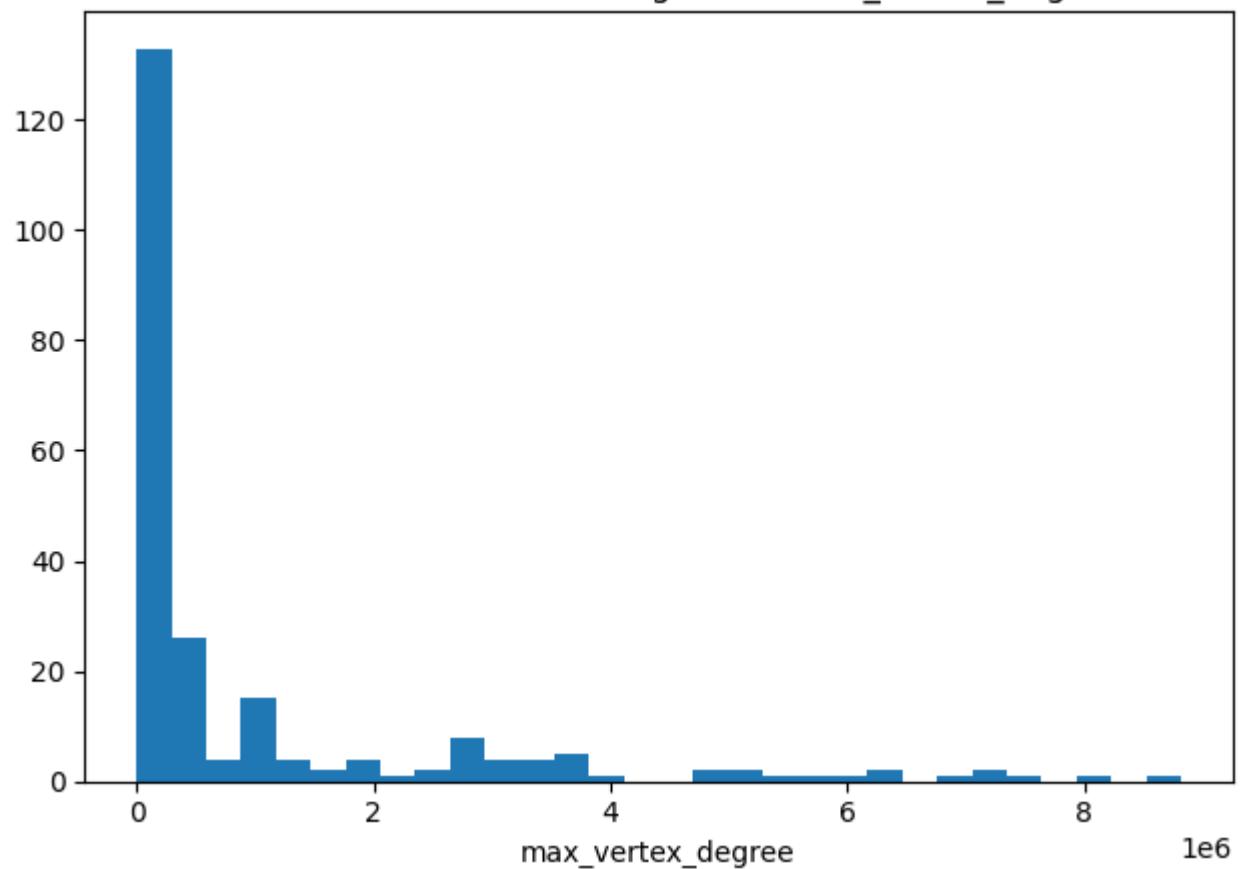


Solver similarity matrix  
(based on SHAP\_summary)

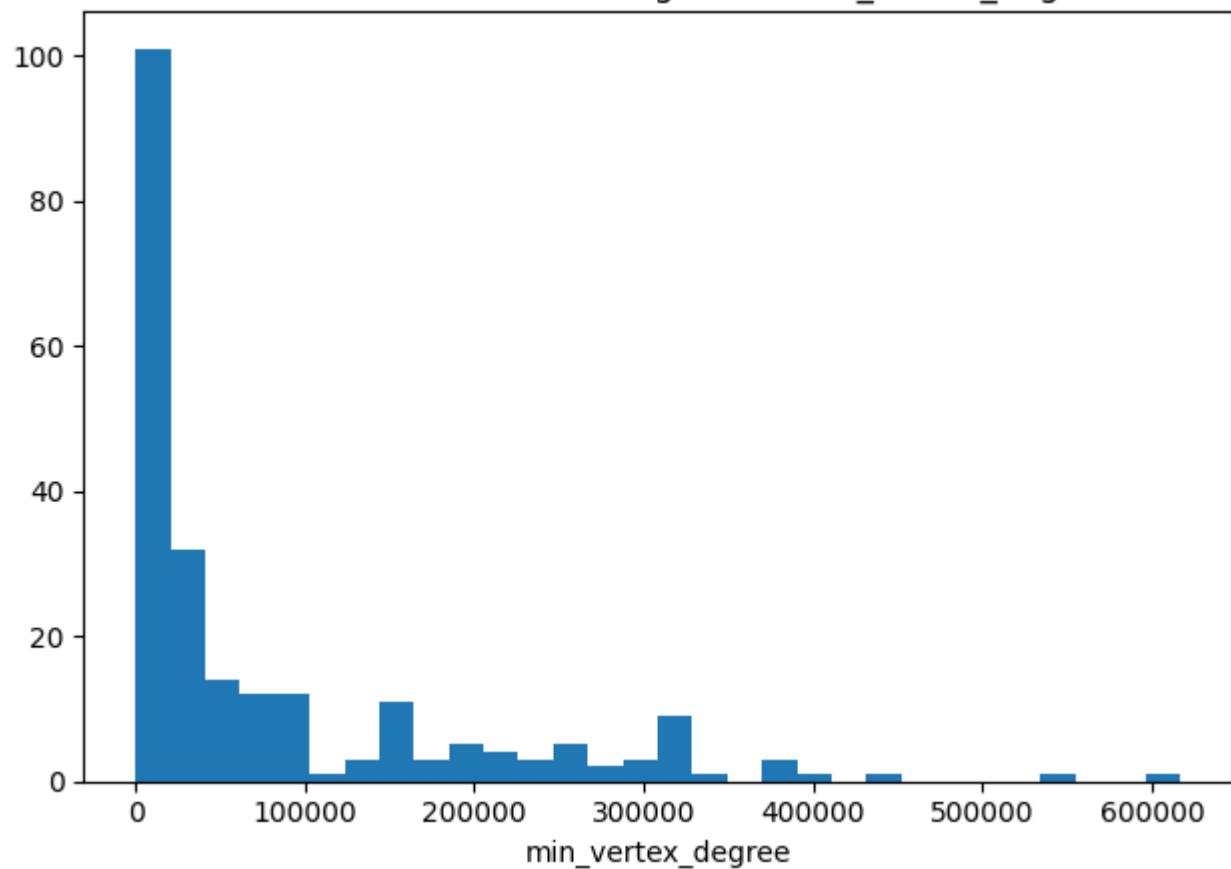




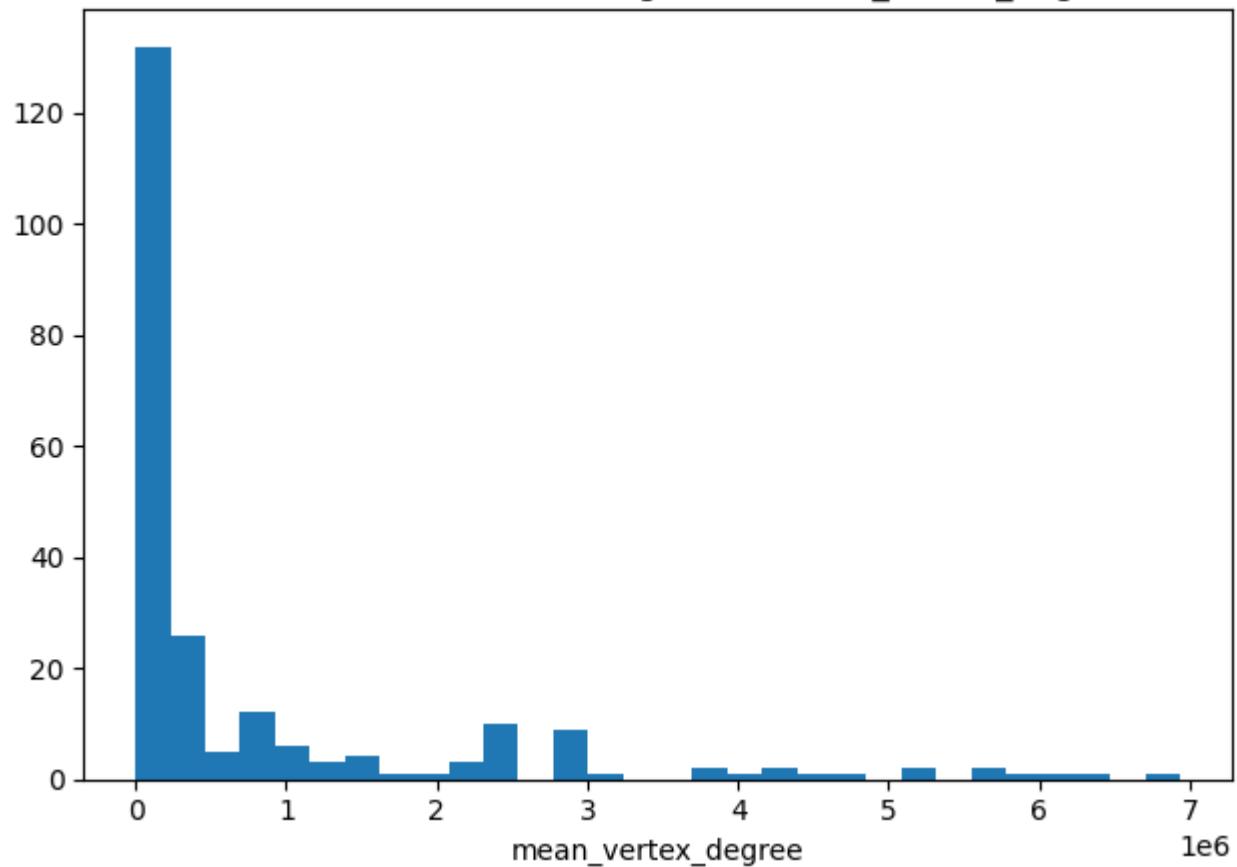
Hamiltonian features: histogram of max\_vertex\_degree



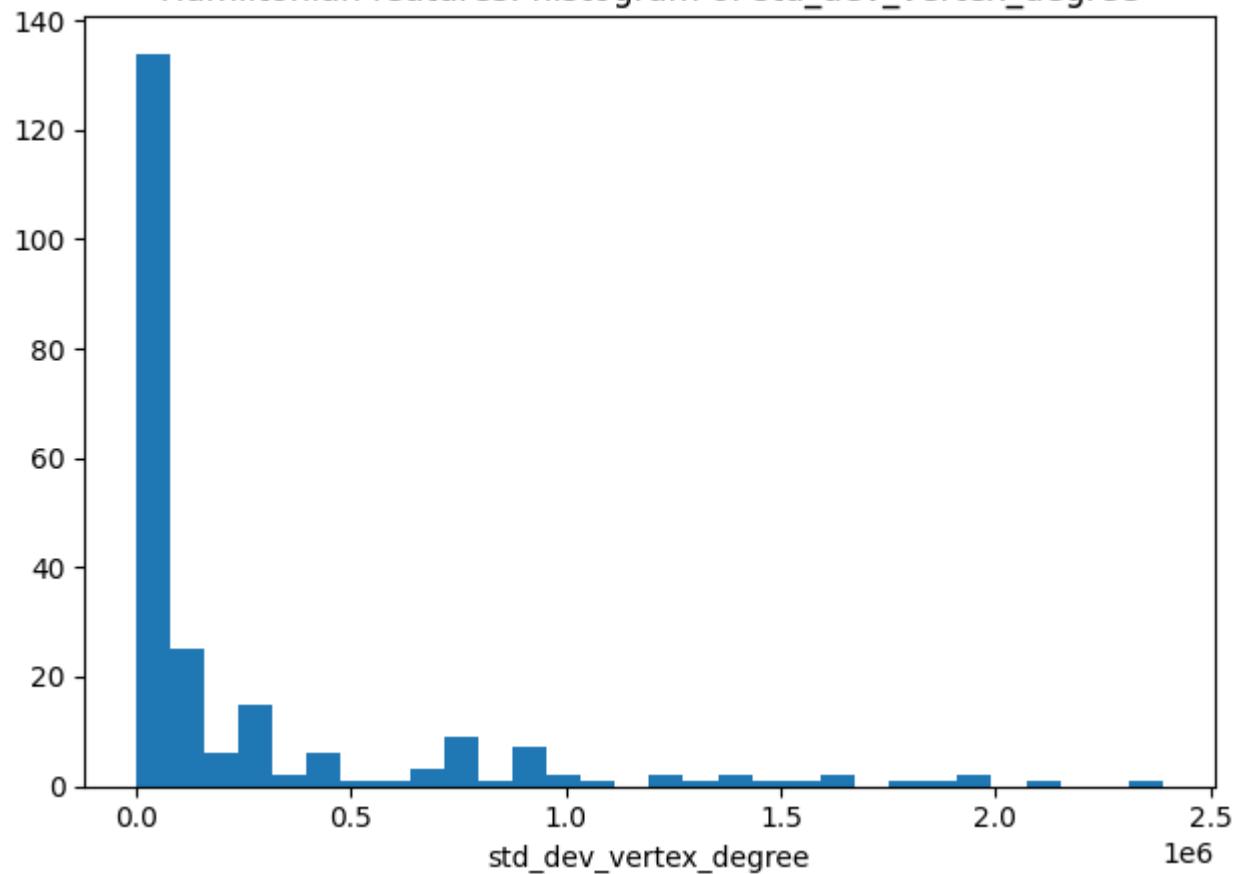
Hamiltonian features: histogram of min\_vertex\_degree



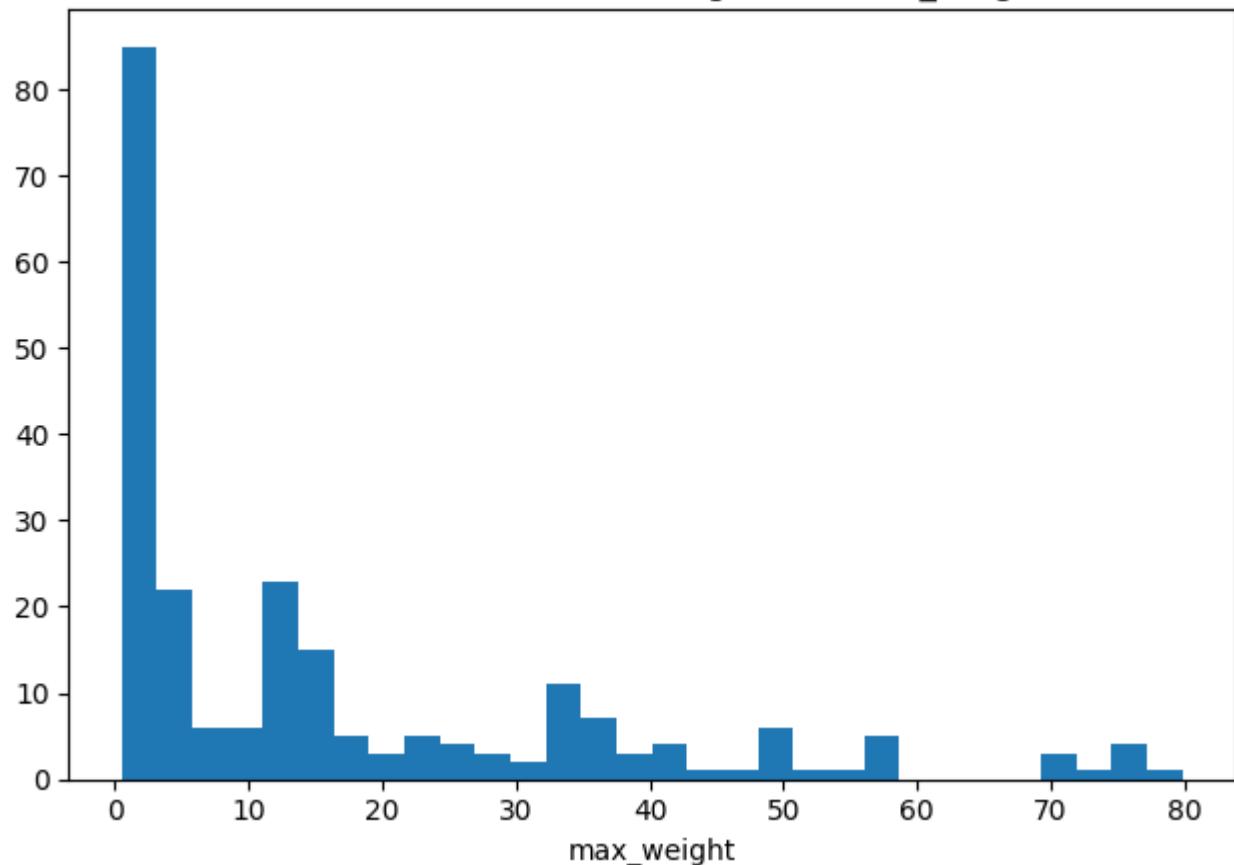
Hamiltonian features: histogram of mean\_vertex\_degree



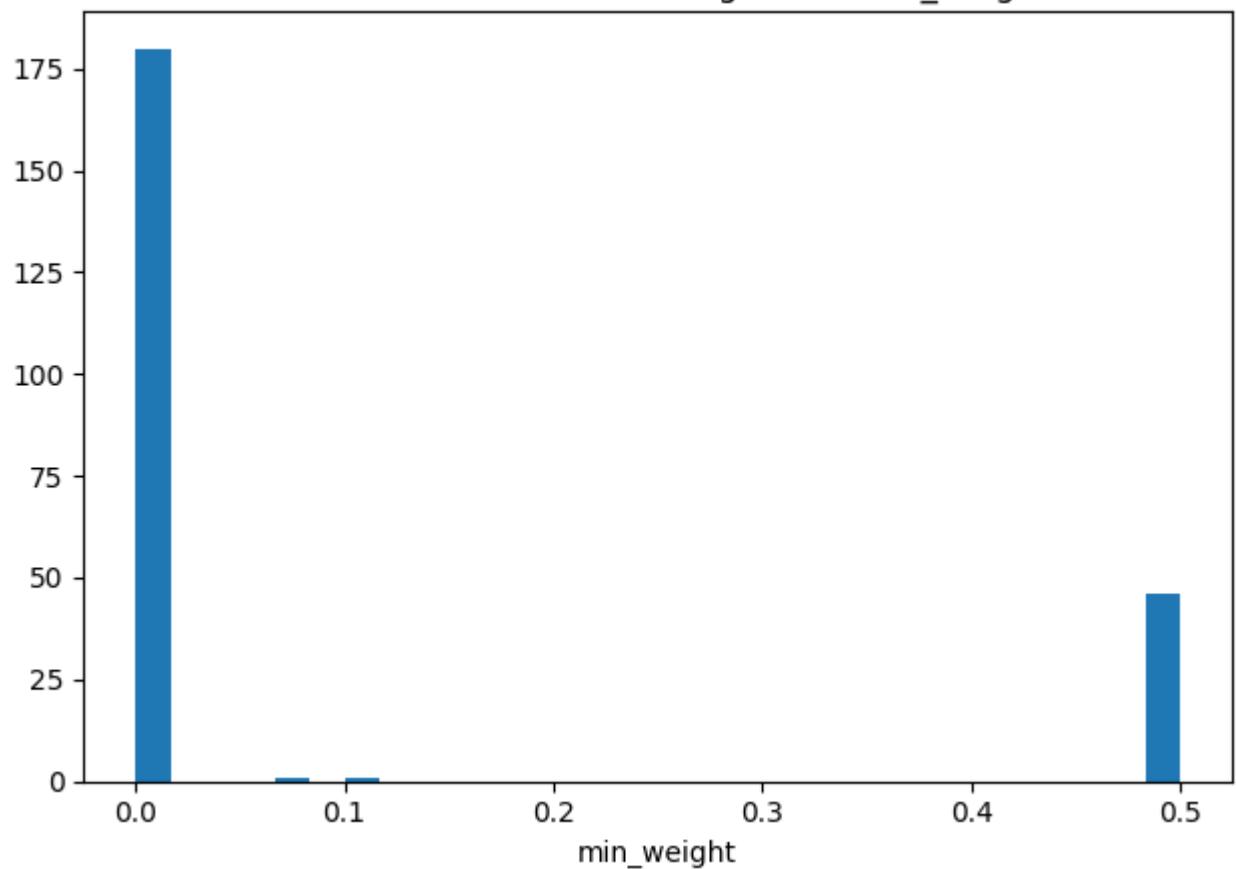
Hamiltonian features: histogram of std\_dev\_vertex\_degree



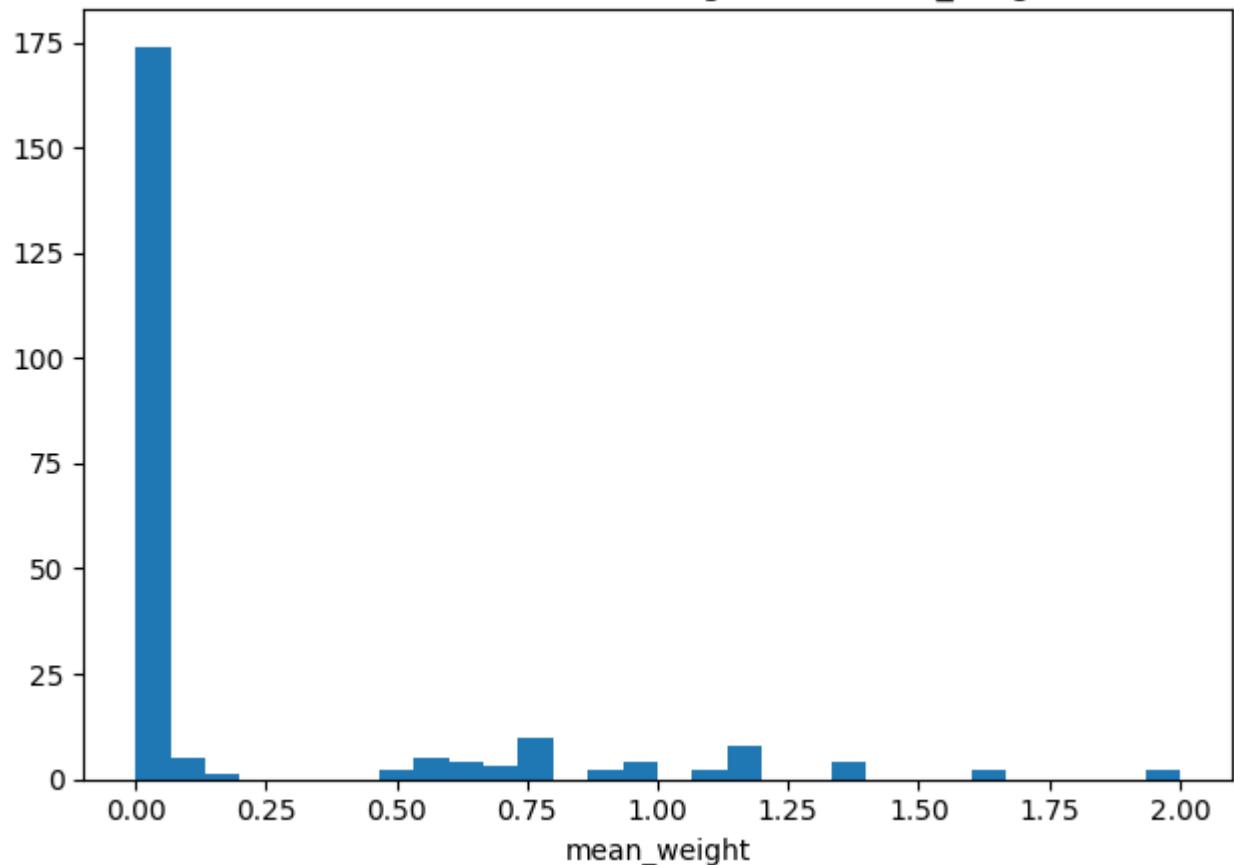
Hamiltonian features: histogram of max\_weight



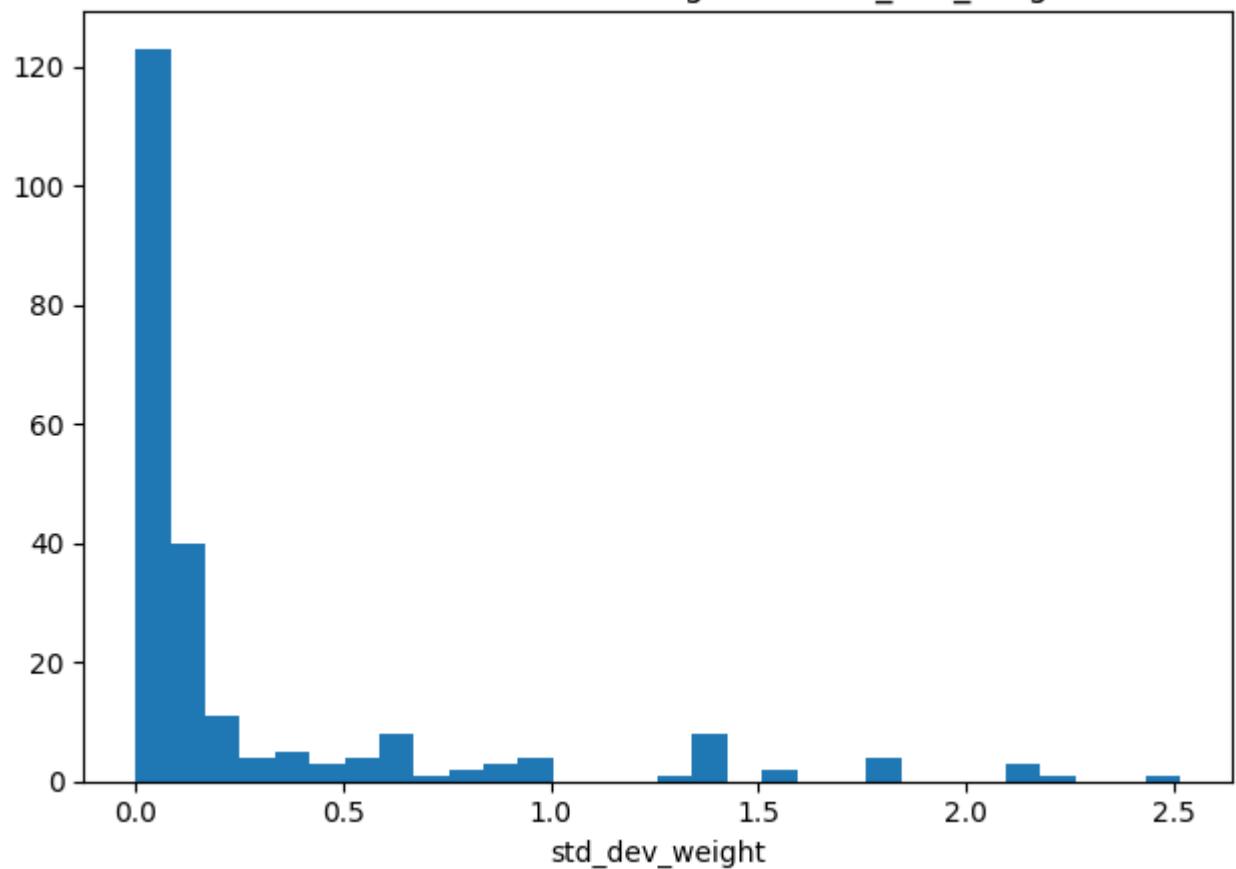
Hamiltonian features: histogram of min\_weight



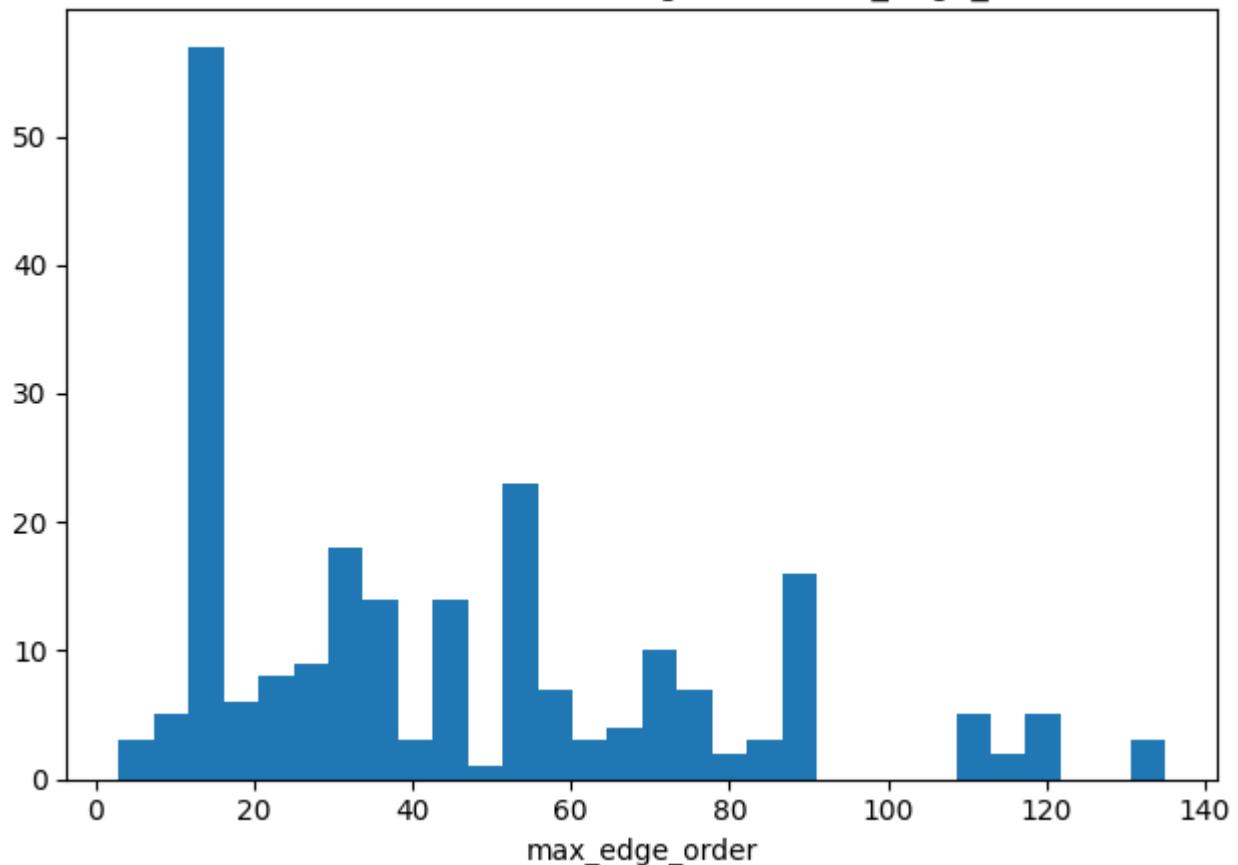
Hamiltonian features: histogram of mean\_weight



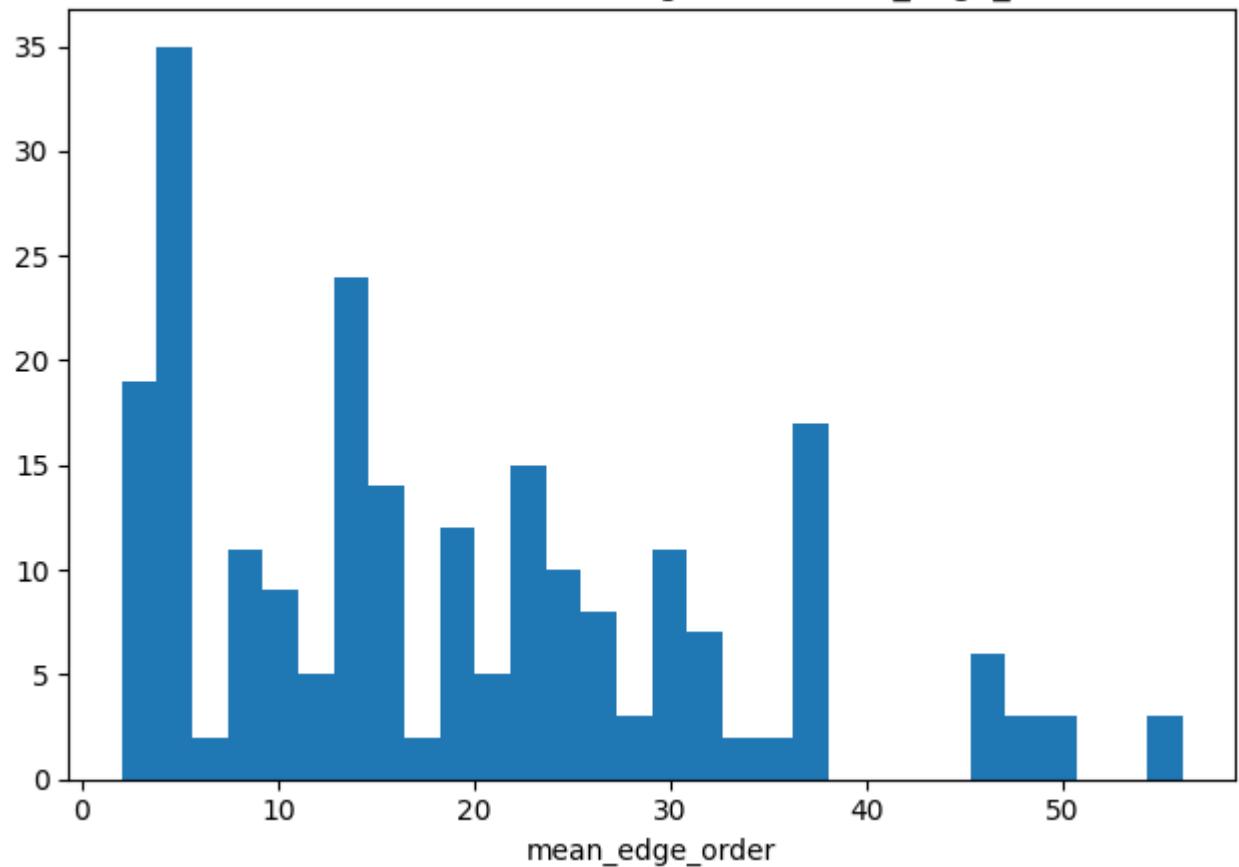
Hamiltonian features: histogram of std\_dev\_weight



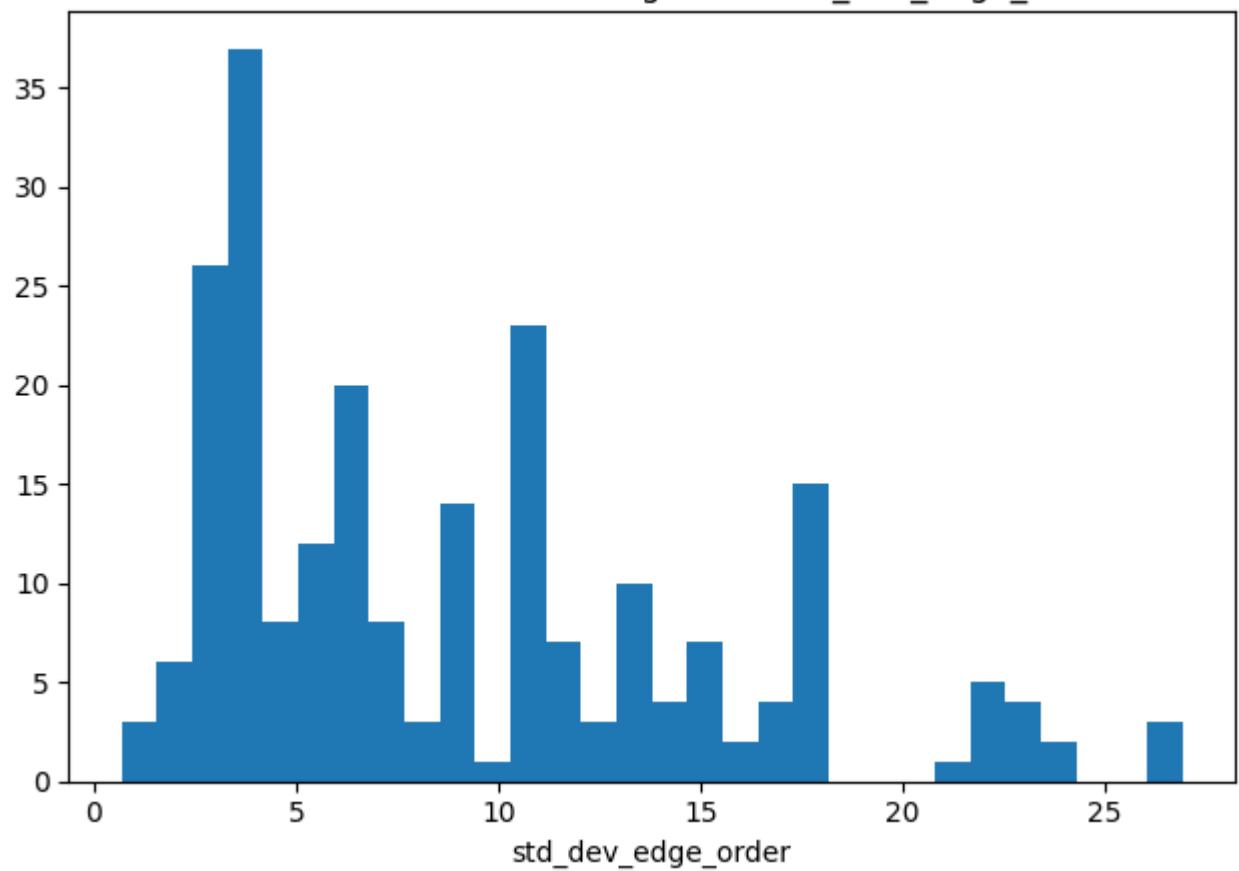
Hamiltonian features: histogram of max\_edge\_order



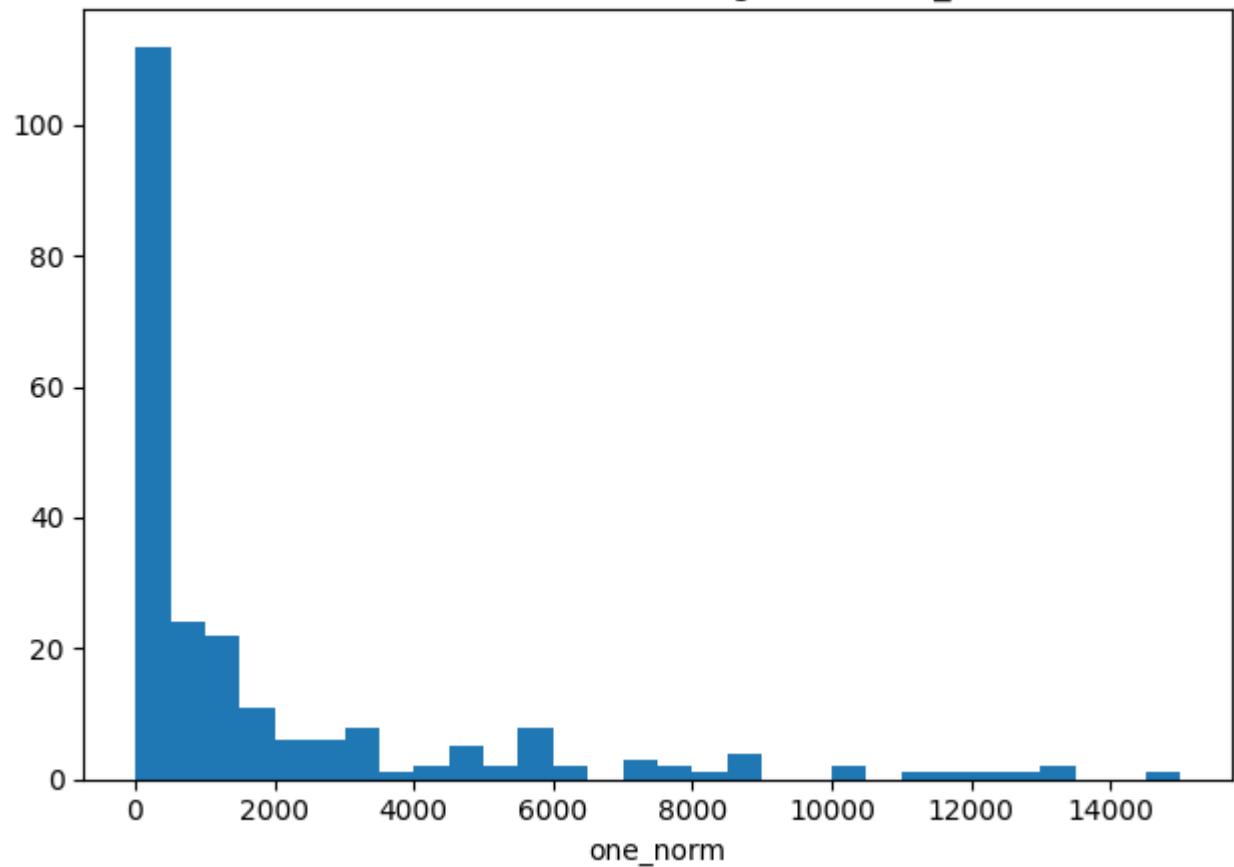
Hamiltonian features: histogram of mean\_edge\_order



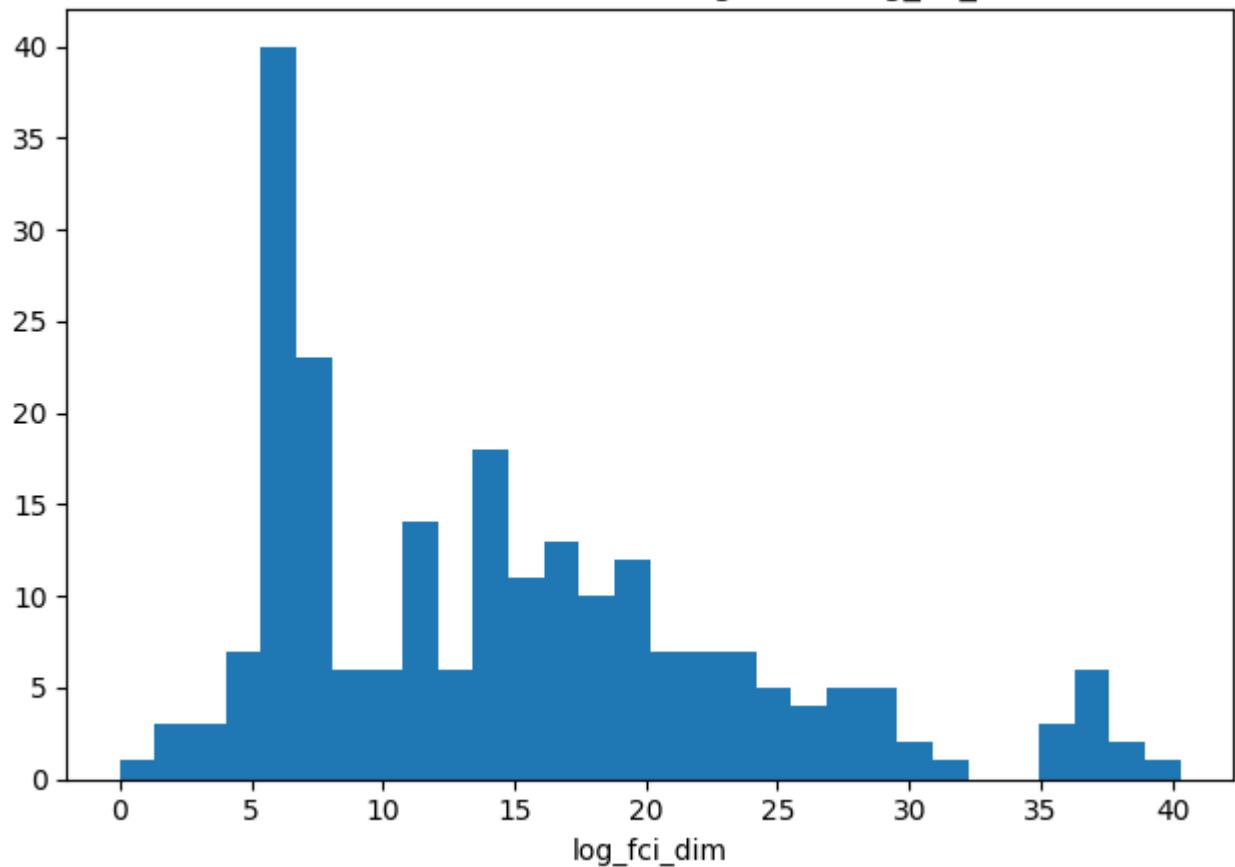
Hamiltonian features: histogram of std\_dev\_edge\_order



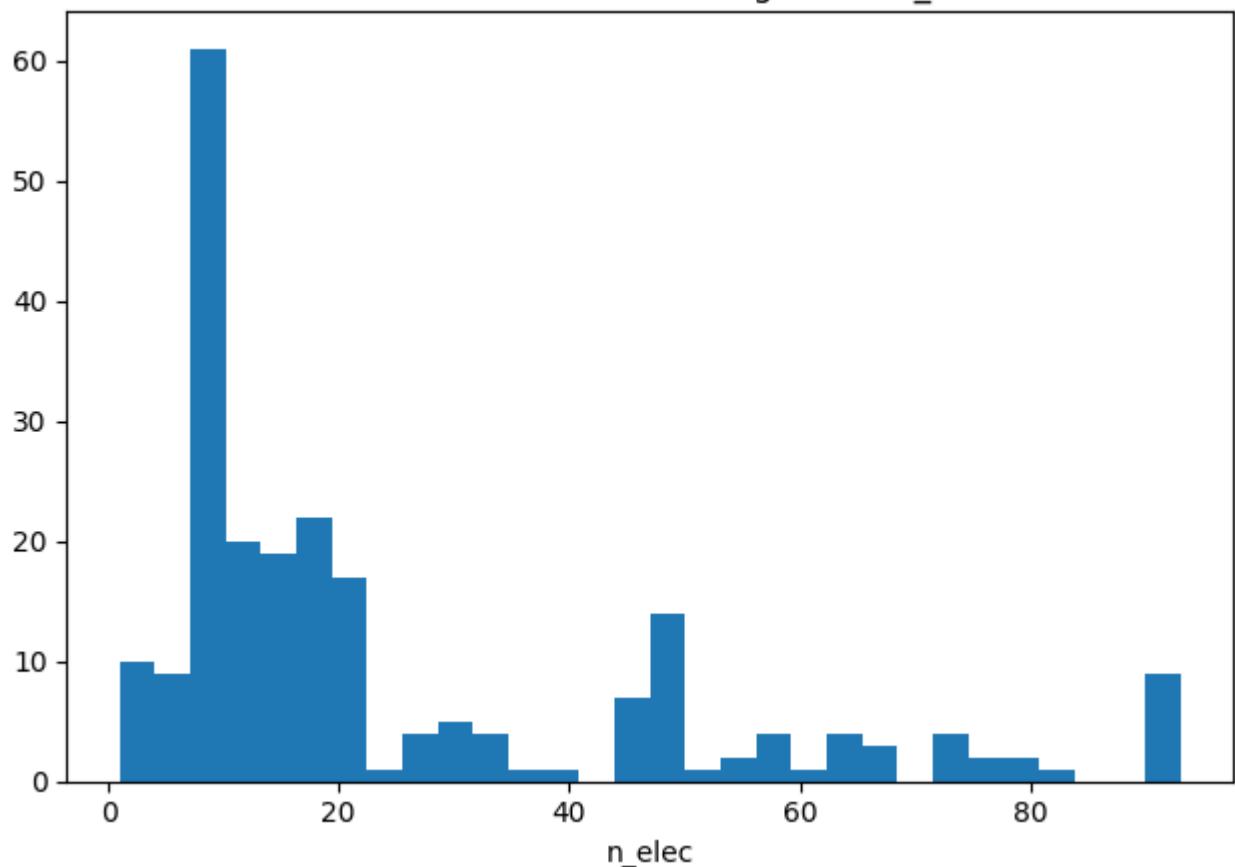
Hamiltonian features: histogram of one\_norm



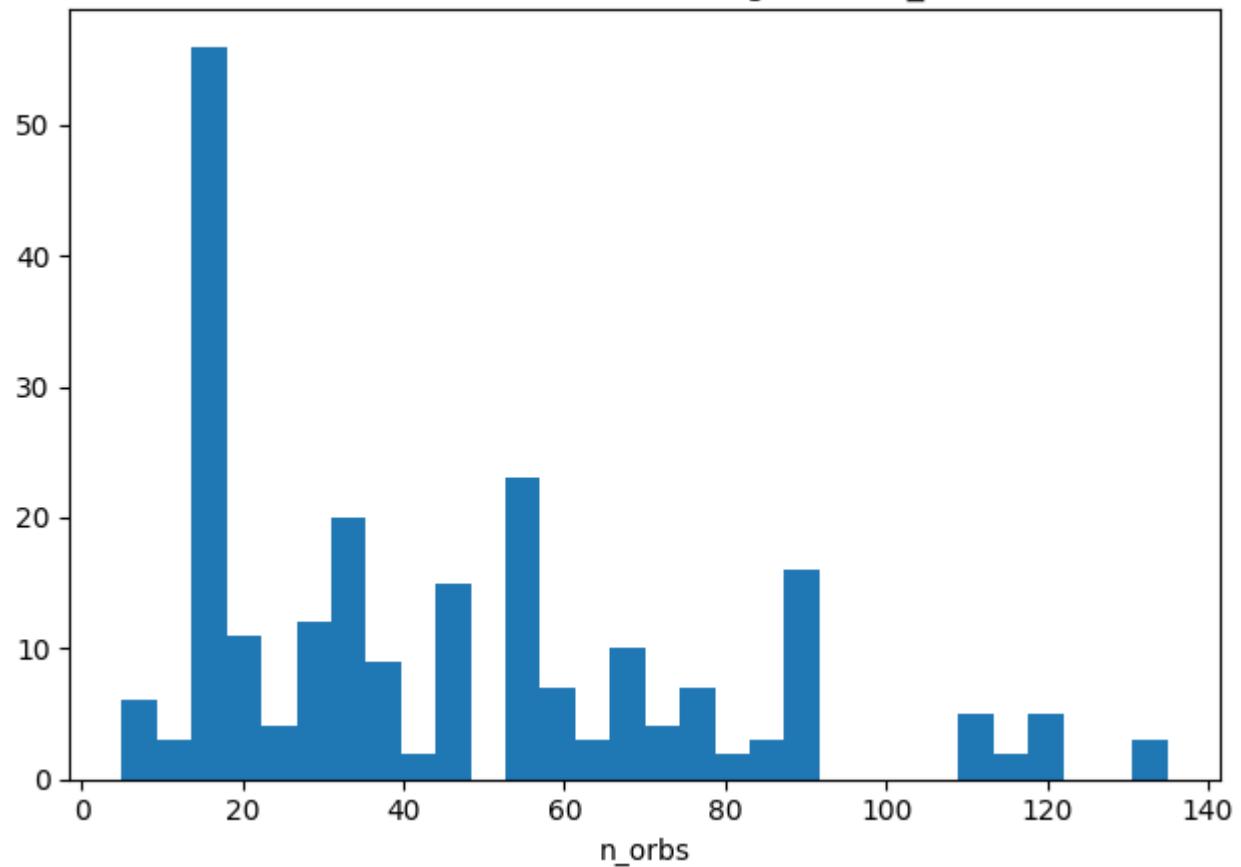
Hamiltonian features: histogram of log\_fci\_dim



Hamiltonian features: histogram of n\_elec



Hamiltonian features: histogram of n\_orbs



Hamiltonian features: histogram of df\_gap

