

GSEE Benchmark Standard Report

Report based on data from 2025-03-06T19:54:13.195807+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Tue Mar 4 15:44:53 2025

Input data: GSEE-
`HC_utility_estimates_all_instances_task_uuids_v2.csv`, last modified
Tue Mar 4 15:44:53 2025

Latest creation time for a `problem_instance.json` file: Tue Mar 4 15:44:53 2025

Latest creation time for a `solution.json` file: Tue Mar 4 15:44:53 2025

Problem Instance Summary Statistics

number of `problem_instances`: 68.

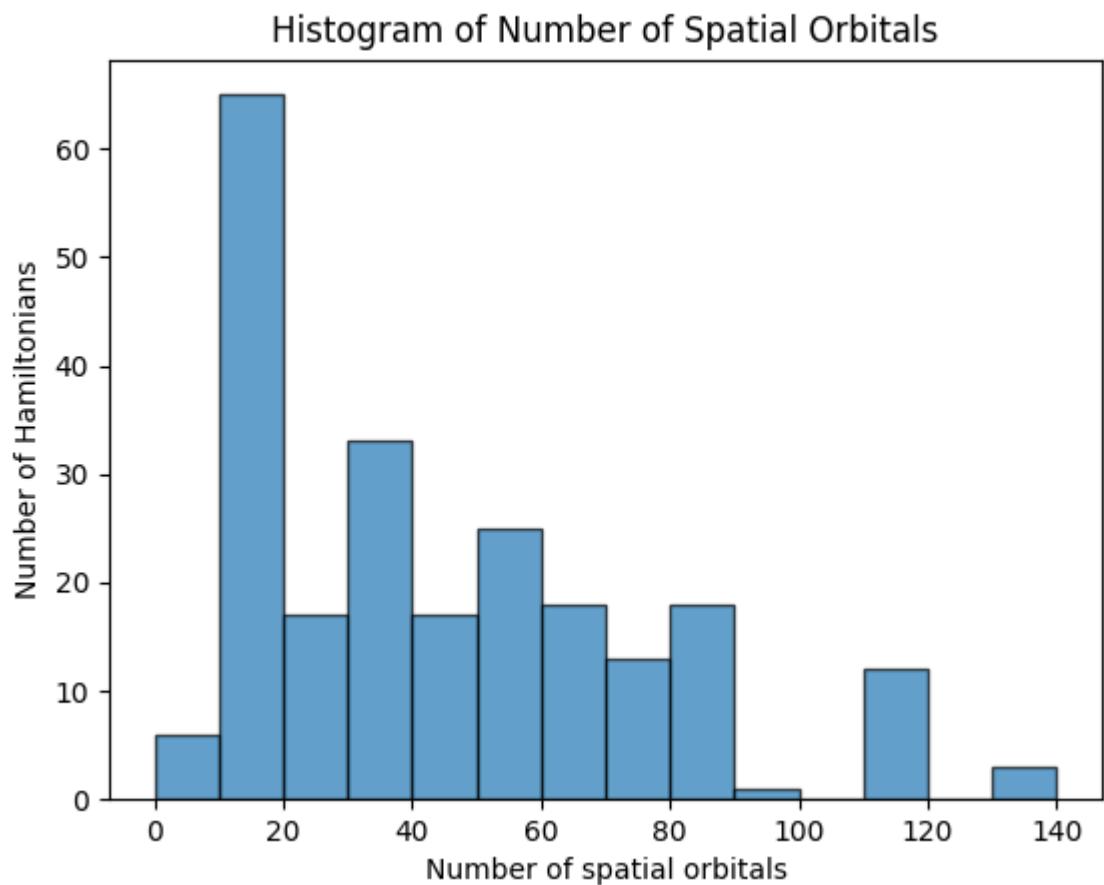
`problem_instance.json` with the most tasks: 30 (`hubbard_square/614c4444-a31a-4348-b24d-01040208651c`)

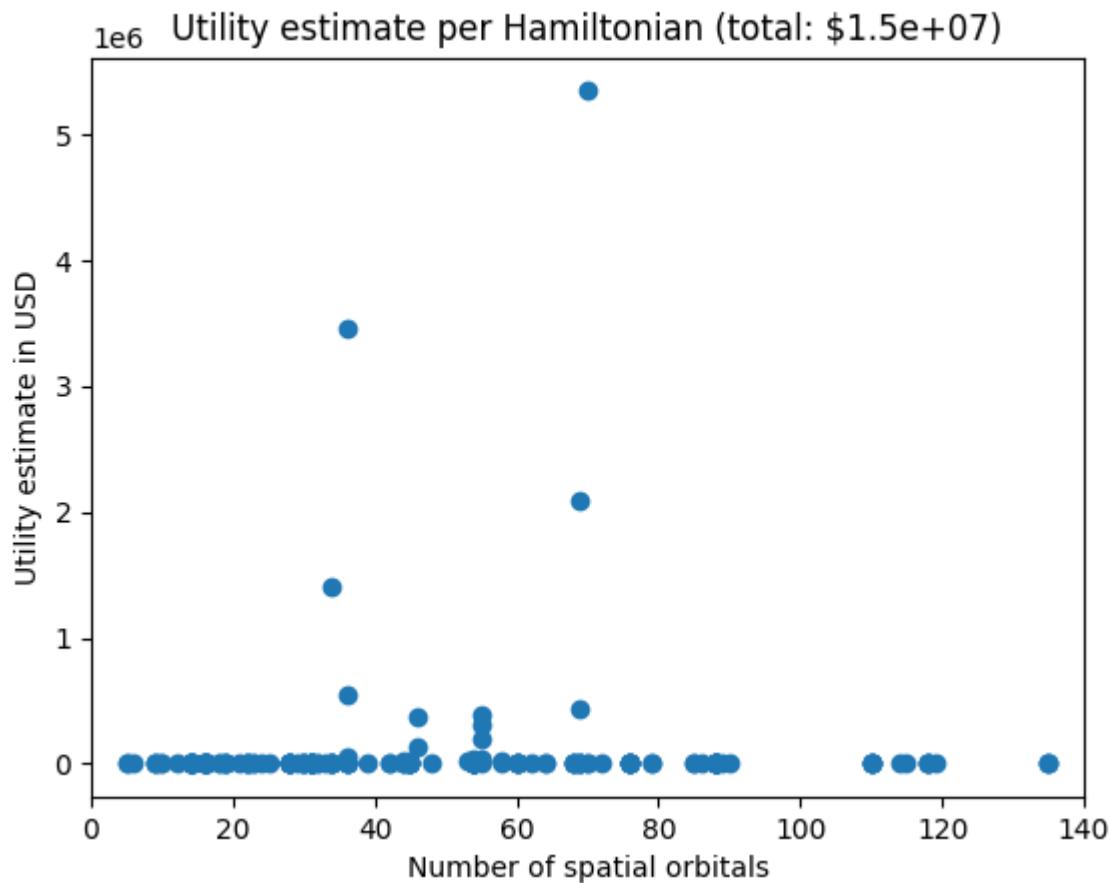
number of Hamiltonians (i.e., tasks) we have features calculated for: 228

minimum number of orbitals: 5

median number of orbitals: 36.0

maximum number of orbitals: 135





Solver Summary Statistics

number of unique participating solvers: 20

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

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/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-b2d6b3dc012, ML Solvability Ratio:
'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98630137 0.71428571]

Solver: MP2/b420358b-5def-41e6-8c5d-b9d93b6aec02, 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]

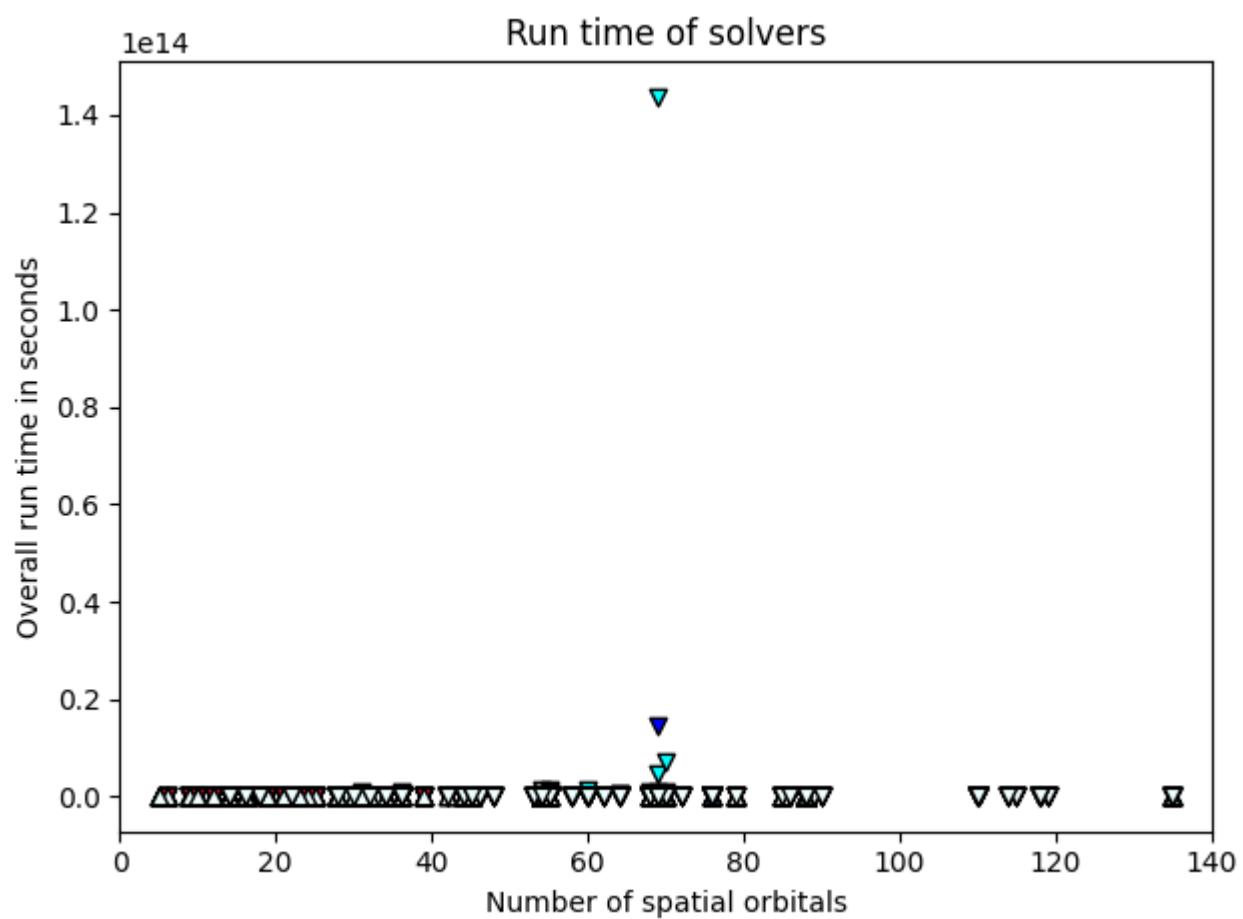
Solver: CCSD(T)/c09217e6-d0f7-4b0f-81c4-79210b7ac878, ML Solvability
Ratio: {'PCA': 0.305, 'NNMF': 0.4969}, F1 Score: [0.95121951 0.94366197]

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

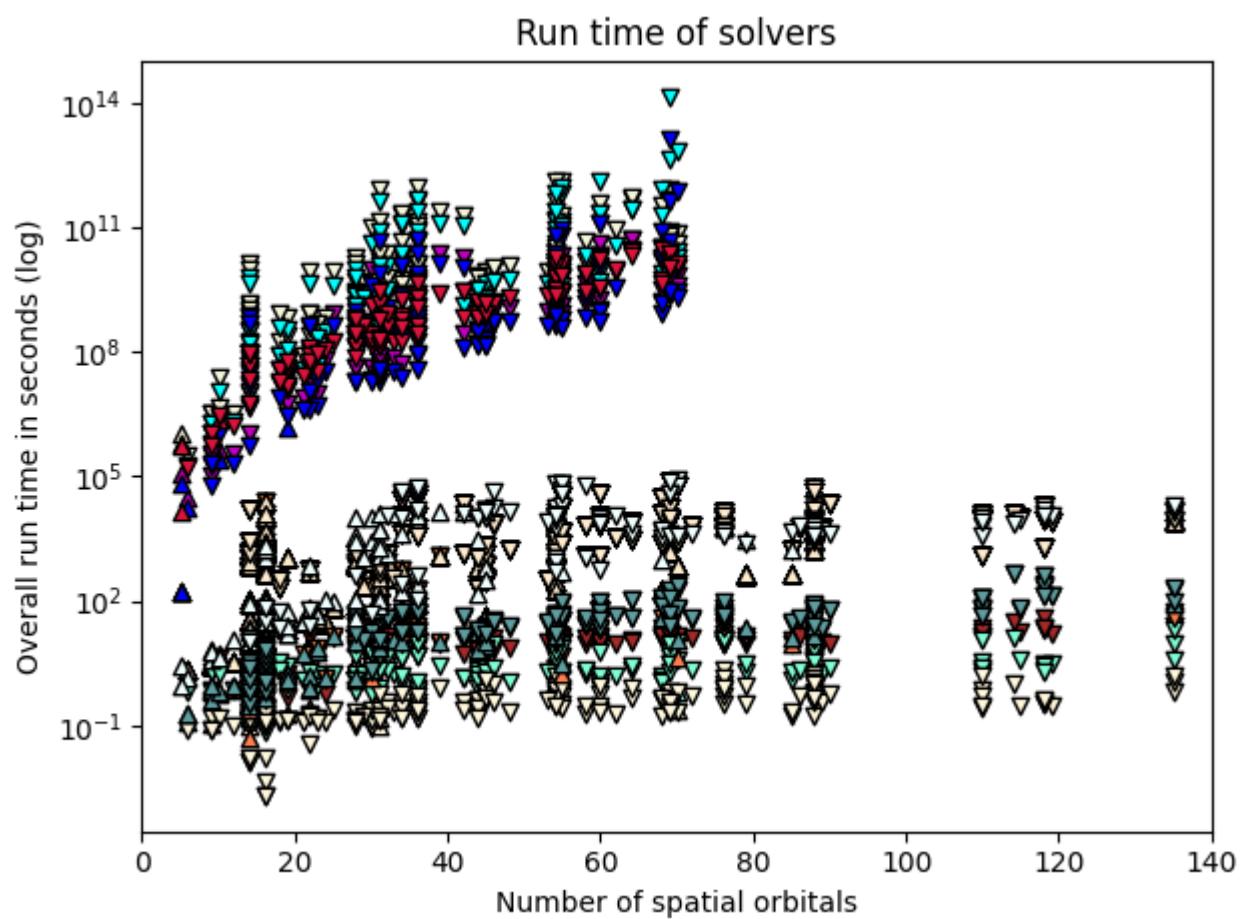
Solver: DF_QPE/f6b36bde-be4a-4eee-975b-2c5f7e553f5f, ML Solvability
Ratio: {'PCA': 0.013, 'NNMF': 0.0006}, F1 Score: [0.99319728 0.83333333]

Solver: DF_QPE/4b07b89f-c66f-4e72-8c24-df3e4222cb41, ML Solvability
Ratio: {'PCA': 0.0, 'NNMF': 0.0}, 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]

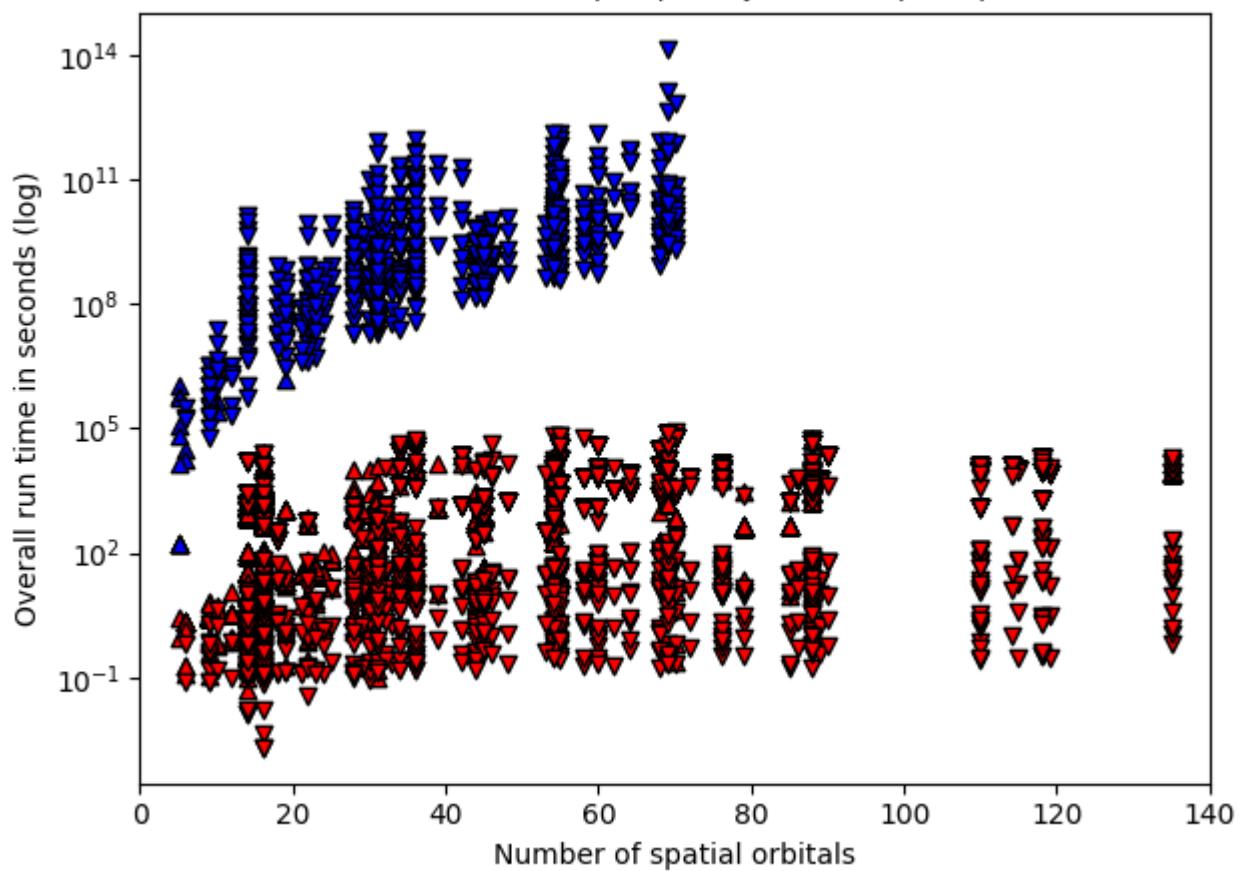


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

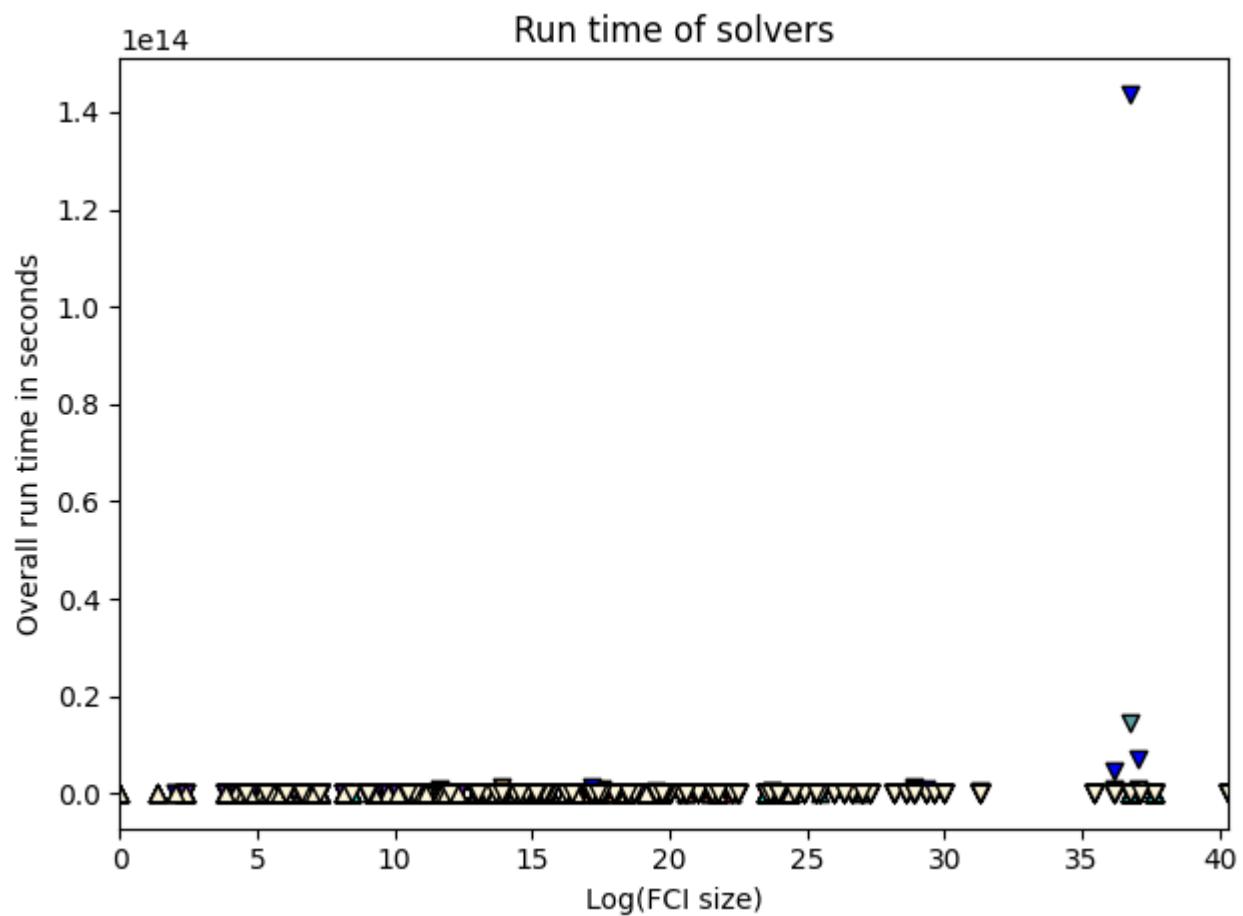


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

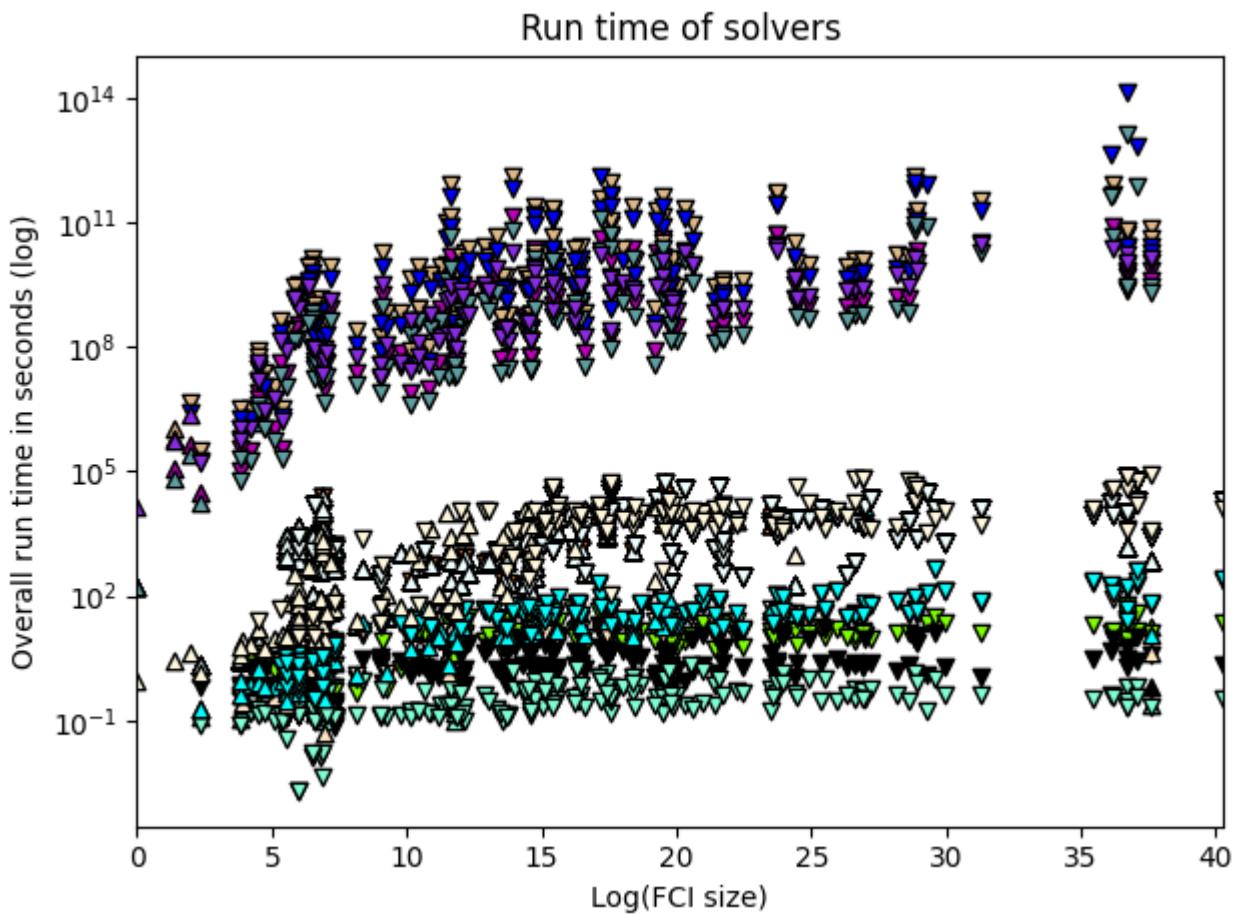
Run time of Classical (red) vs Quantum (blue) solvers



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

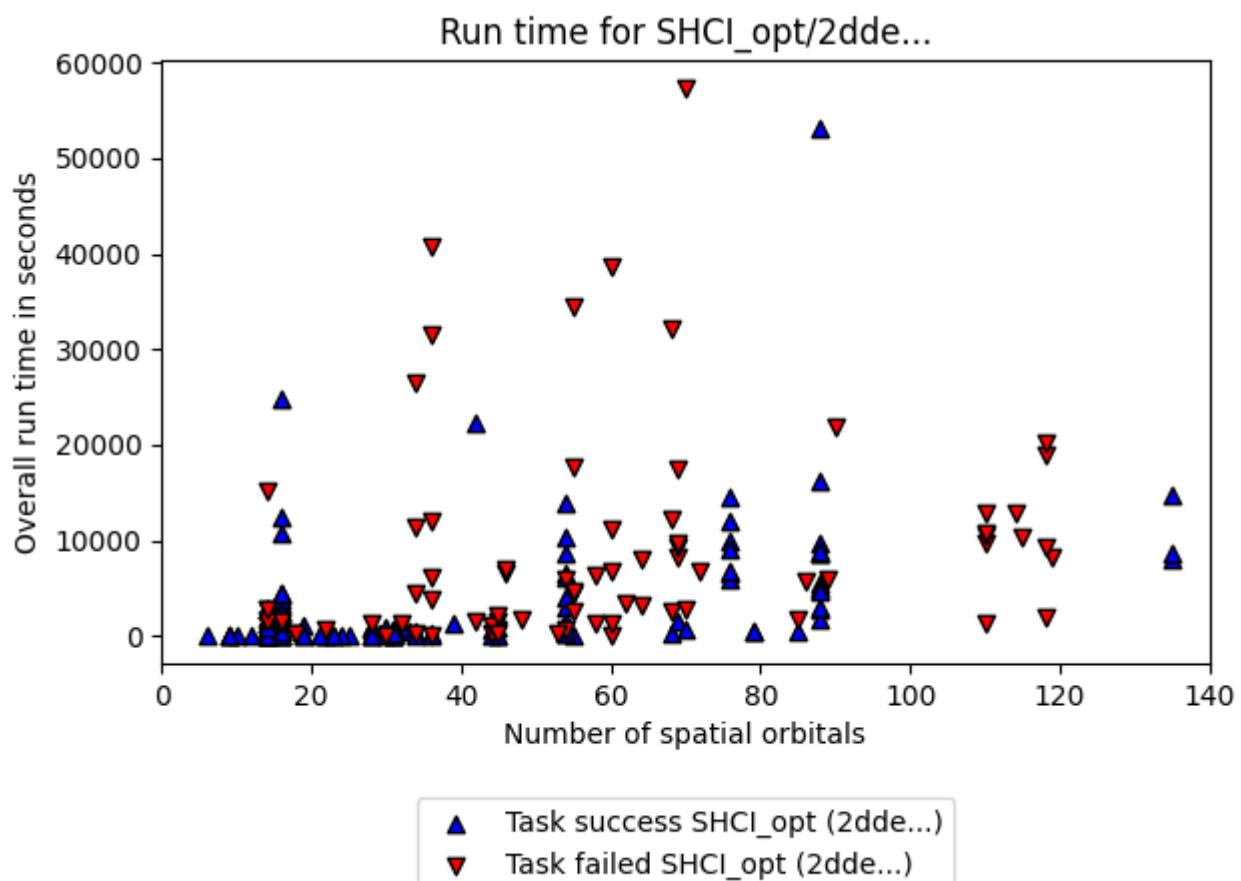
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance_metrics_uuid: b336d306-0018-4e80-9d79-5006455b000f

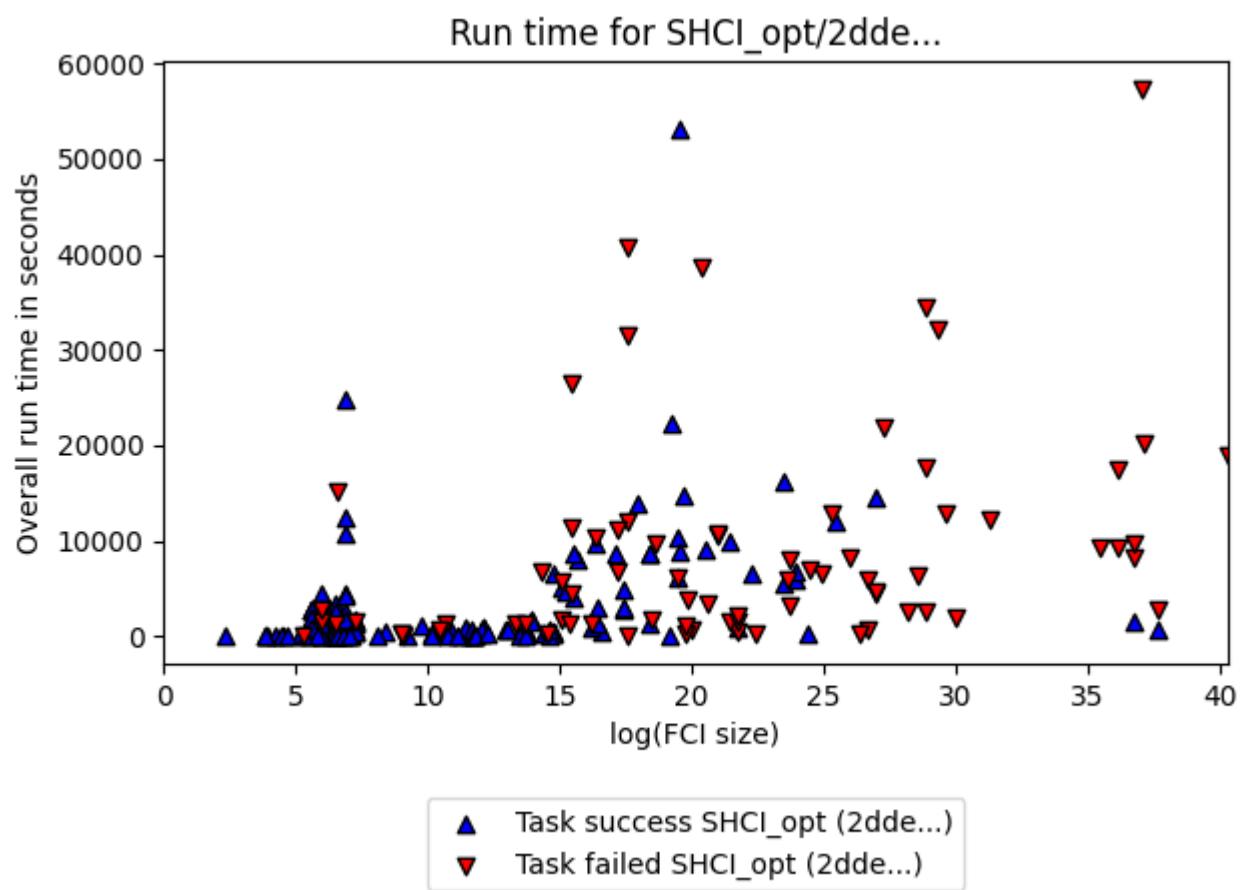
creation_timestamp: 2025-03-06T19:54:13.195807+00:00

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
comment: solvability ratio based on PCA embedding.
f1_score: [0.8571428571428571, 0.9894736842105263]
ml_metrics_calculator_version: 1



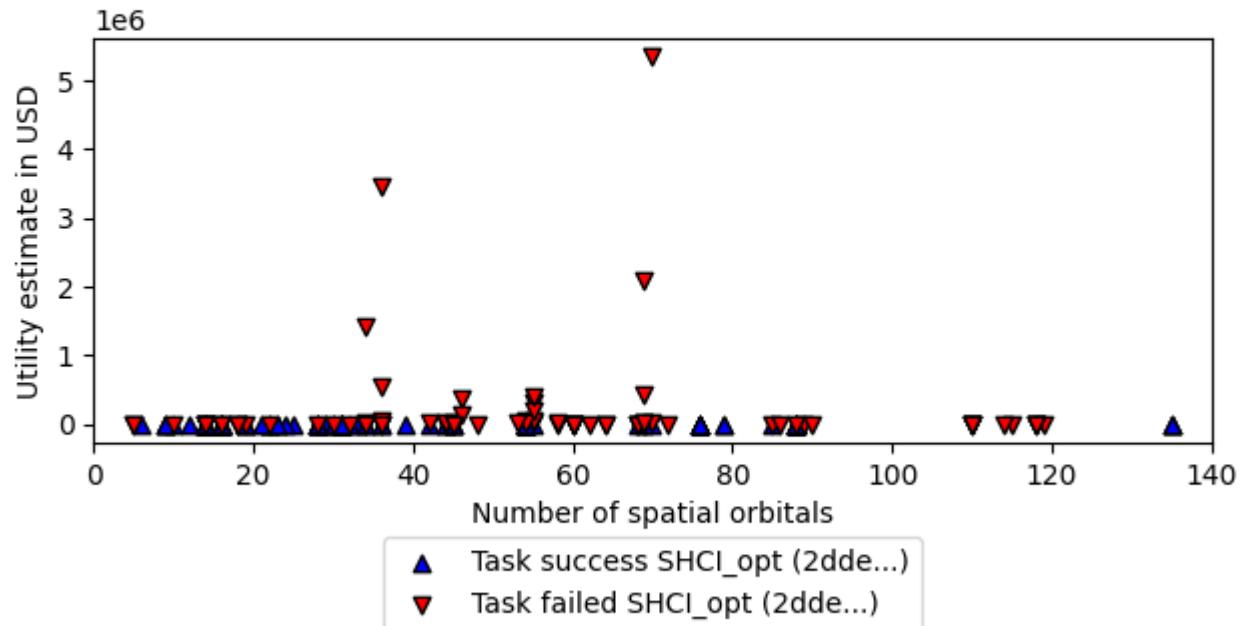
Note: plot only contains attempted tasks.



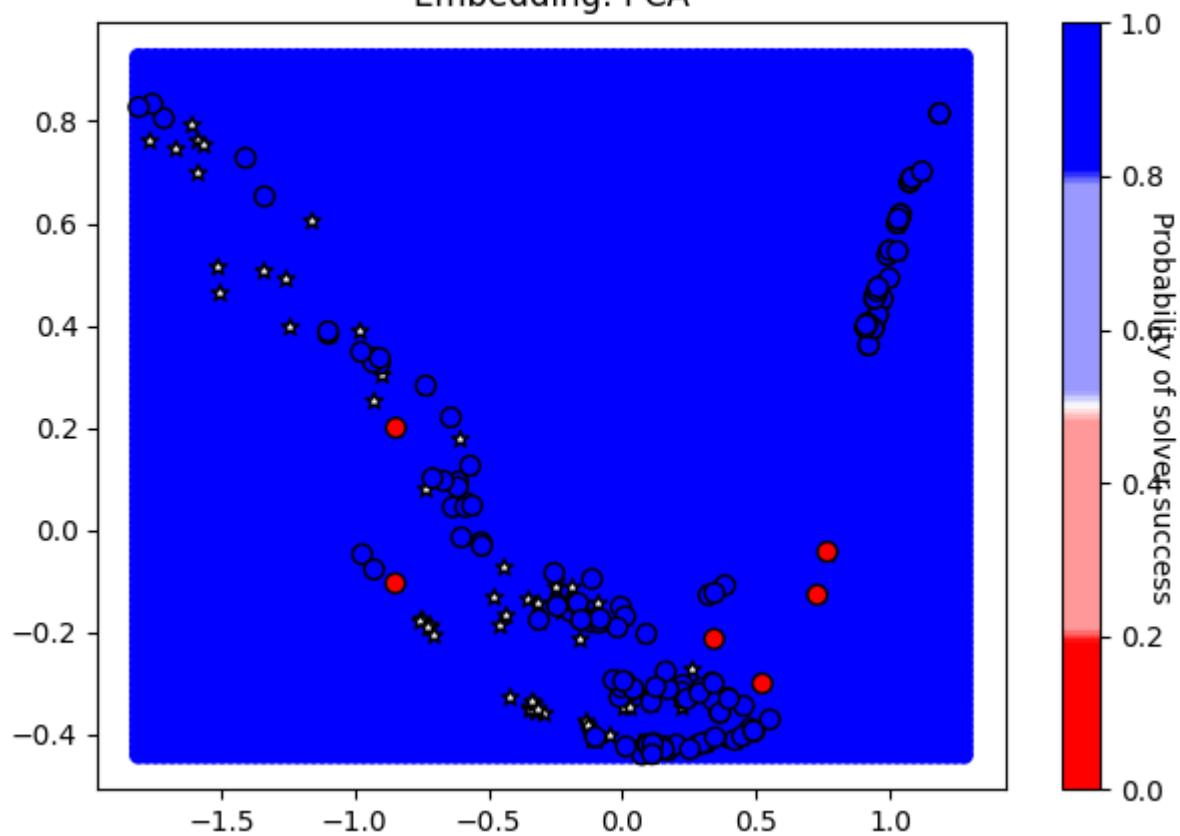
Note: plot only contains attempted tasks.

Utility capture from SHCI_opt/2dde...

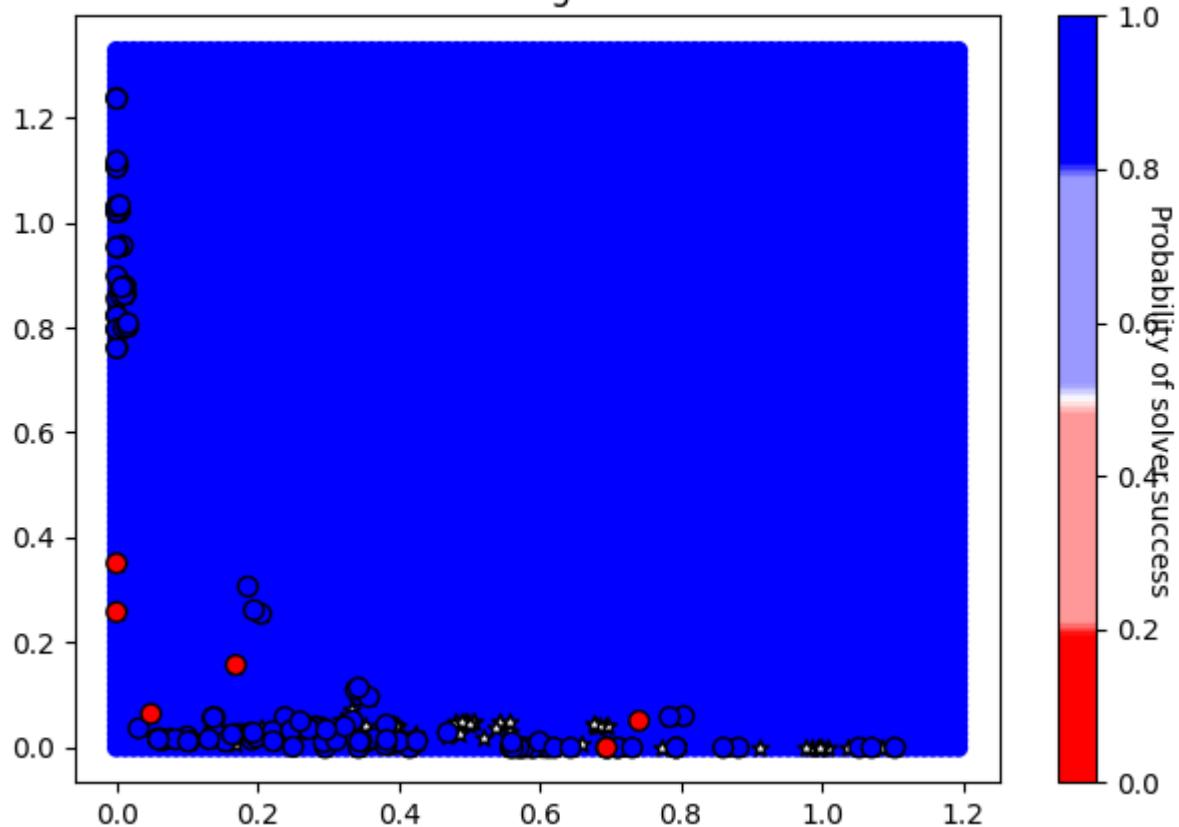
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



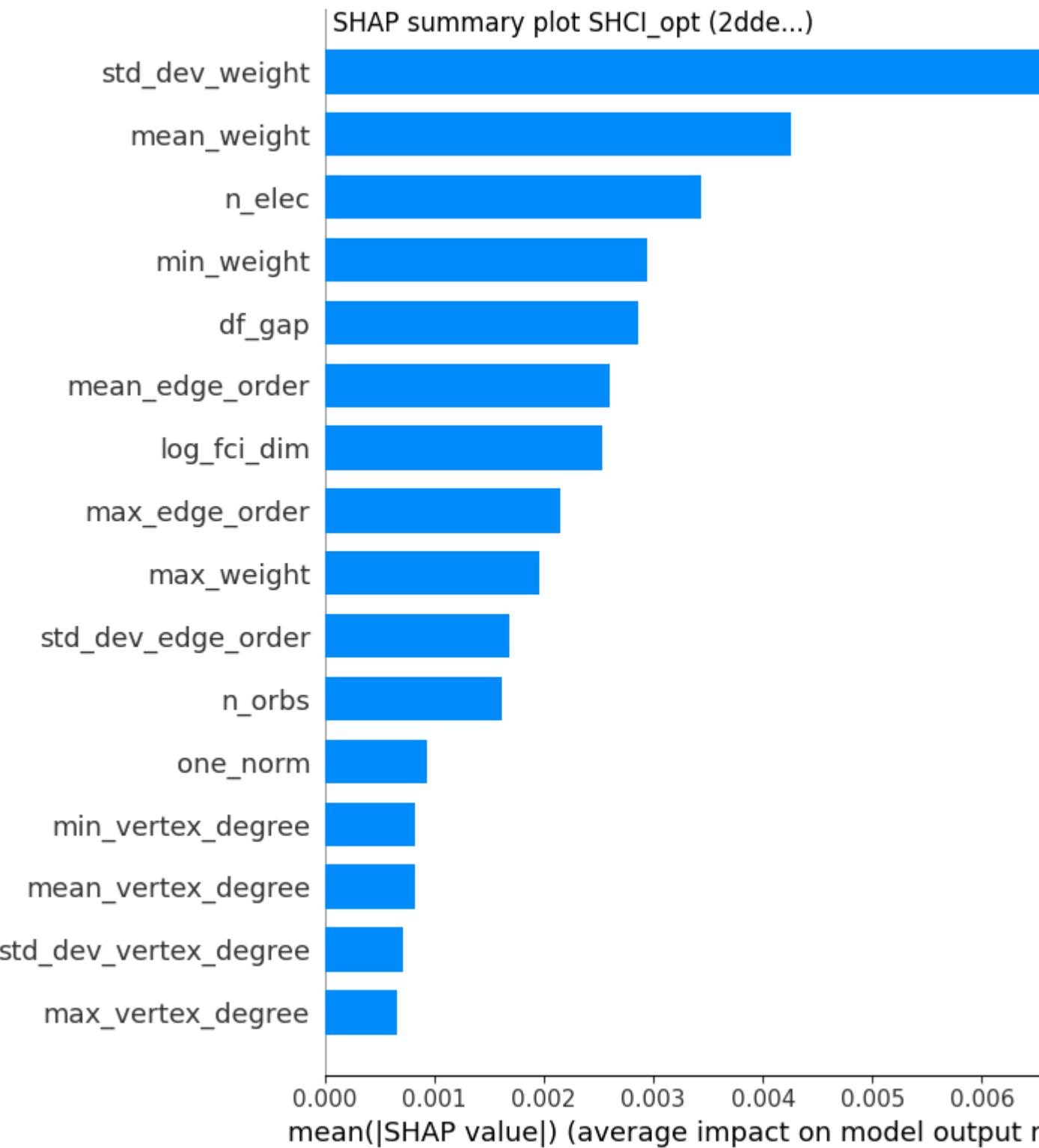
Solver SHCI_opt (2dde...)
Embedding: PCA



Solver SHCI_opt (2ddee...)
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, 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': '1.3.4'}, {'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': '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:2f90da87-a699-4de4-98ad-a78231385822

logical_resource_estimate_solver_uuid:f2d73e1f-3058-43c4-a634-b6c267c84ff1

performance_metrics_uuid: 808f9c9c-306b-485f-979b-e28a24e38d80

creation_timestamp: 2025-03-06T19:54:13.195807+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: 139406856747.7868

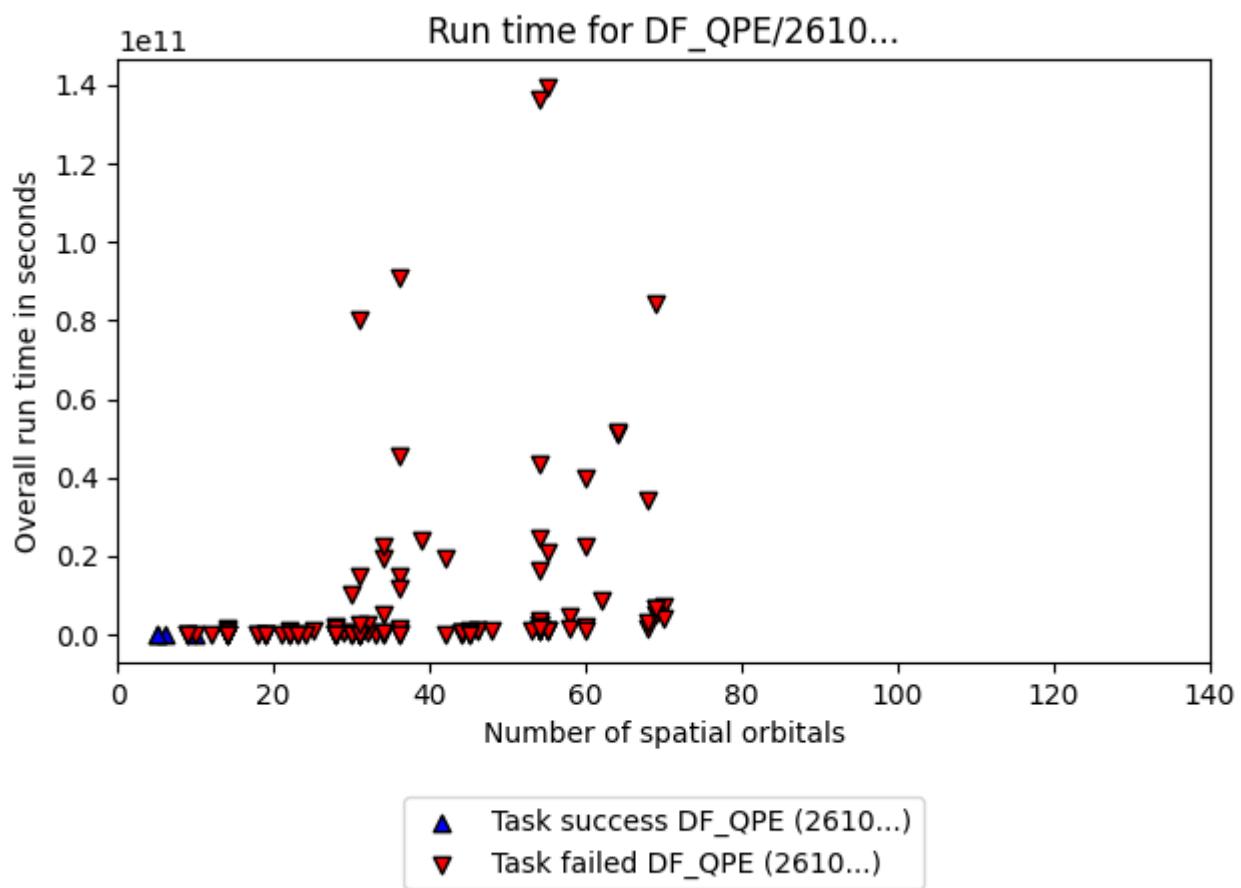
sum_of_run_time_of_attempted_tasks: 1131474650773.224

solvability_ratio: 0.0716

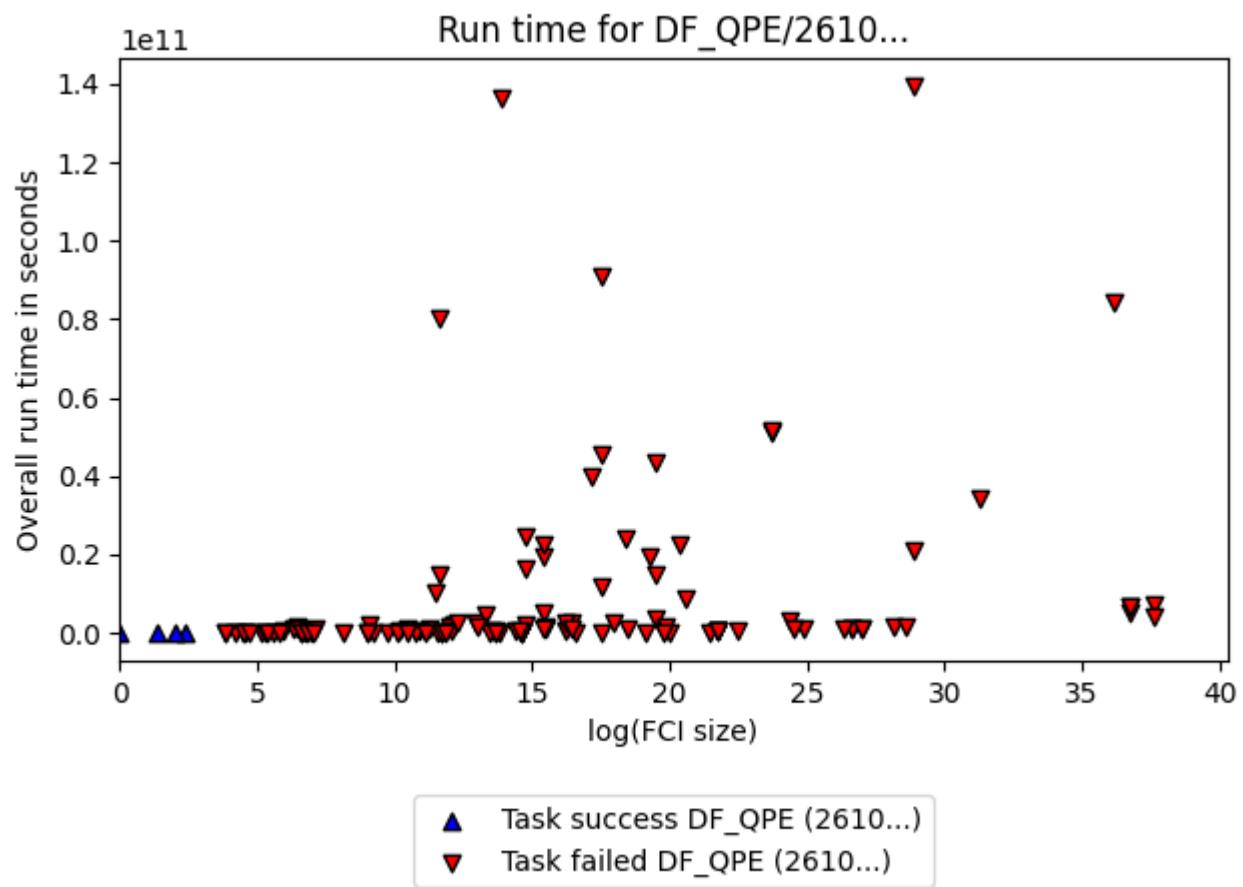
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



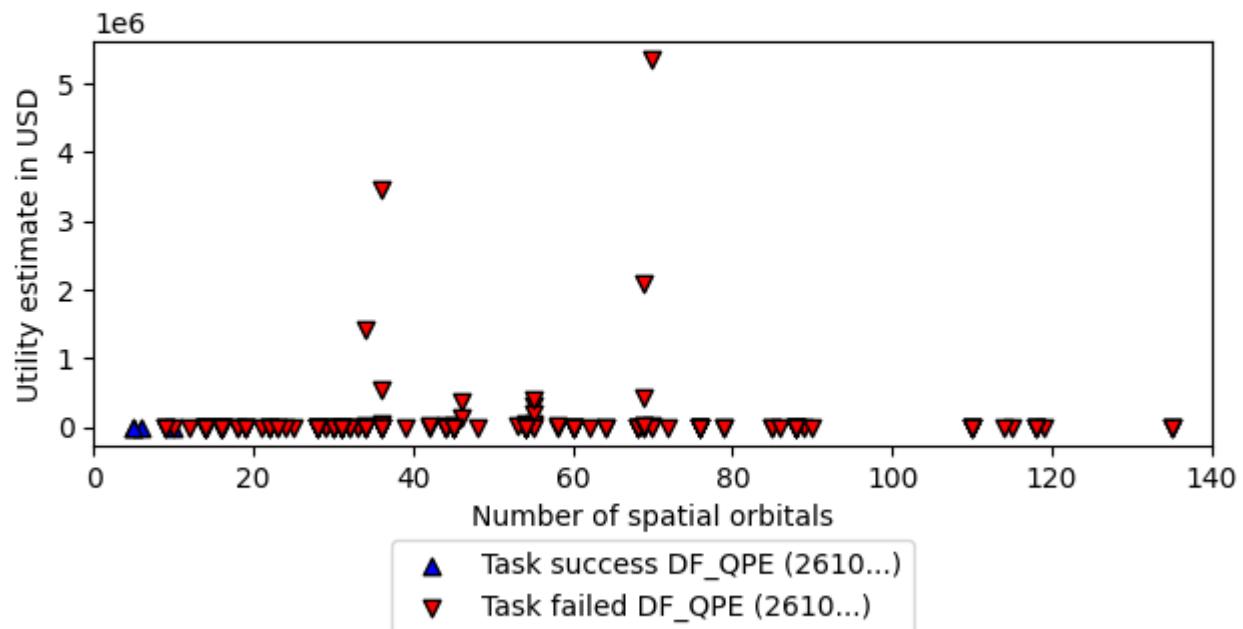
Note: plot only contains attempted tasks.



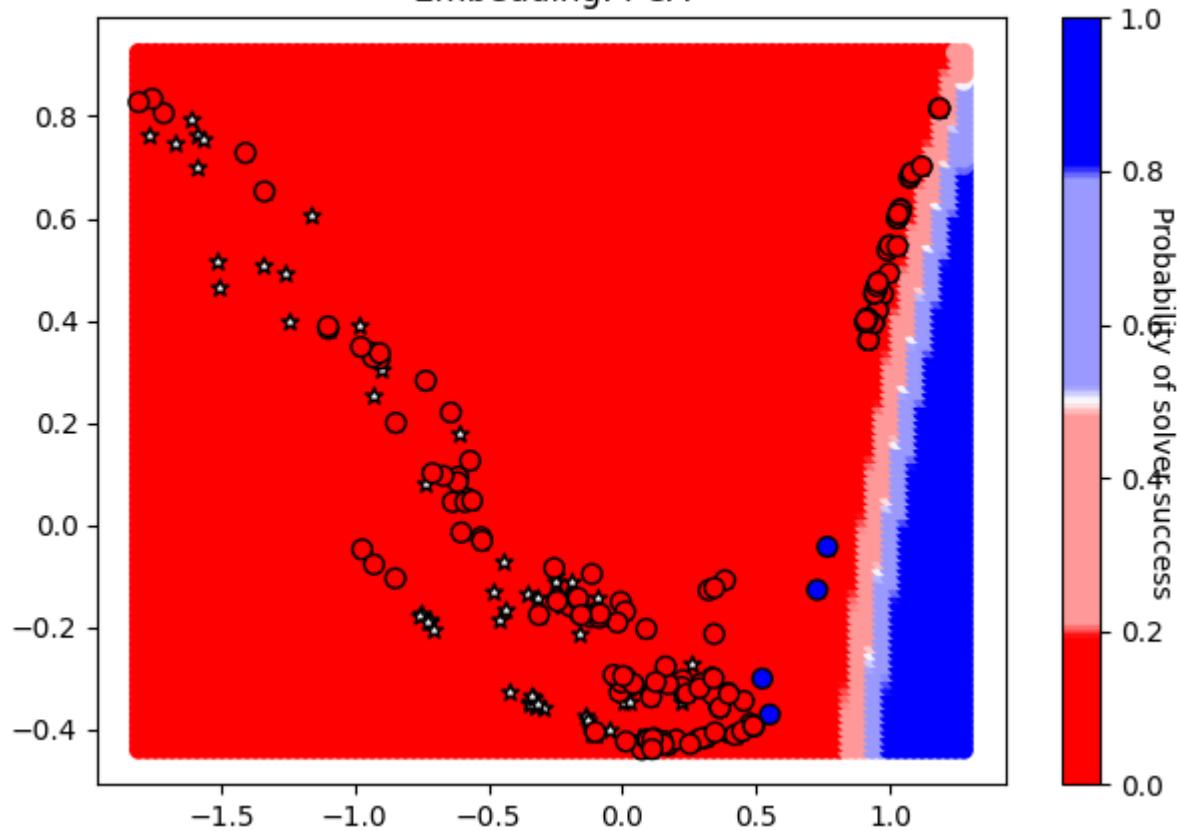
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/2610...

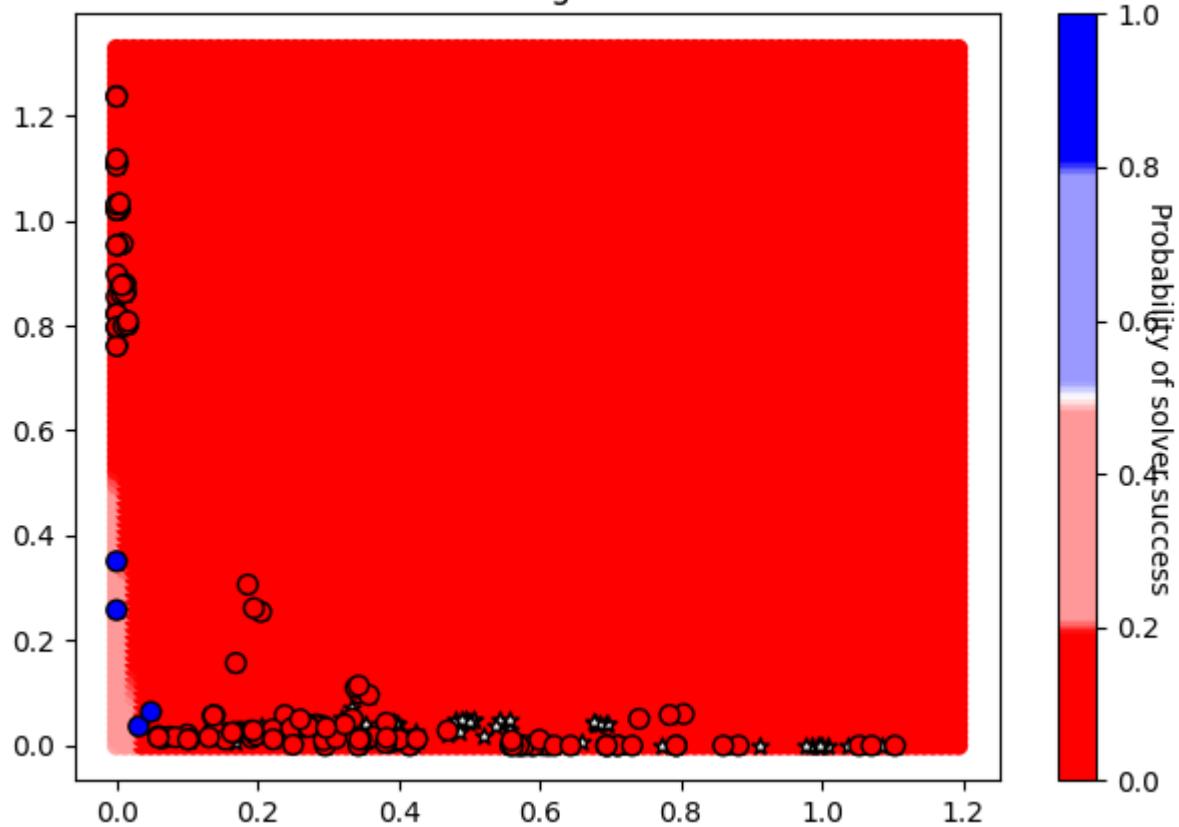
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



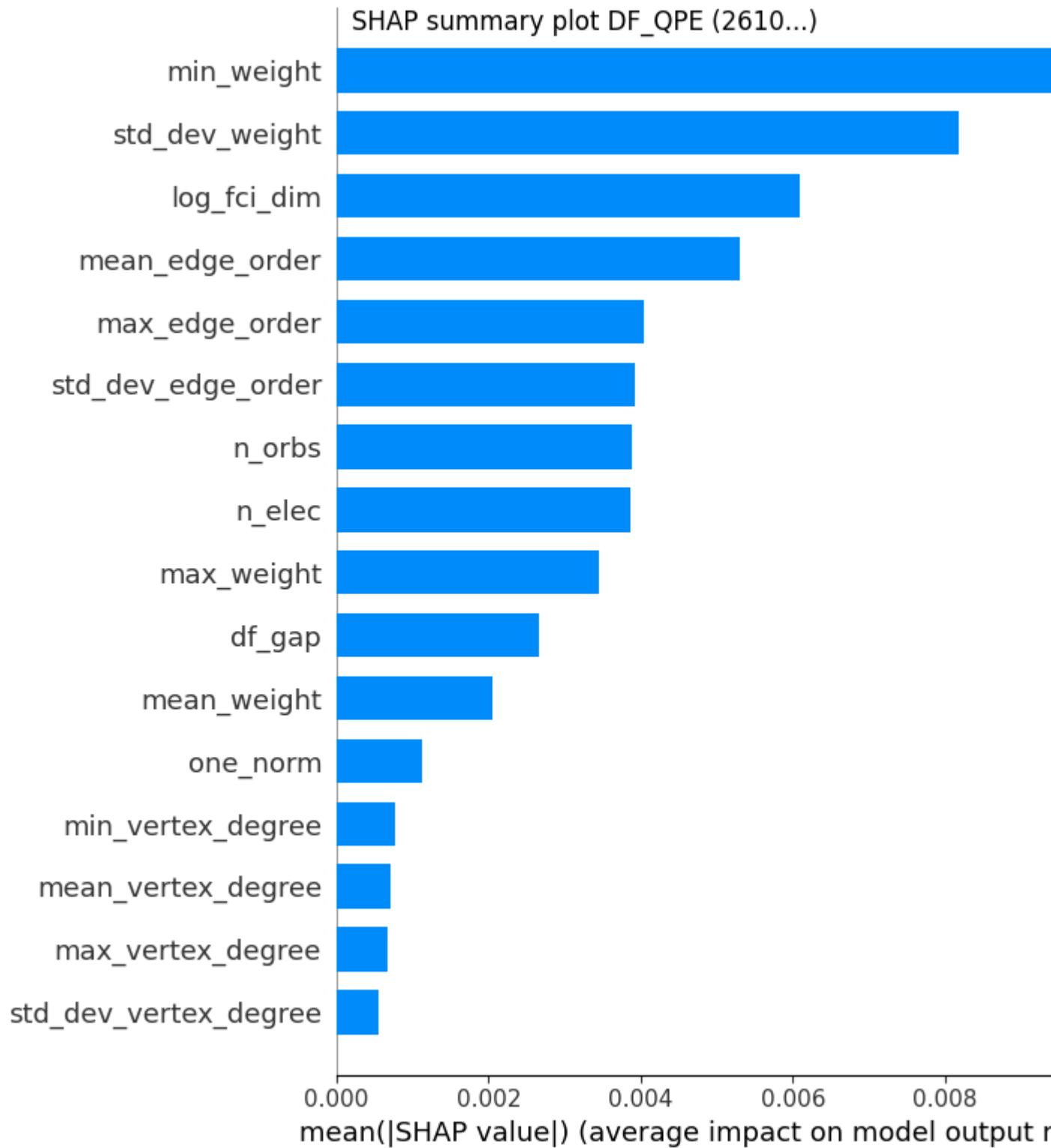
Solver DF_QPE (2610...)
Embedding: PCA



Solver DF_QPE (2610...)
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.

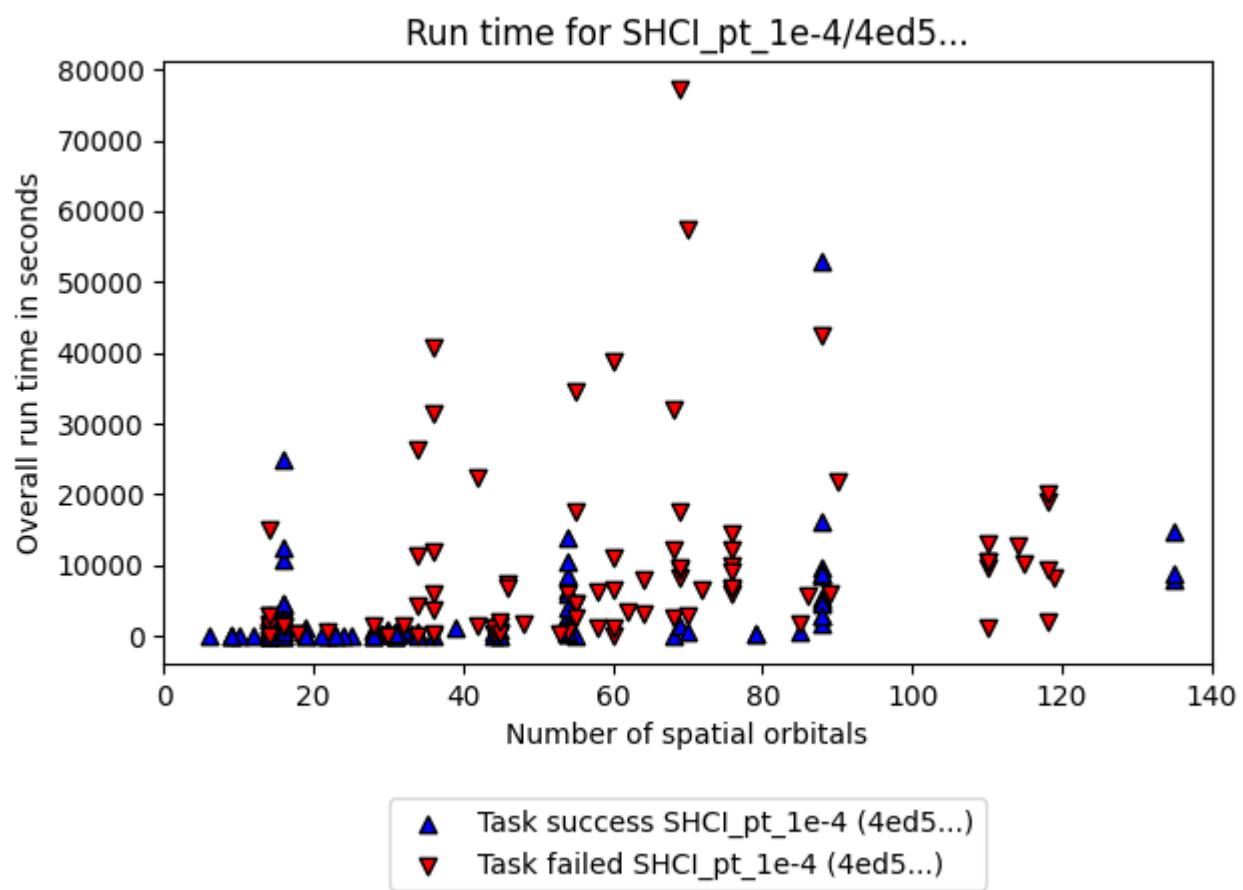


Solver SHCI_pt_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4

solver_uuid:4ed500f1-0650-41e3-af00-e4d0359394b4

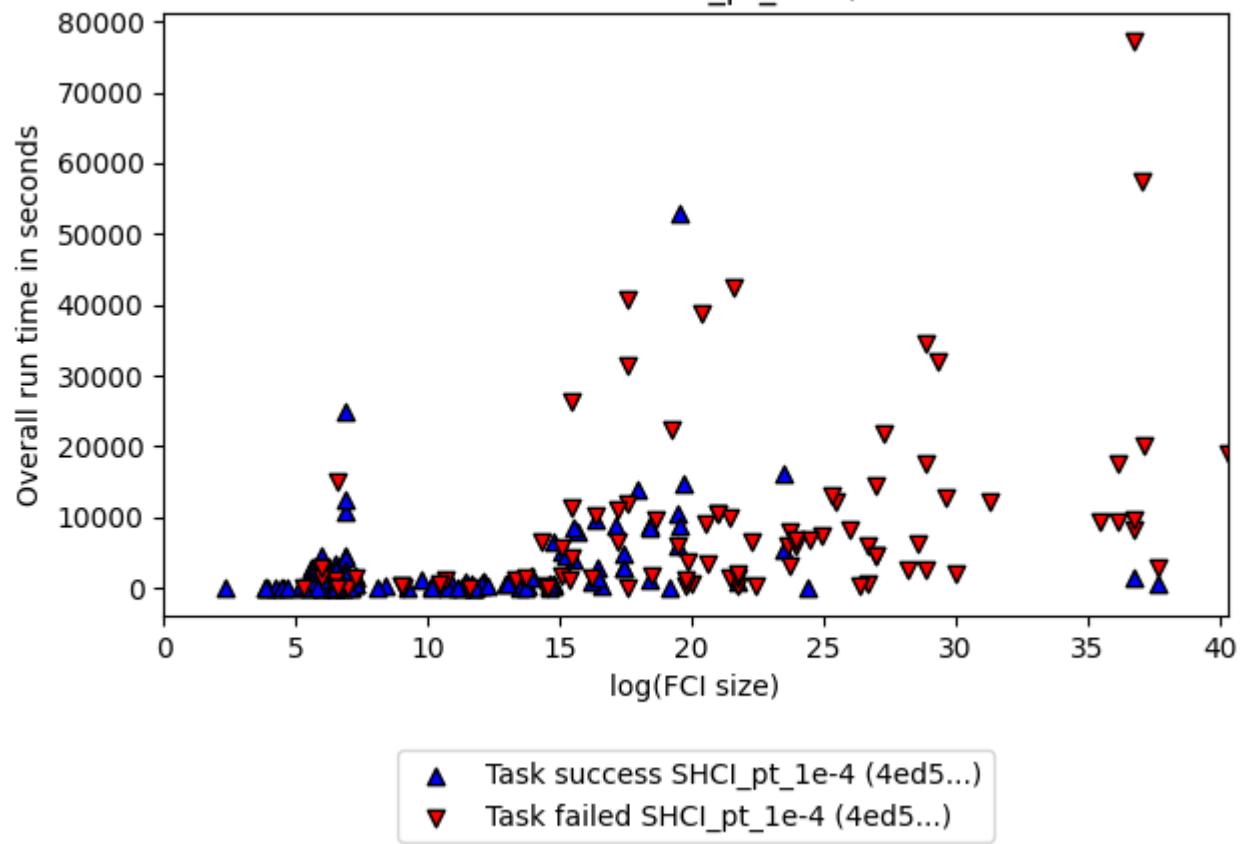
solver_short_name:SHCI_pt_1e-4

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: 6da59c70-de11-49d5-bc8d-7e67bef15ad3
creation.timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.7058823529411765, 0.9632352941176471]
ml.metrics_calculator_version: 1



Note: plot only contains attempted tasks.

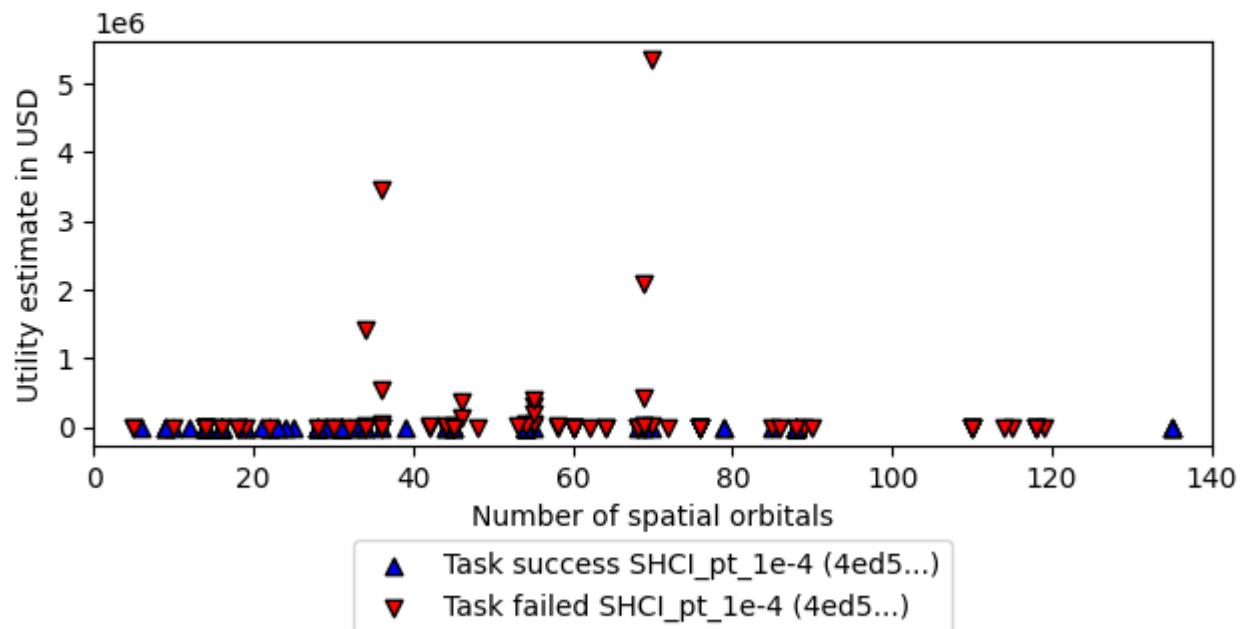
Run time for SHCI_pt_1e-4/4ed5...



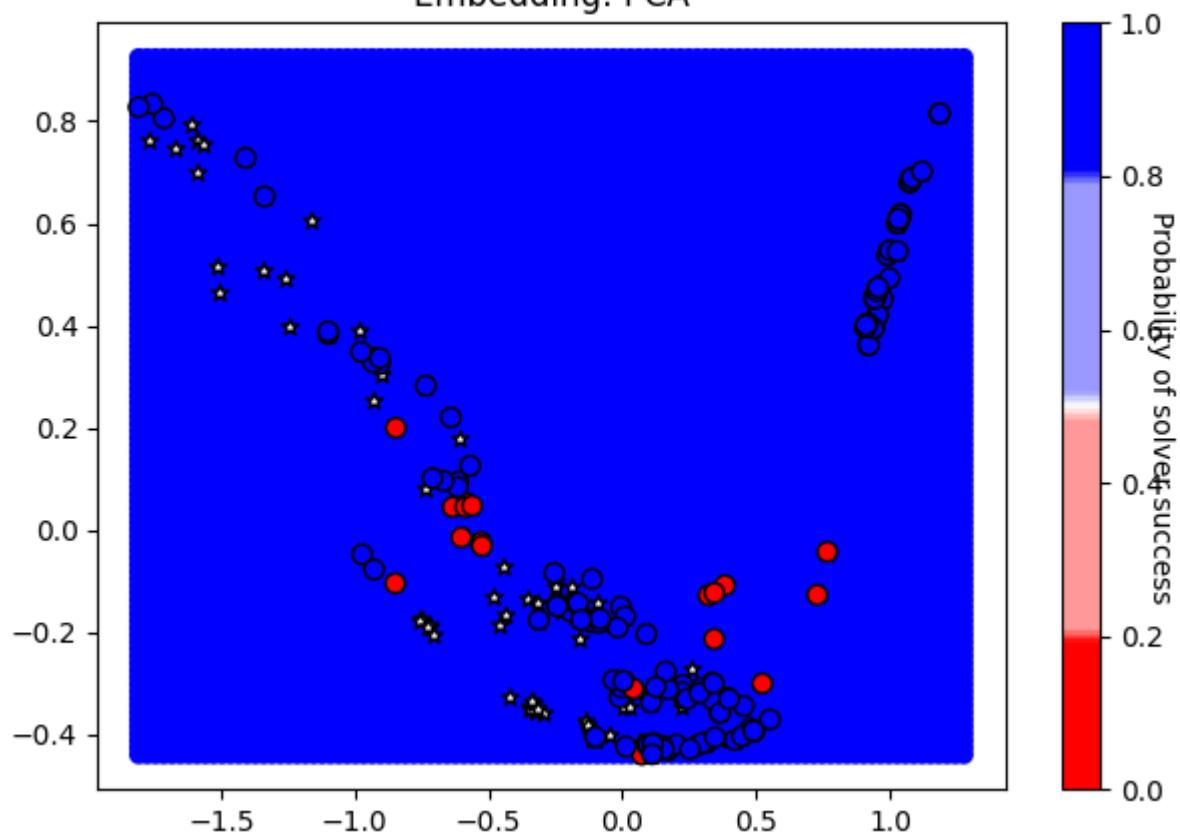
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_1e-4/4ed5...

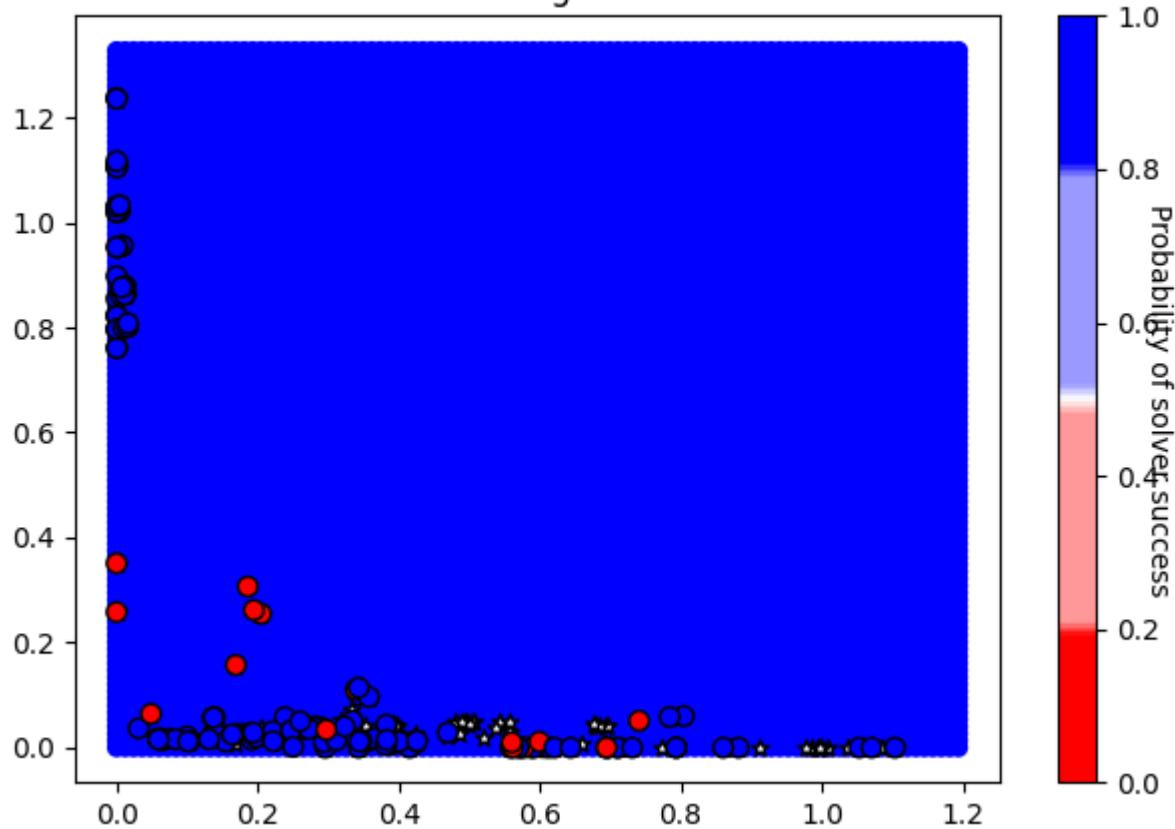
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



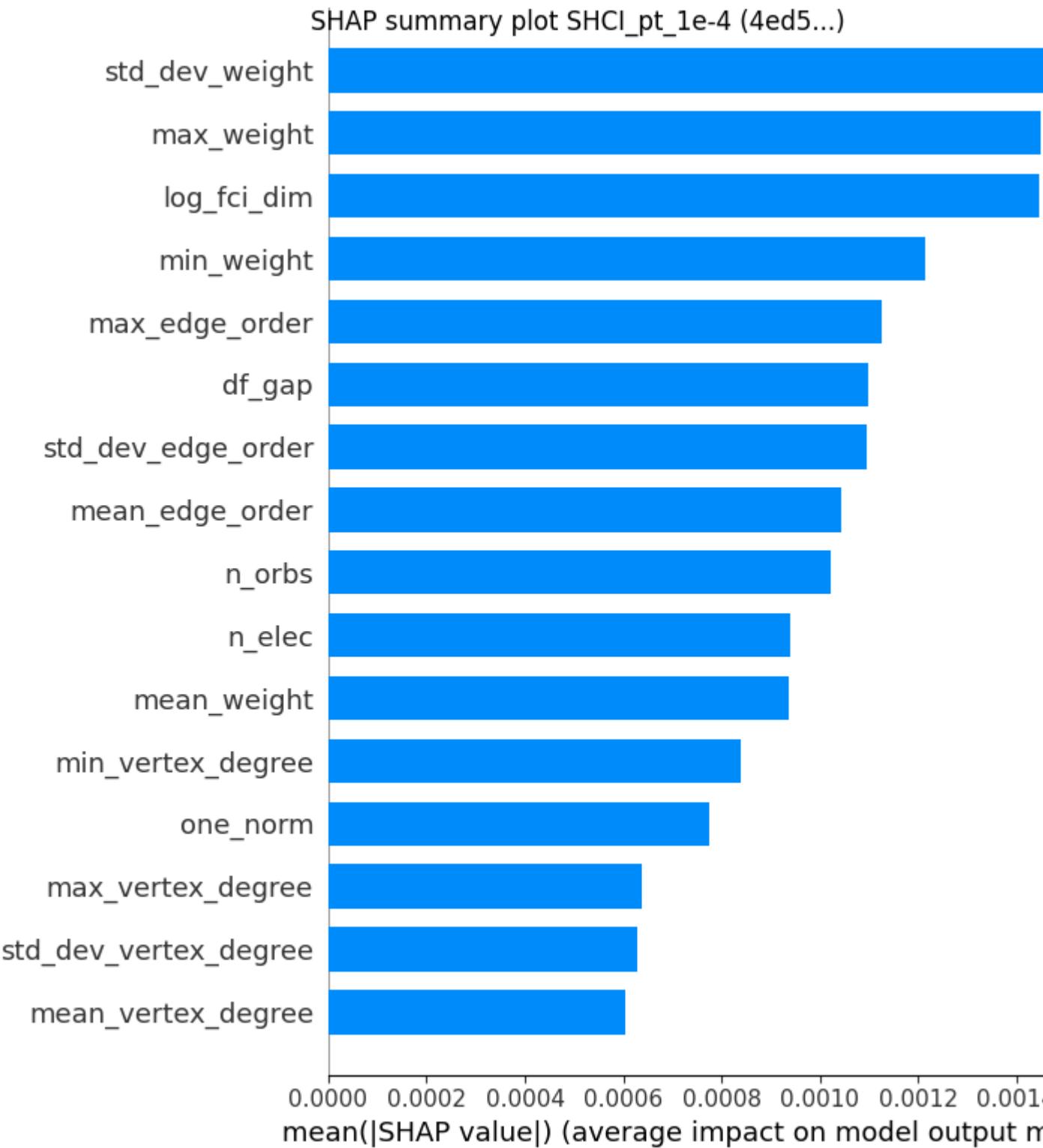
Solver SHCI_pt_1e-4 (4ed5...)
Embedding: PCA



Solver SHCI_pt_1e-4 (4ed5...)
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.

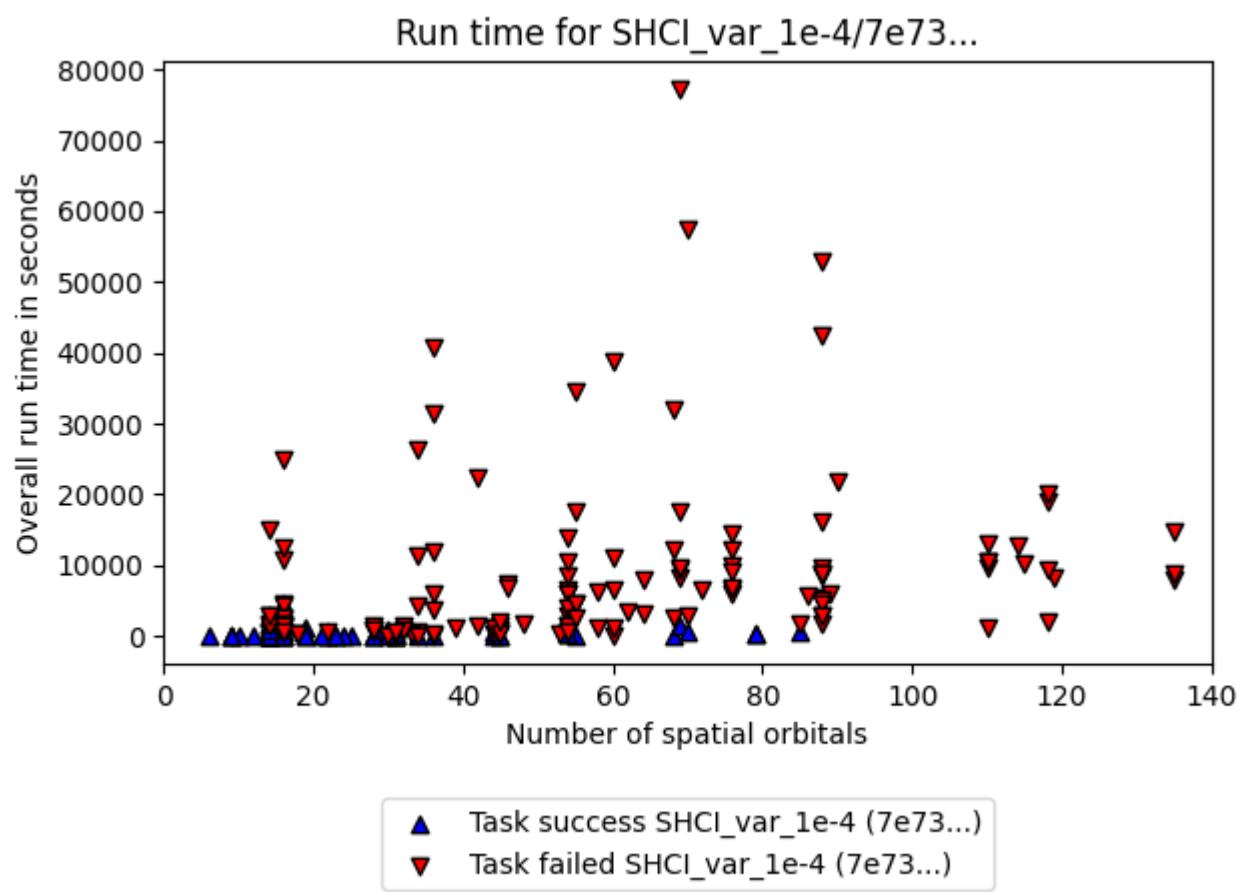


Solver SHCI_var_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54

solver_uuid:7e730dfb-57ee-480b-a8a1-4b73f5f07c54

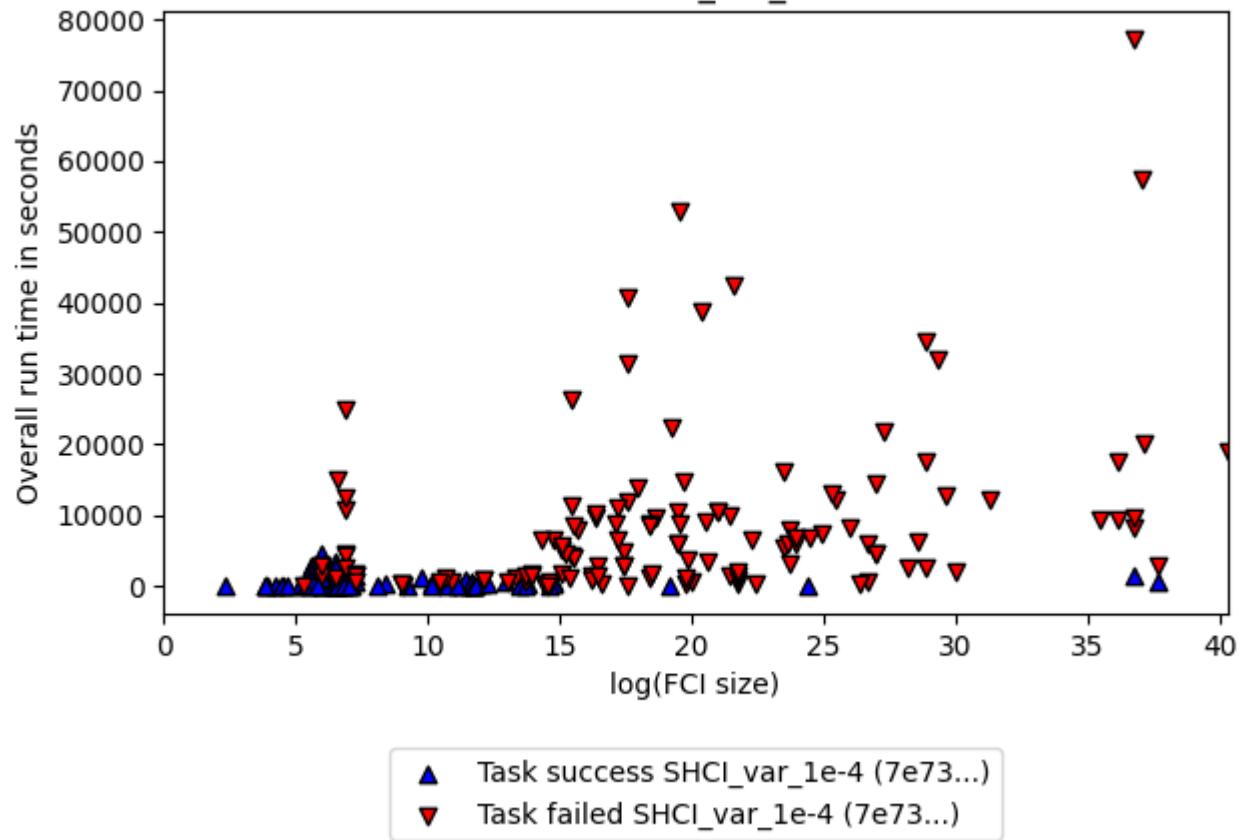
solver_short_name:SHCI_var_1e-4

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: 5cb45704-8216-41a3-a6cd-837cc7567967
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.98484848484849, 0.9885057471264368]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

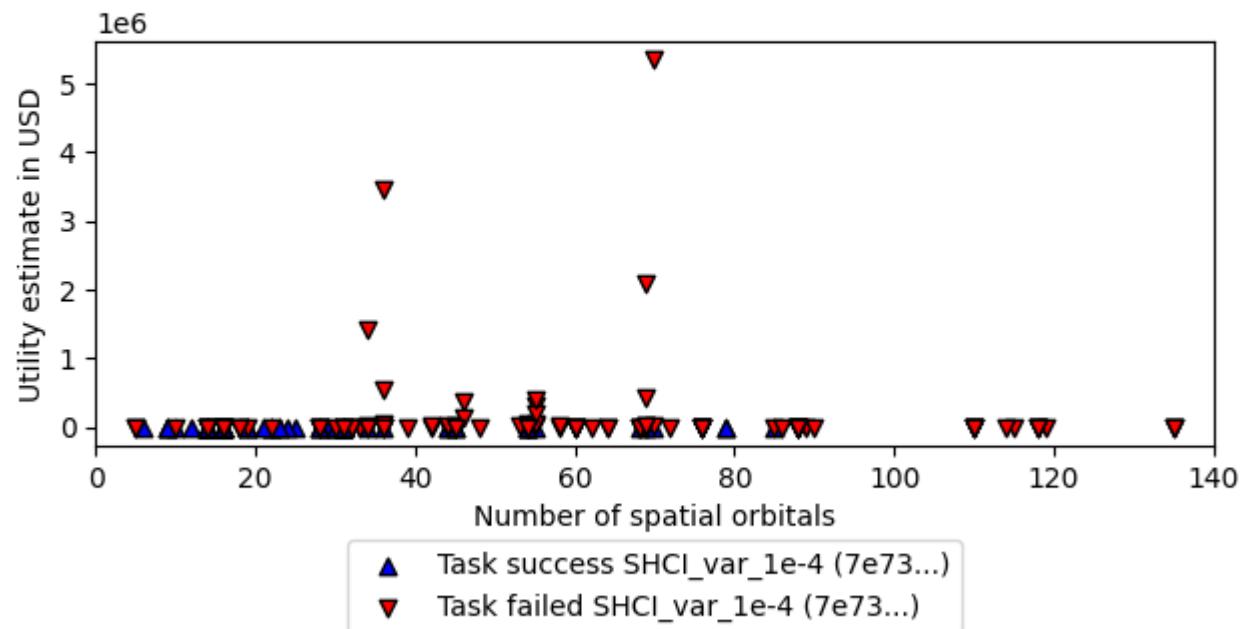
Run time for SHCI_var_1e-4/7e73...



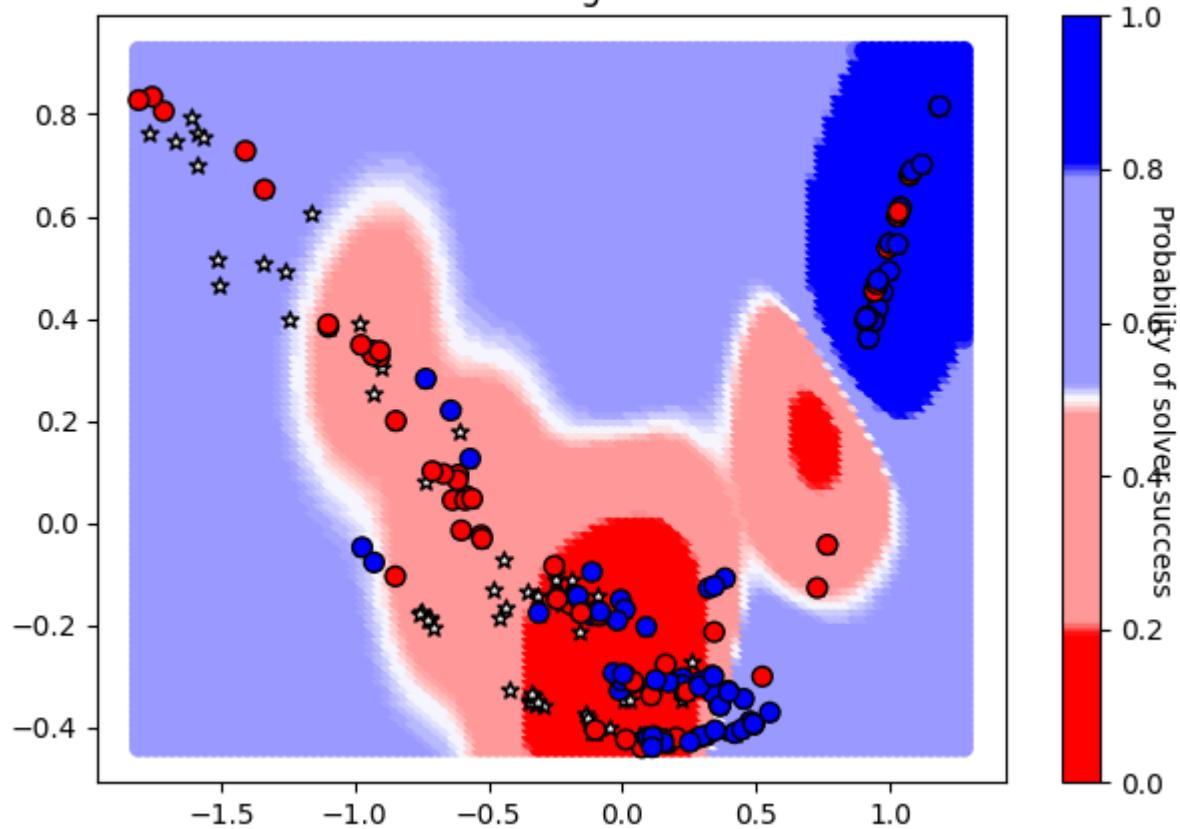
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_1e-4/7e73...

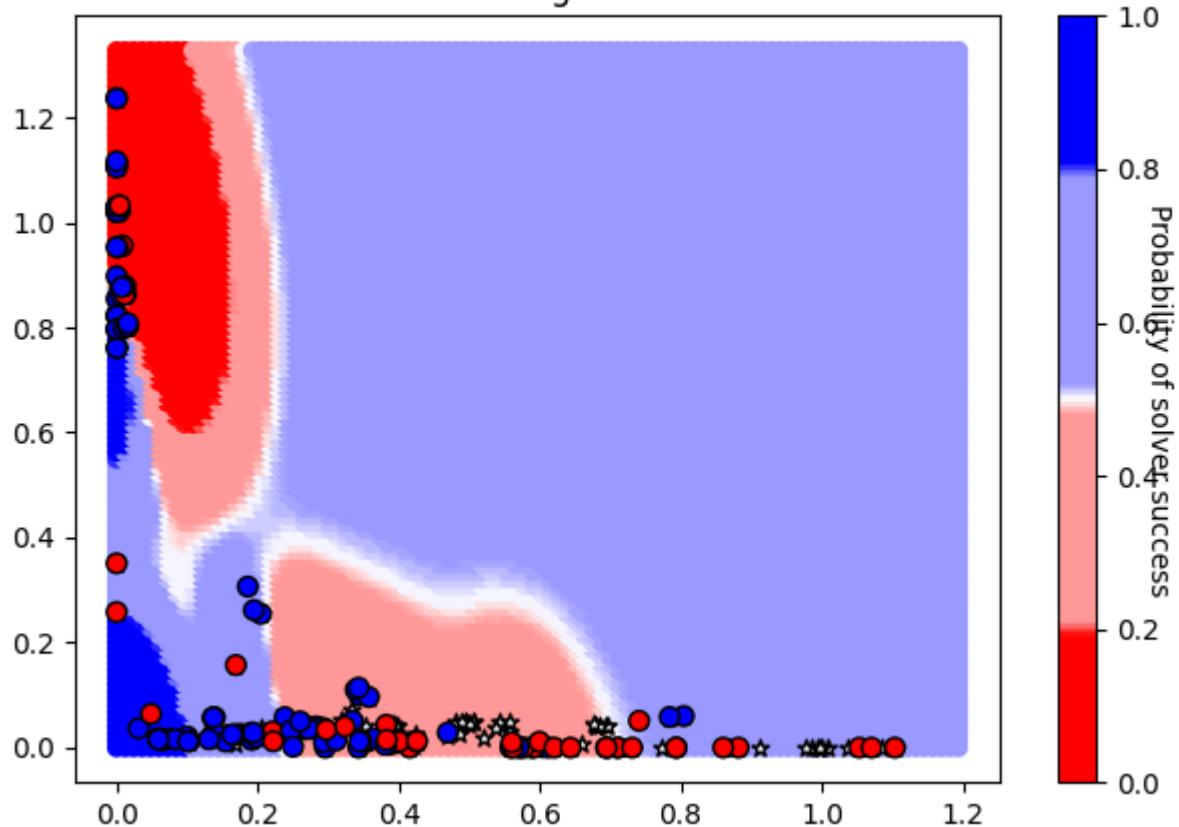
(captured: $\$1.0\text{e}+02/1.5\text{e}+07$, approximately $6.8\text{e}-04\%$)



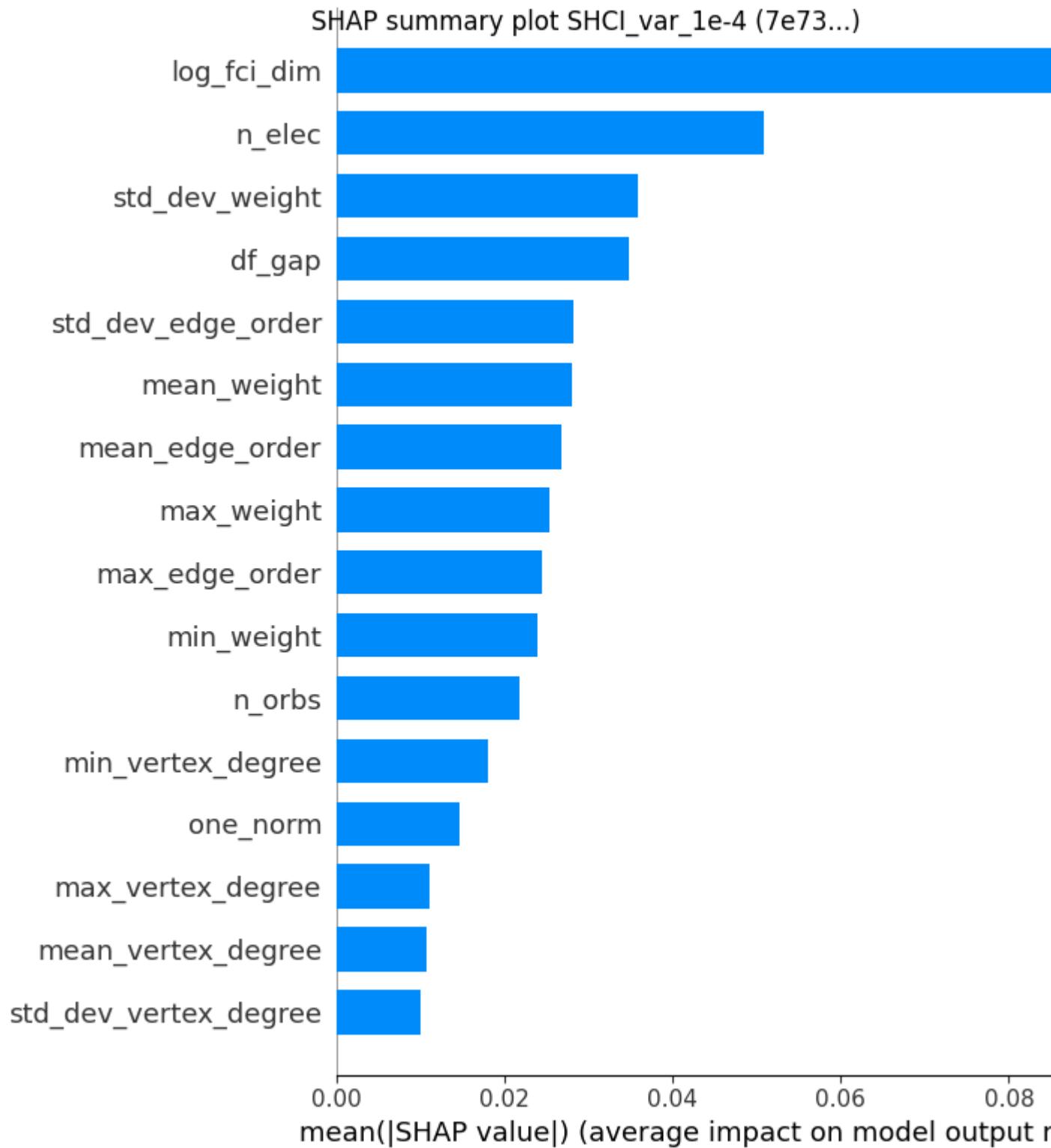
Solver SHCI_var_1e-4 (7e73...)
Embedding: PCA



Solver SHCI_var_1e-4 (7e73...)
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.



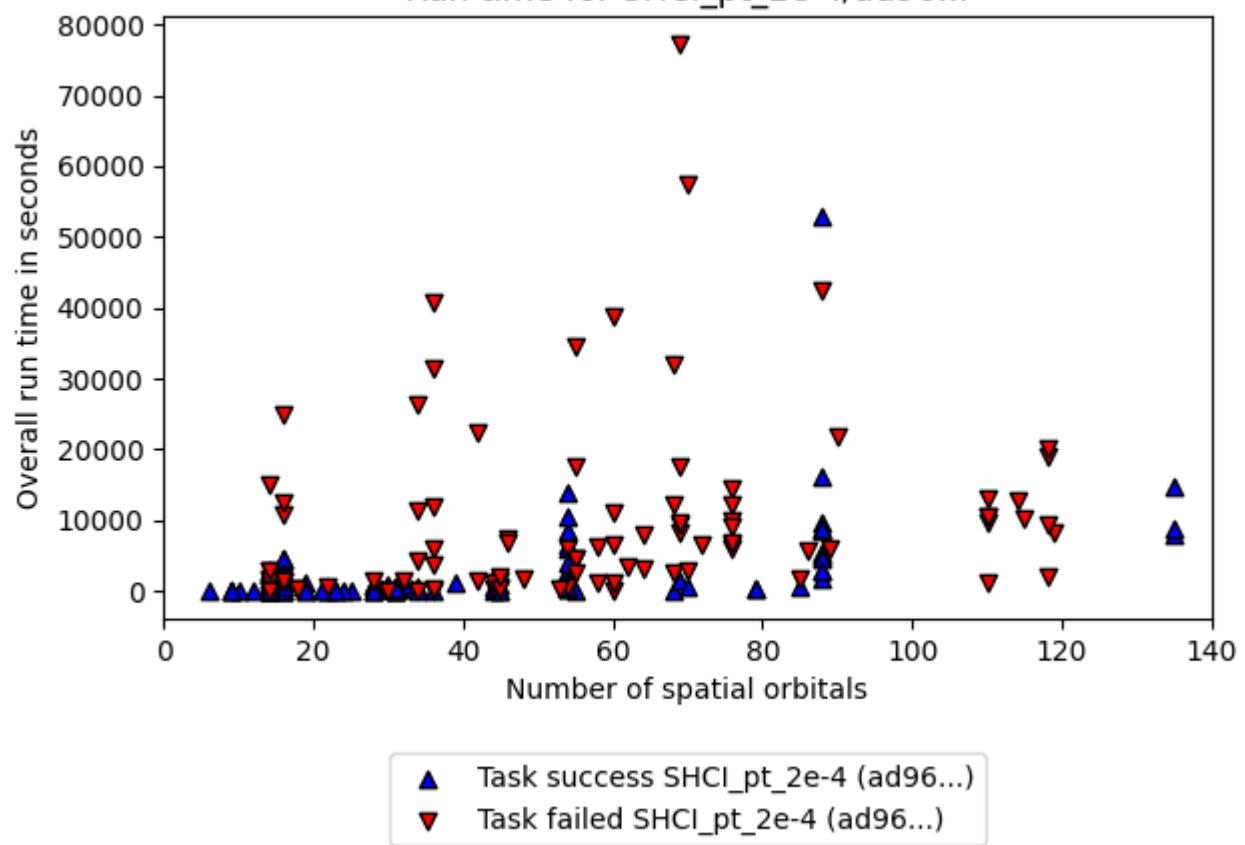
Solver SHCI_pt_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb

solver_uuid:ad964781-302e-4728-a26d-39918e0a6cdb

solver_short_name:SHCI_pt_2e-4

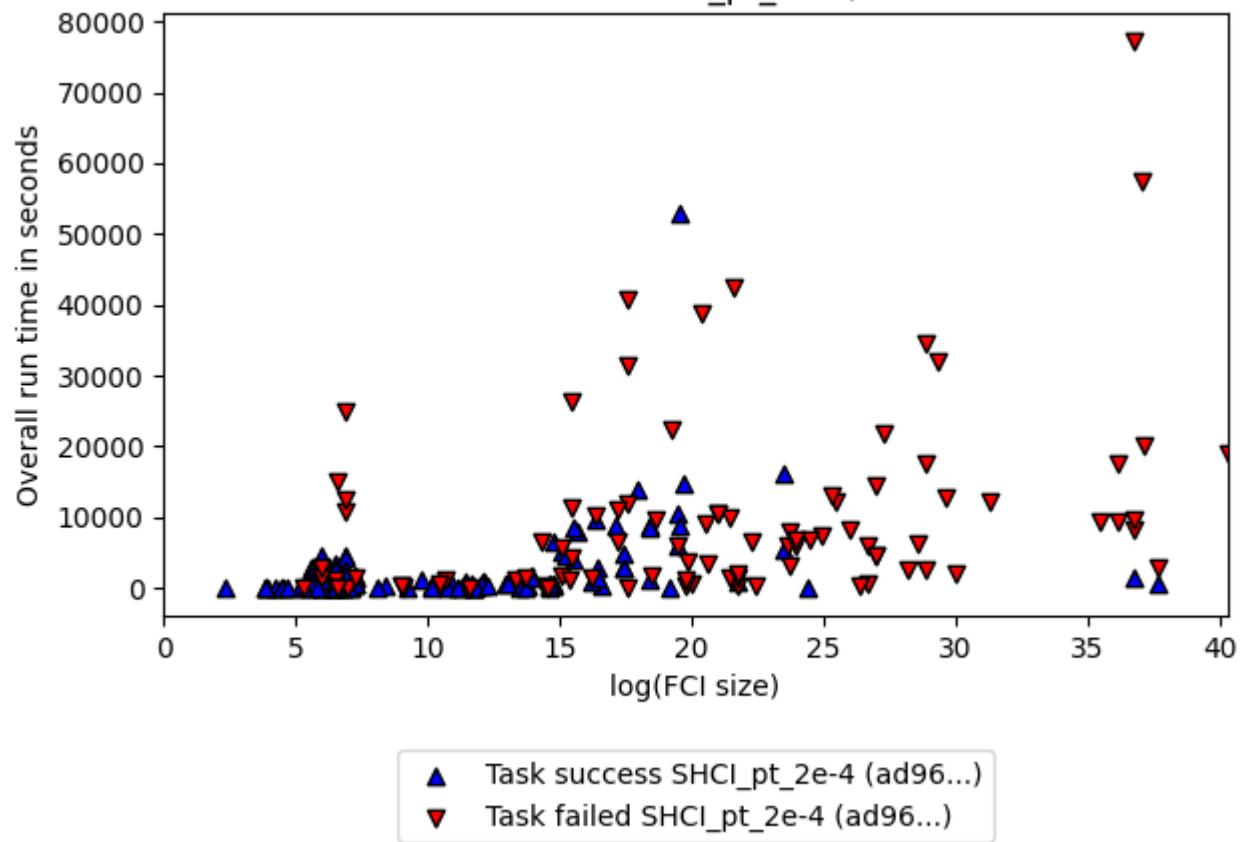
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:SHCI with eps_var 2e-4 + PT
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: ee3f073f-c432-4625-bde3-4980da92270e
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.6486486486486487, 0.9516728624535316]
ml_metrics_calculator_version: 1

Run time for SHCI_pt_2e-4/ad96...



Note: plot only contains attempted tasks.

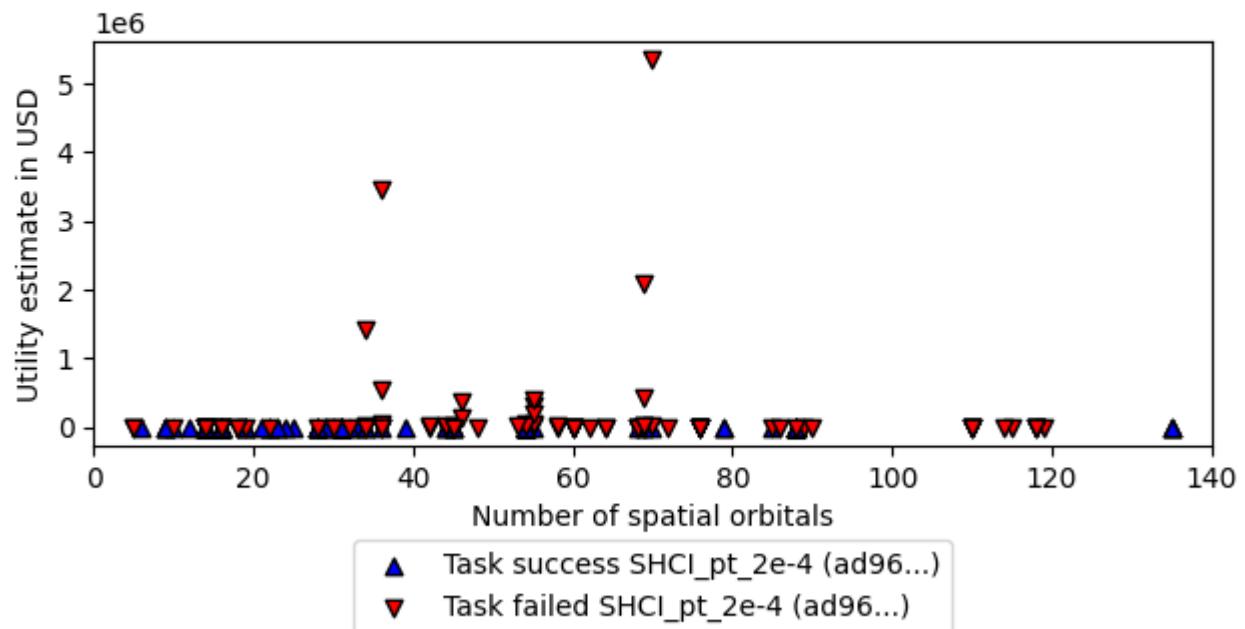
Run time for SHCI_pt_2e-4/ad96...



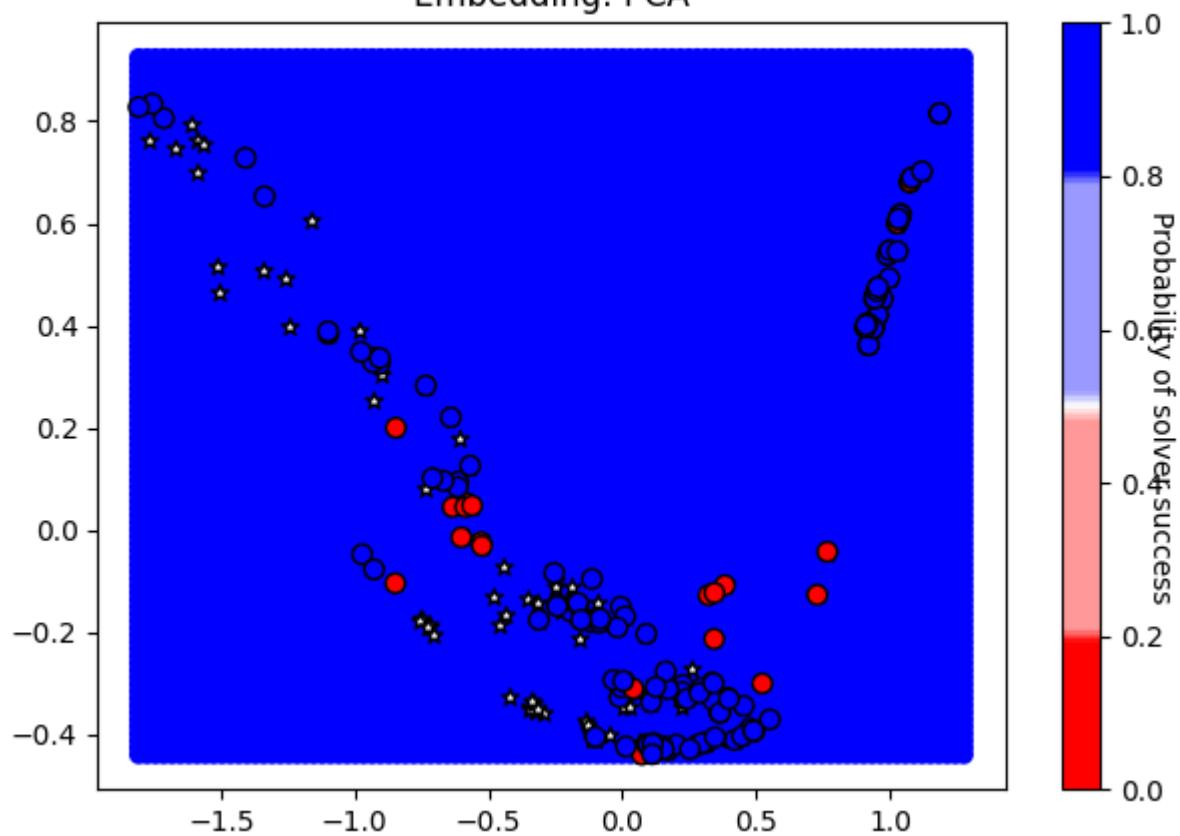
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-4/ad96...

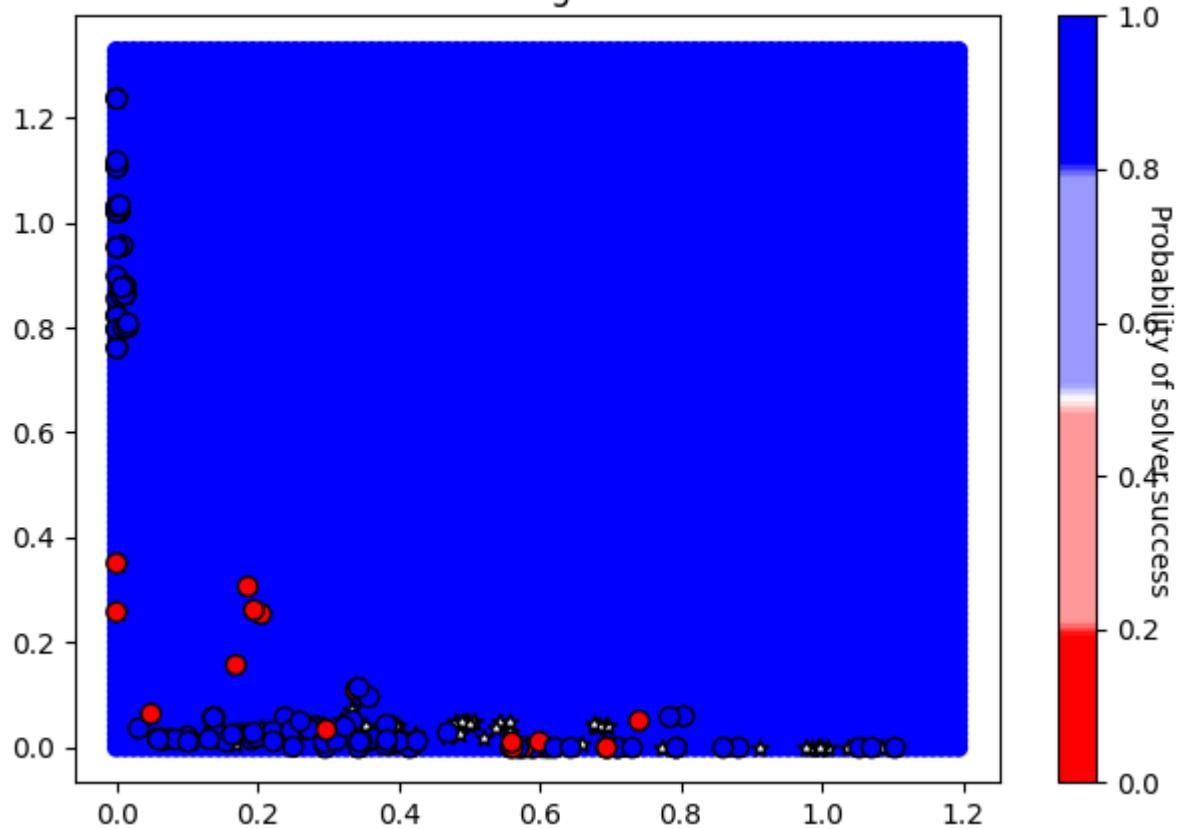
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



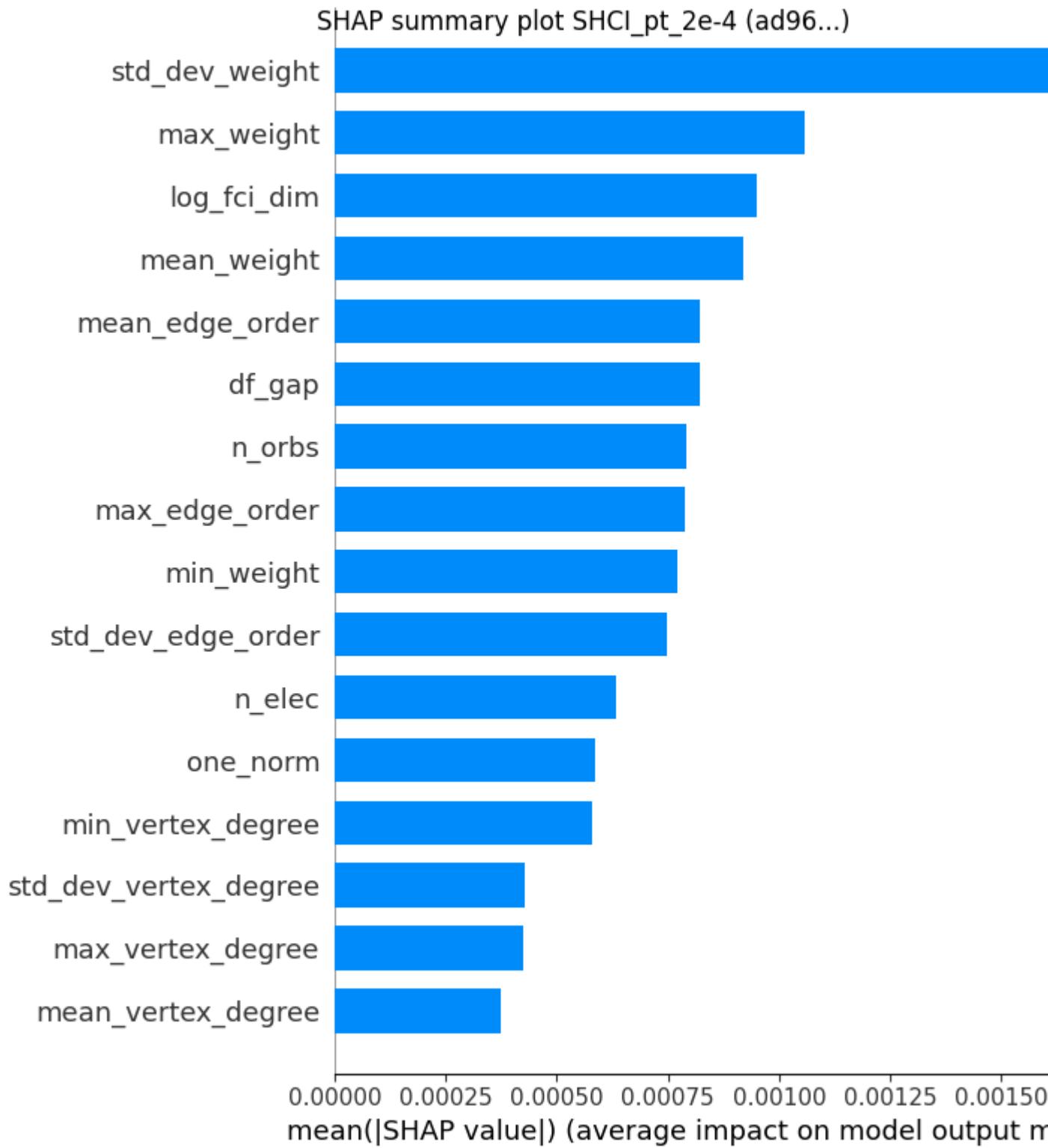
Solver SHCI_pt_2e-4 (ad96...)
Embedding: PCA



Solver SHCI_pt_2e-4 (ad96...)
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.



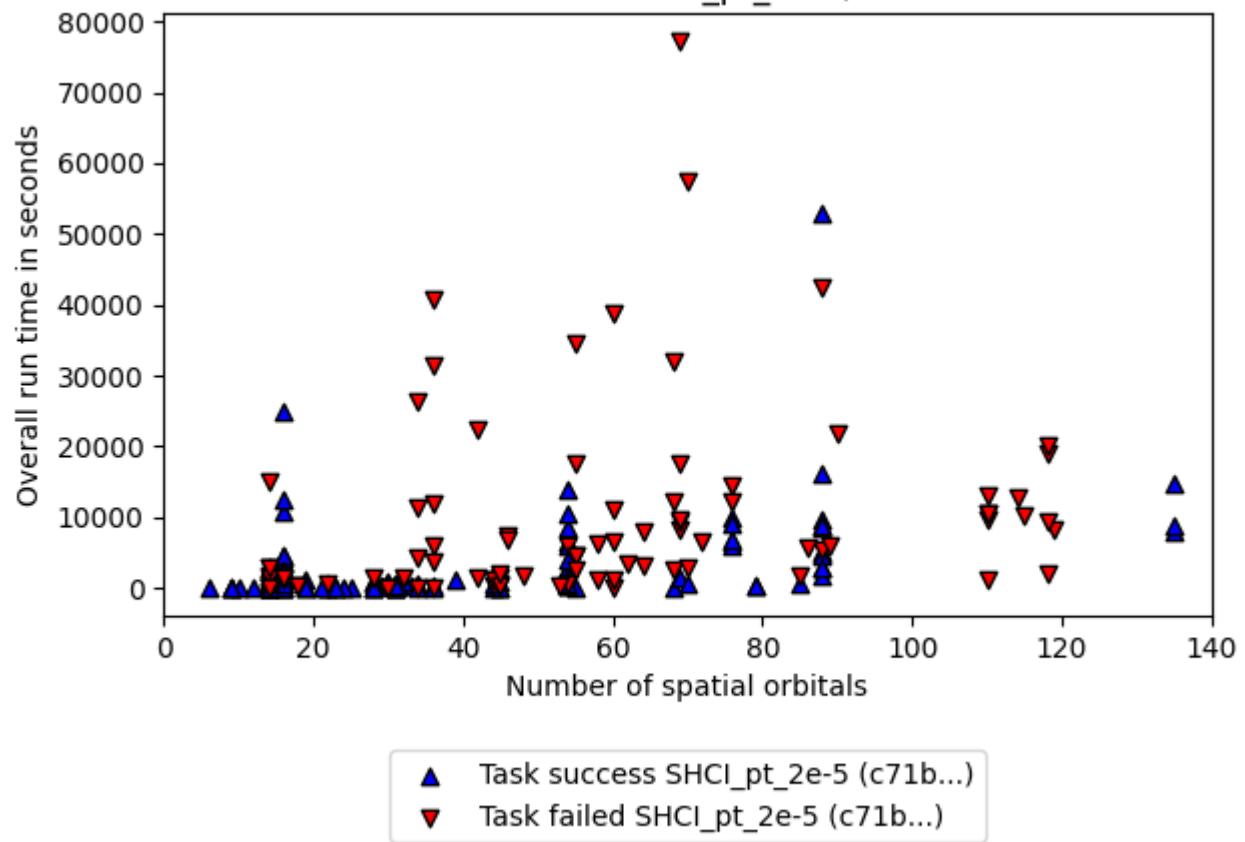
Solver SHCI_pt_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6

solver_uuid:c71b90bd-3250-4c0c-b4e7-fc9878f141f6

solver_short_name:SHCI_pt_2e-5

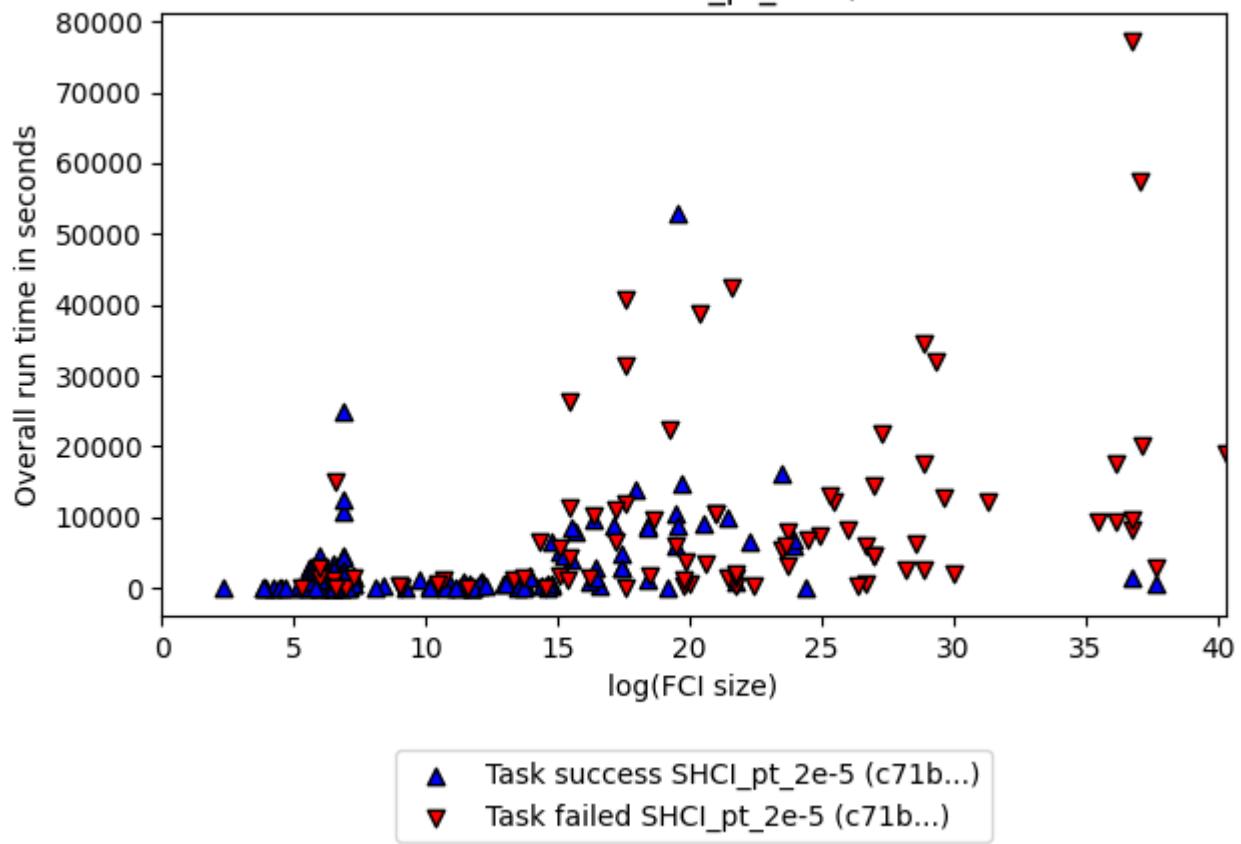
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-5 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: 9a81088b-b64e-4d02-b9c4-7d0b6851cf31
creation.timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.7428571428571429, 0.966789667896679]
ml.metrics_calculator_version: 1

Run time for SHCI_pt_2e-5/c71b...



Note: plot only contains attempted tasks.

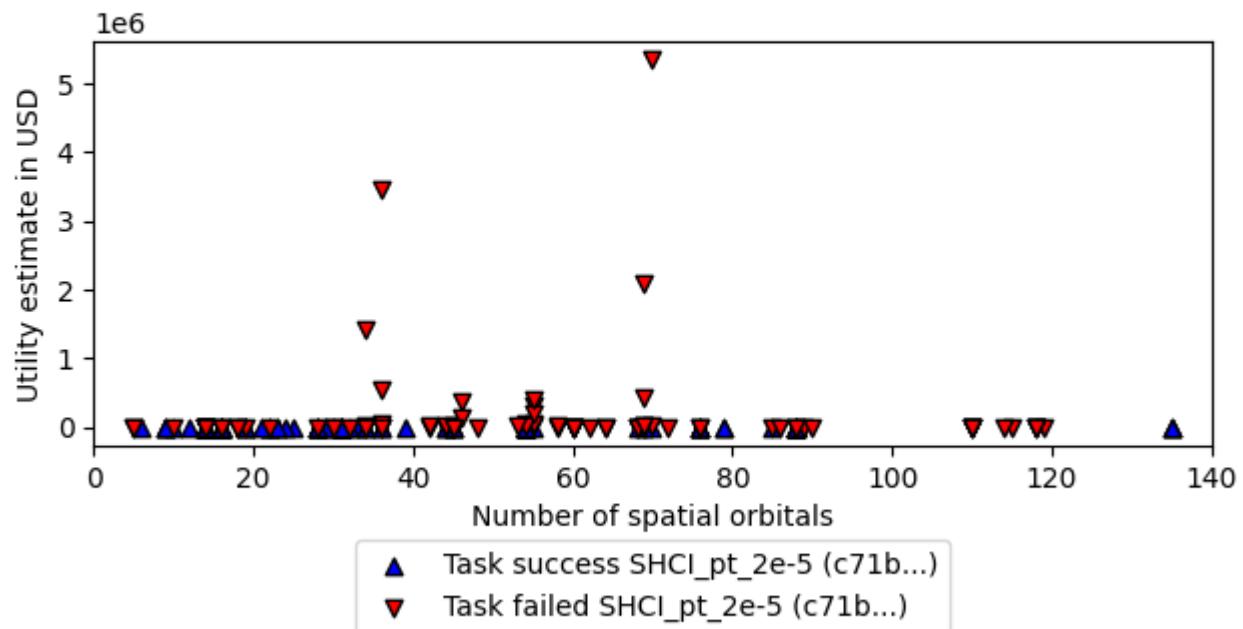
Run time for SHCI_pt_2e-5/c71b...



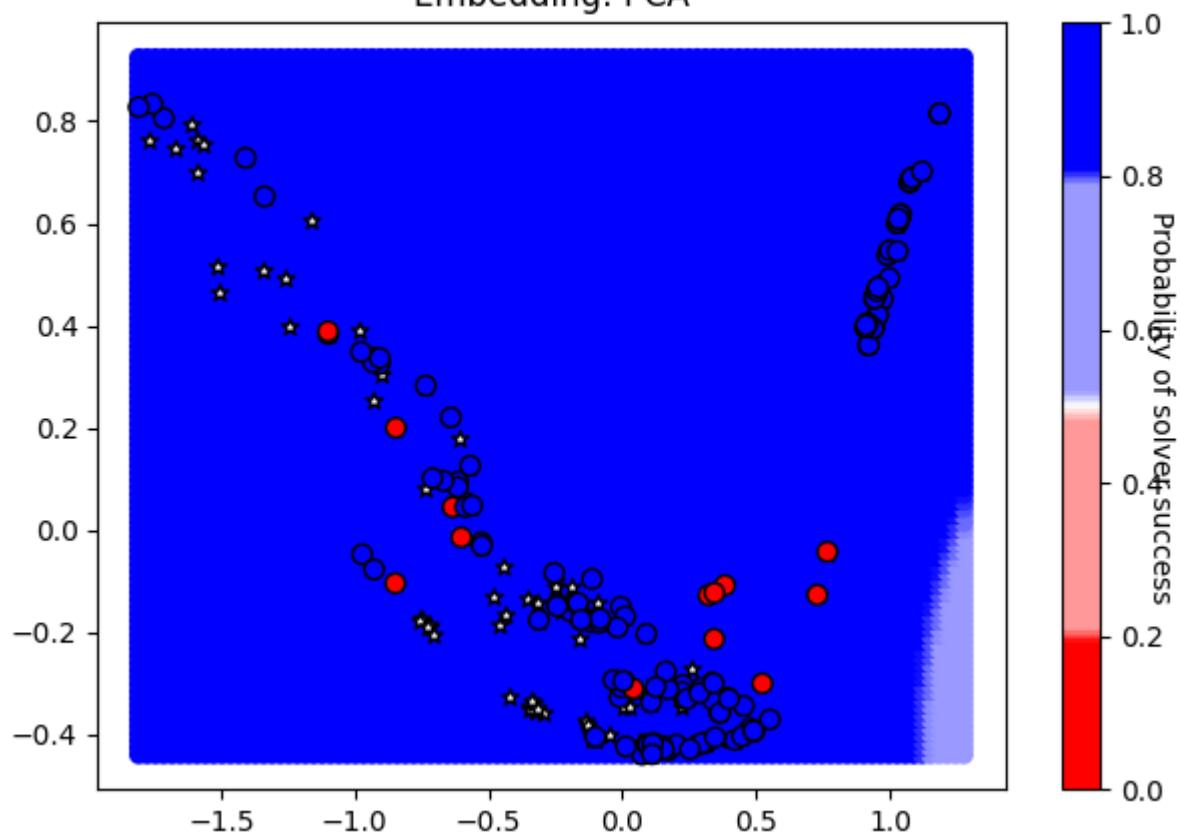
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-5/c71b...

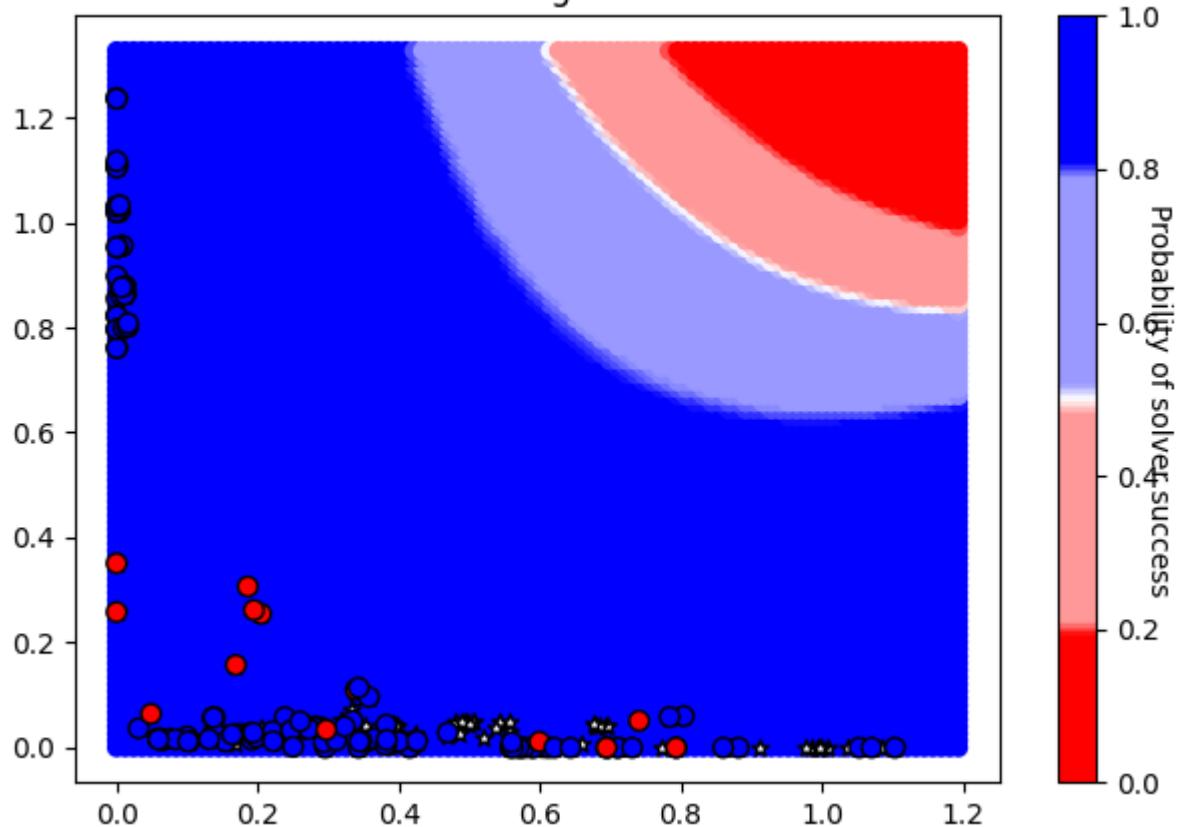
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



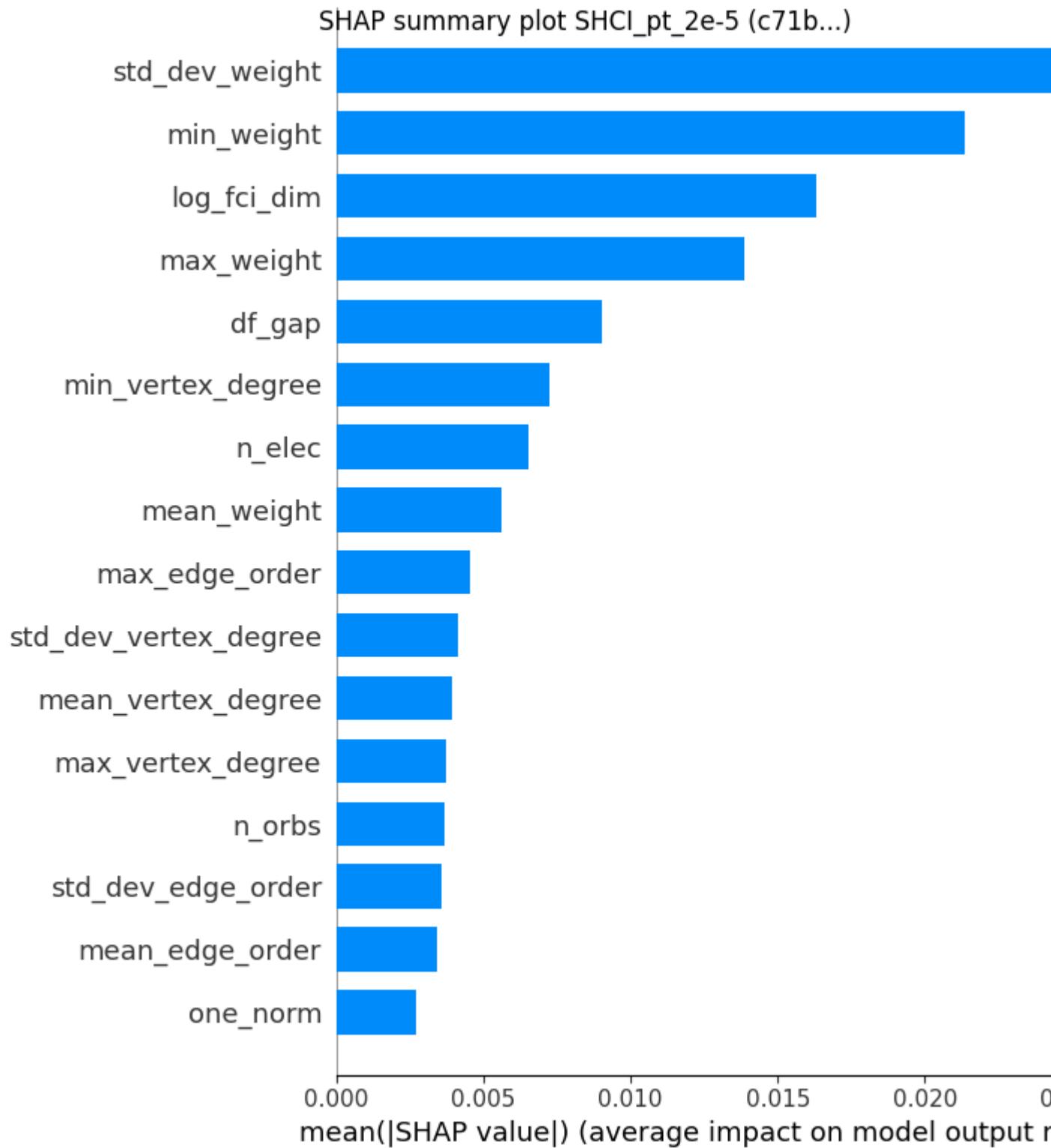
Solver SHCI_pt_2e-5 (c71b...)
Embedding: PCA



Solver SHCI_pt_2e-5 (c71b...)
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.

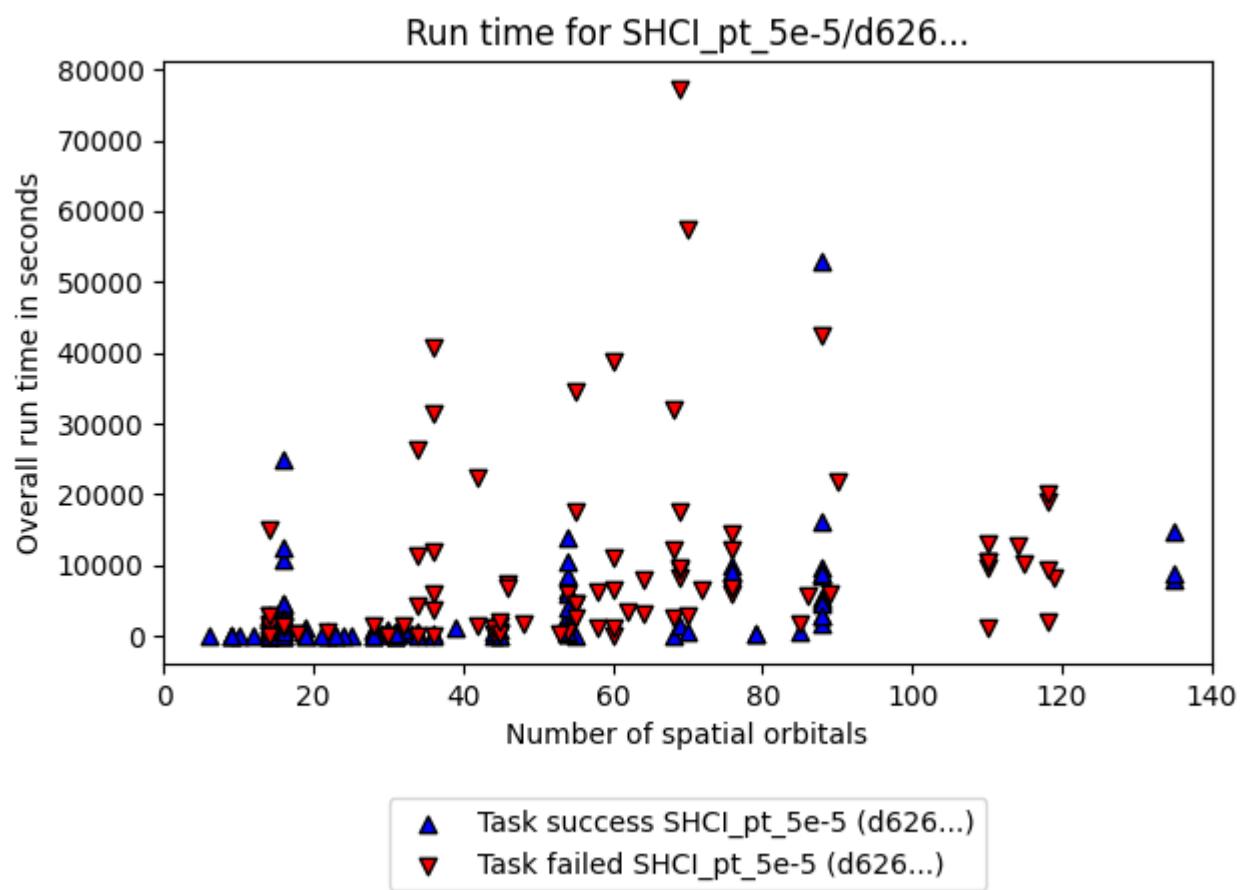


Solver SHCI_pt_5e-5, d626506c-7aae-4ad6-802a-b29af5f2bb93

solver_uuid:d626506c-7aae-4ad6-802a-b29af5f2bb93

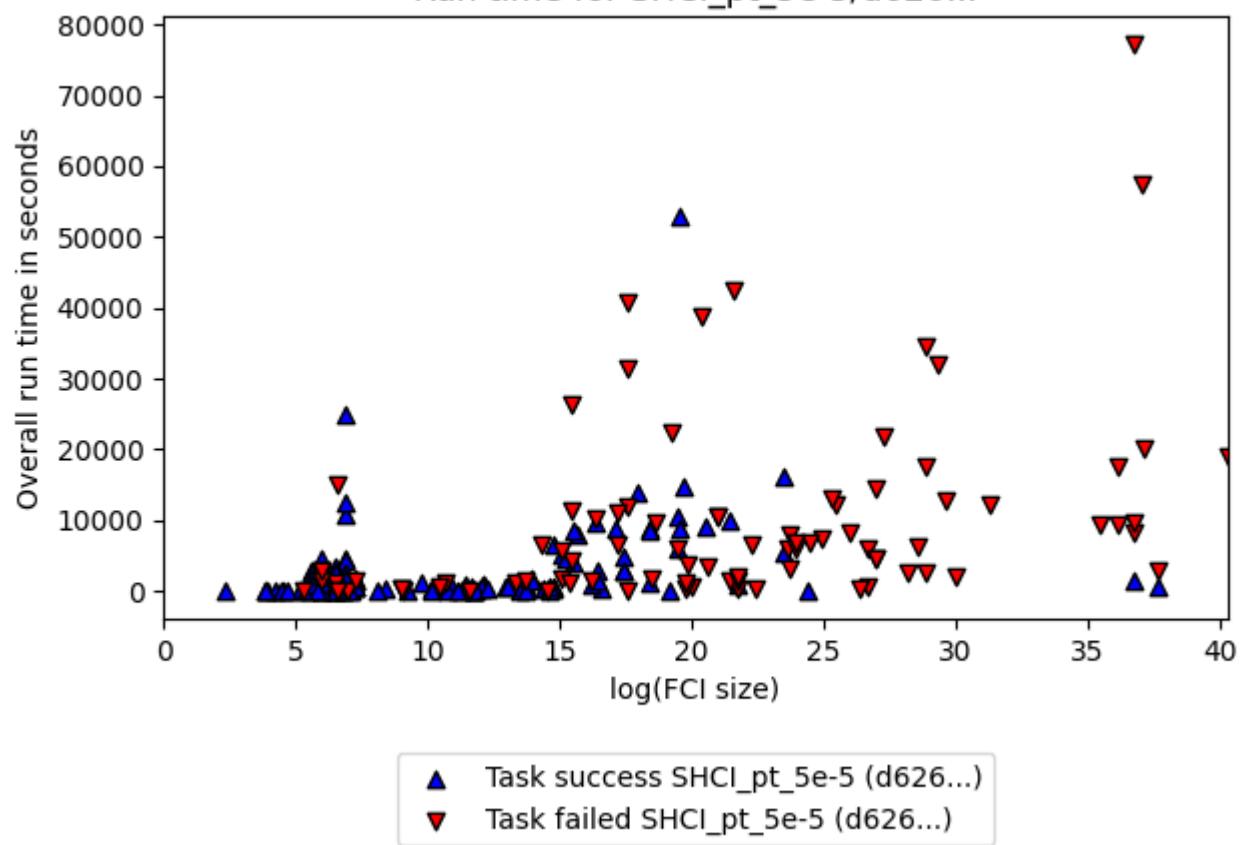
solver_short_name:SHCI_pt_5e-5

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: a96b0ab8-df1a-4eb2-b416-e59b9a1319b6
creation.timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.8, 0.974169741697417]
ml.metrics_calculator_version: 1



Note: plot only contains attempted tasks.

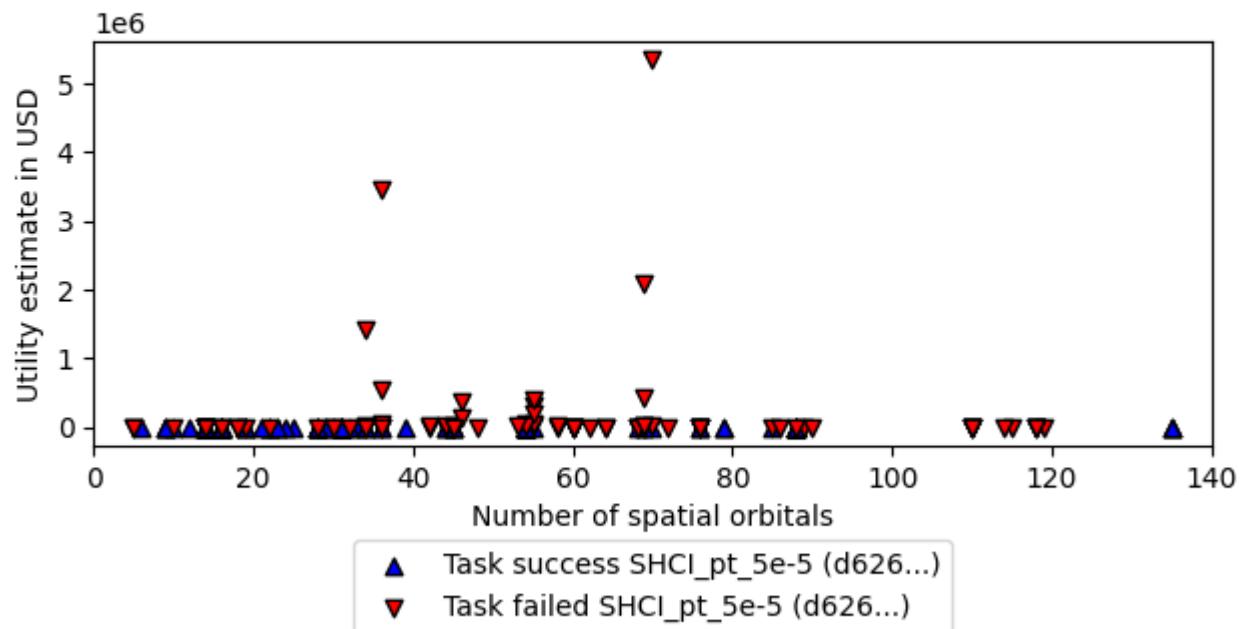
Run time for SHCI_pt_5e-5/d626...



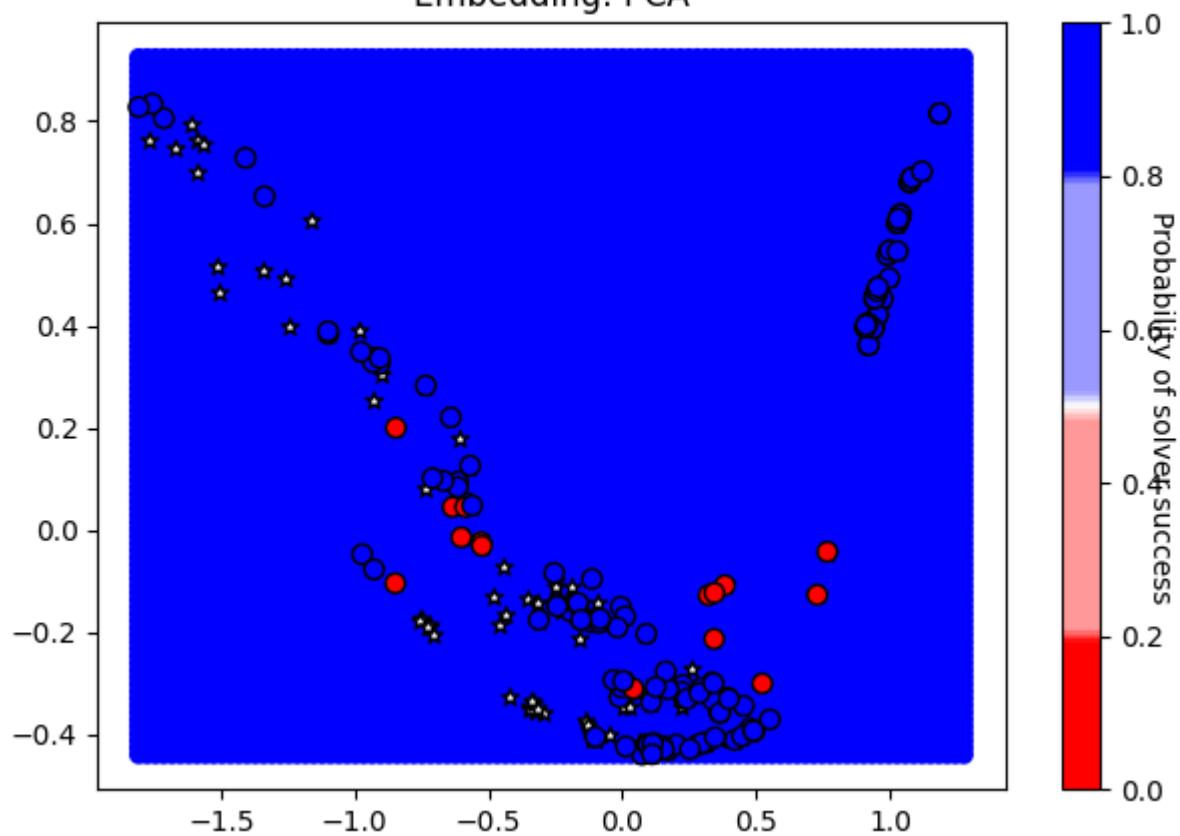
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_5e-5/d626...

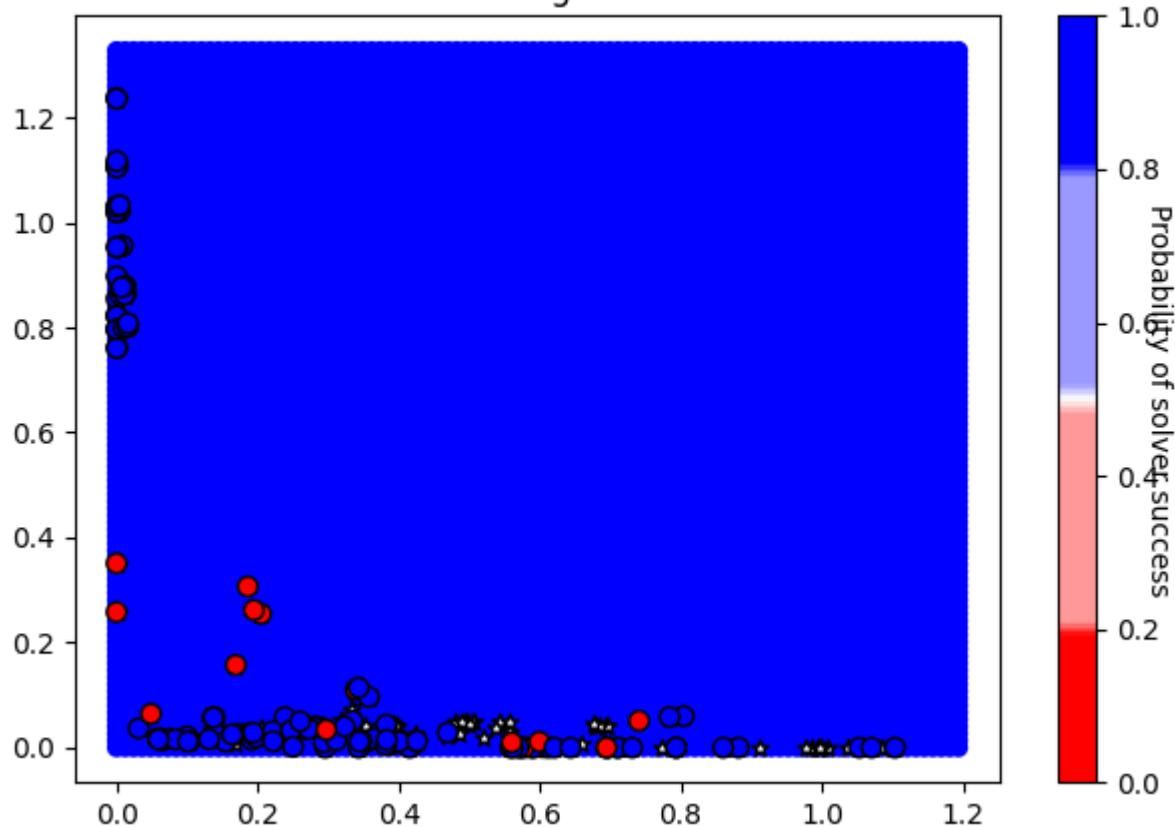
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



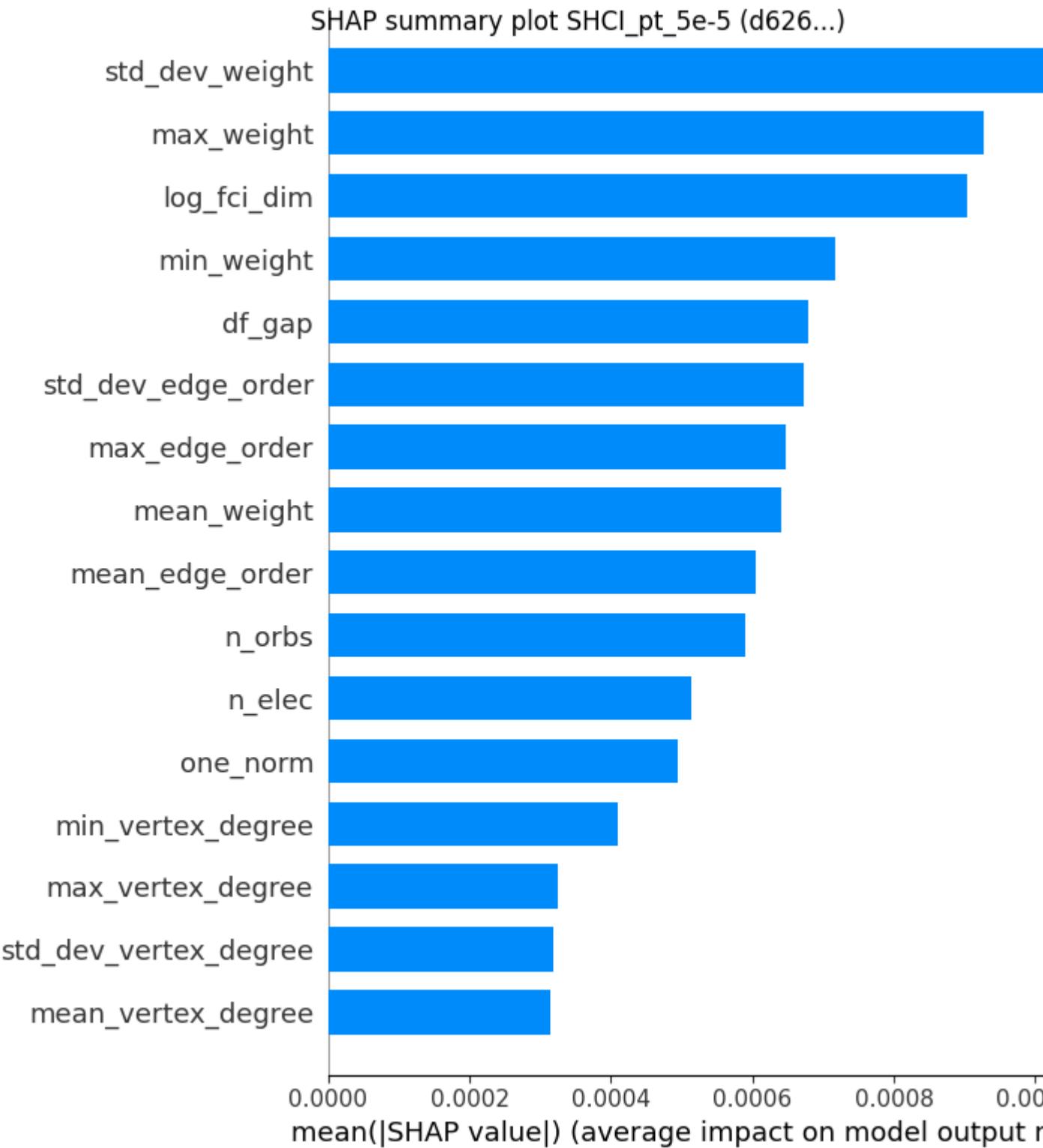
Solver SHCI_pt_5e-5 (d626...)
Embedding: PCA



Solver SHCI_pt_5e-5 (d626...)
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.

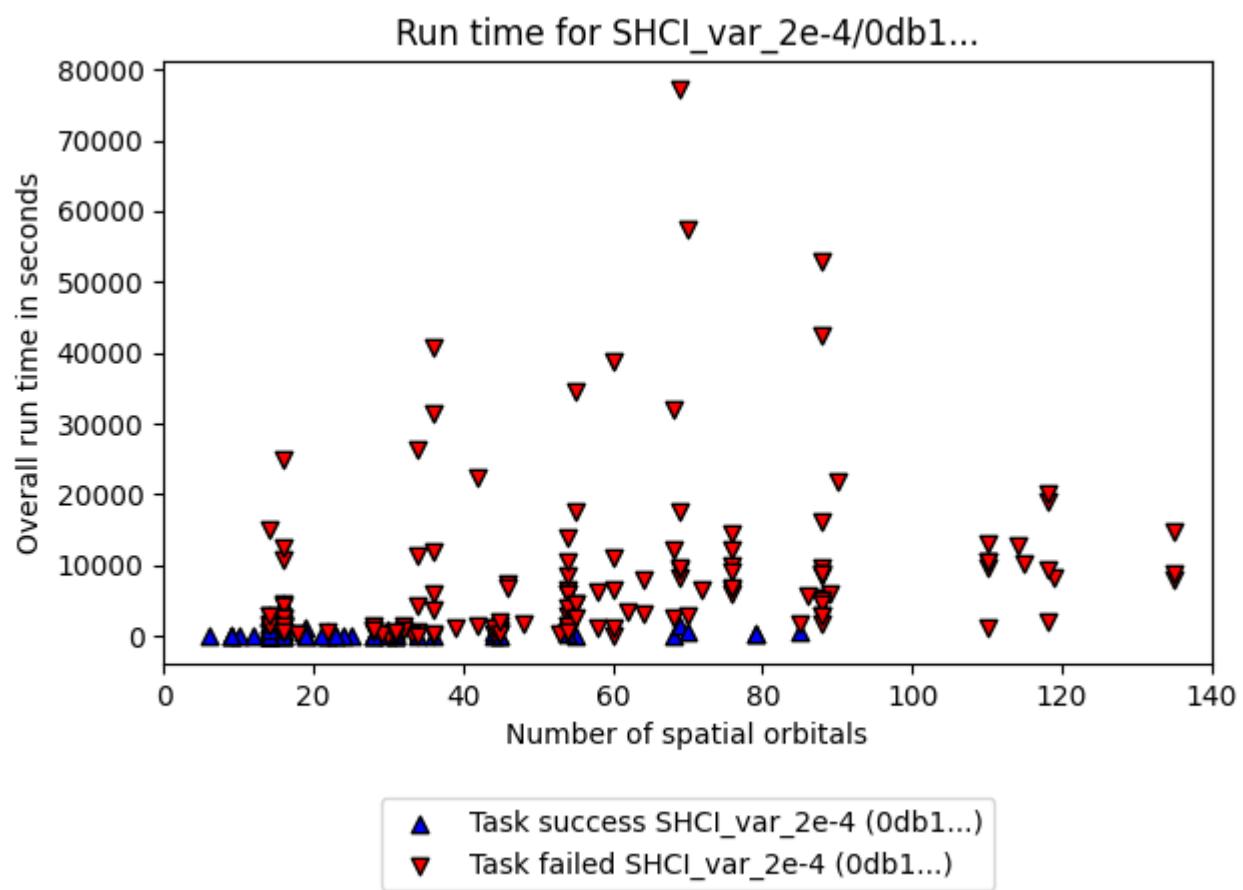


Solver SHCI_var_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a

solver_uuid:0db183e3-a86d-491b-9125-599556e37c7a

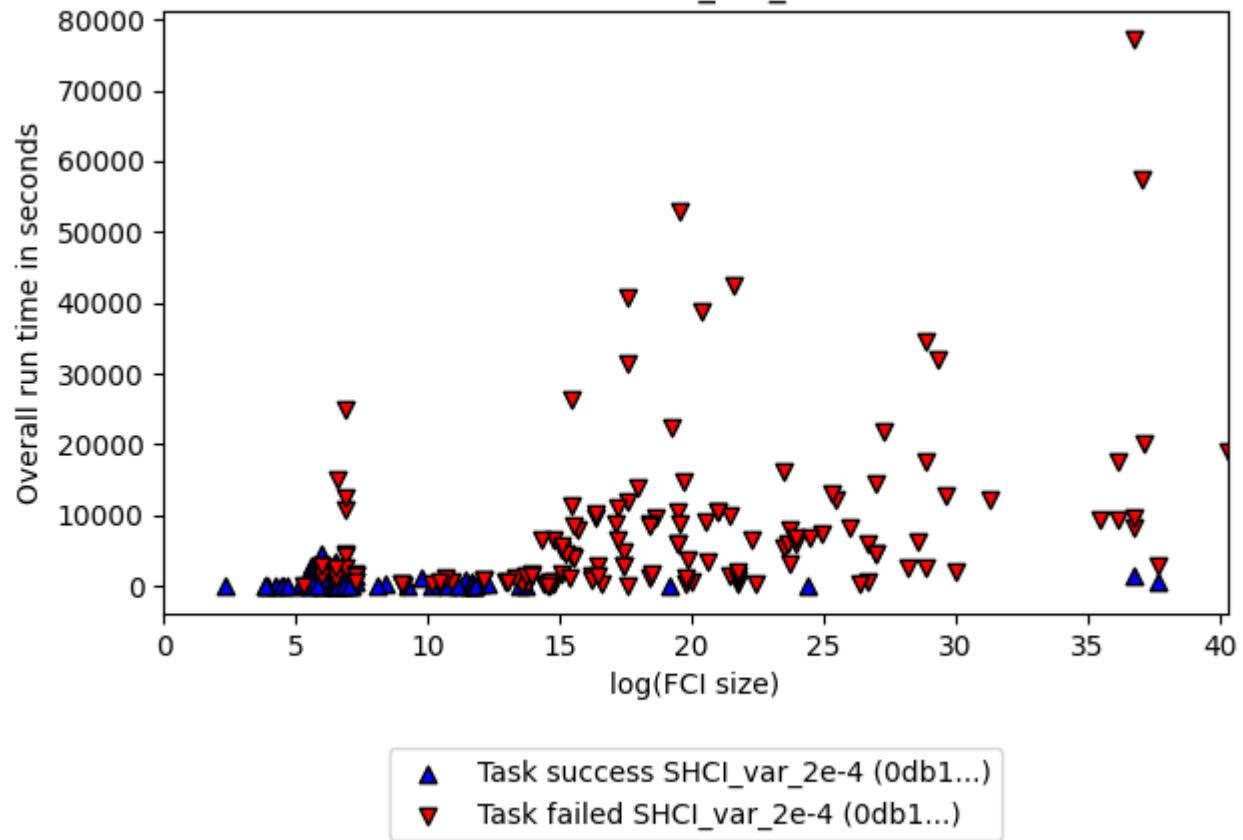
solver_short_name:SHCI_var_2e-4

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: 56a31017-d890-4943-86fb-75ca6082630f
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9863013698630136, 0.9875]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

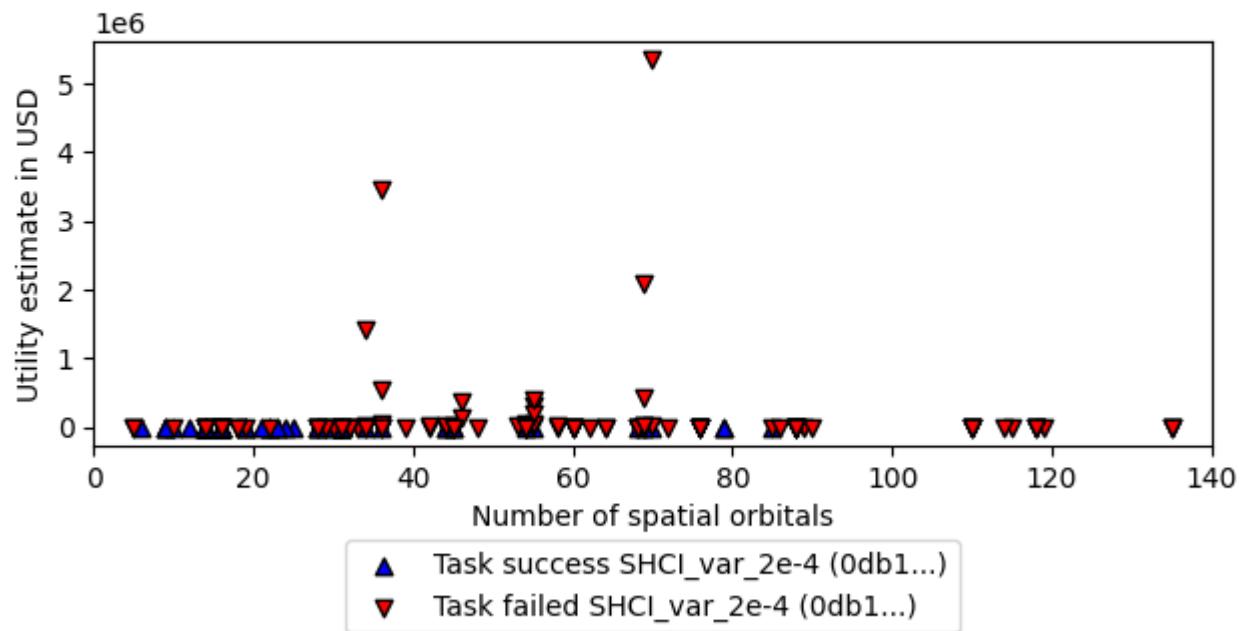
Run time for SHCI_var_2e-4/0db1...



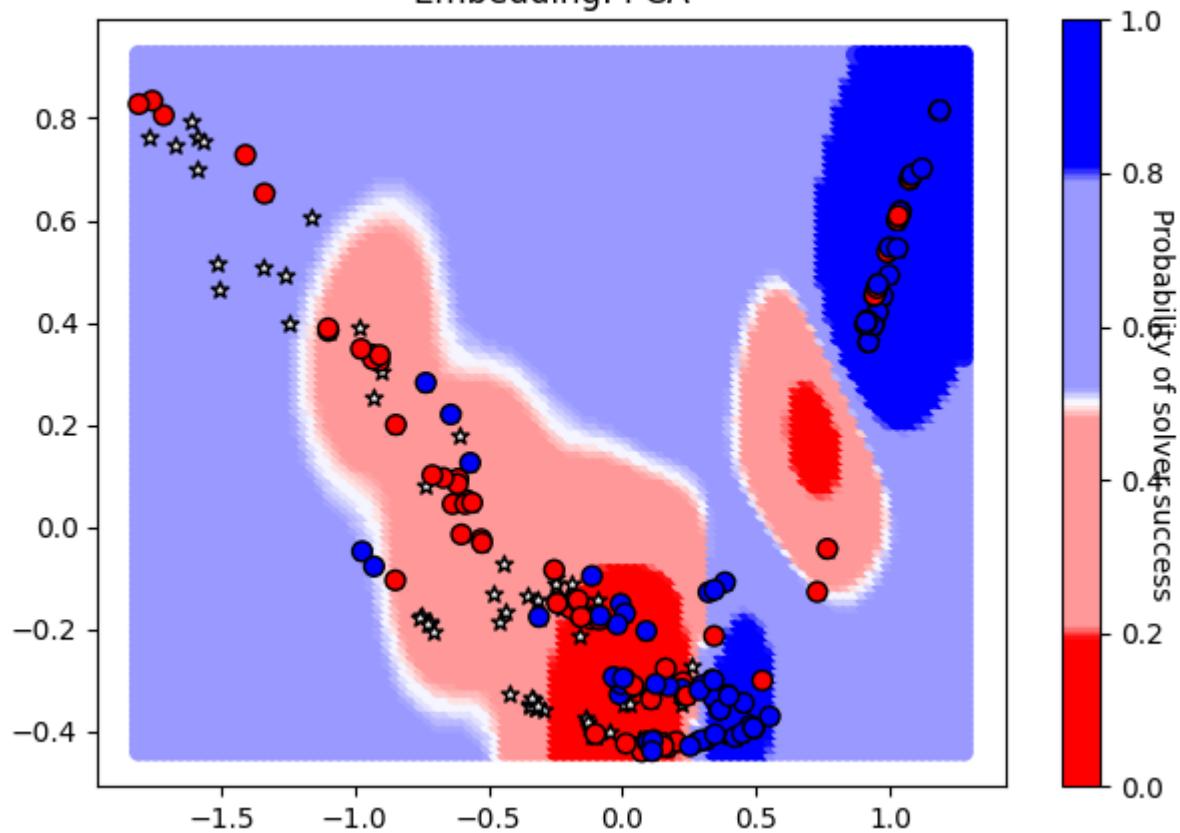
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_2e-4/0db1...

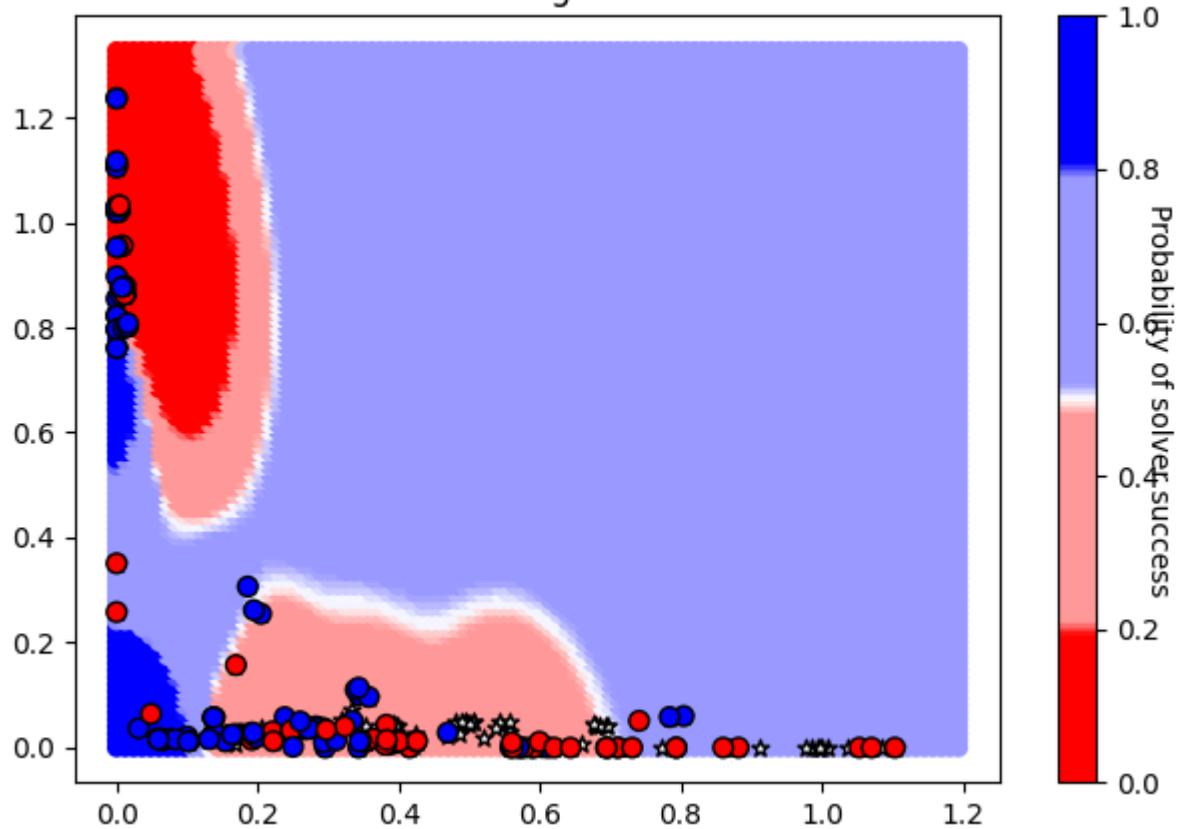
(captured: $\$8.6\text{e+}01/1.5\text{e+}07$, approximately $5.8\text{e-}04\%$)



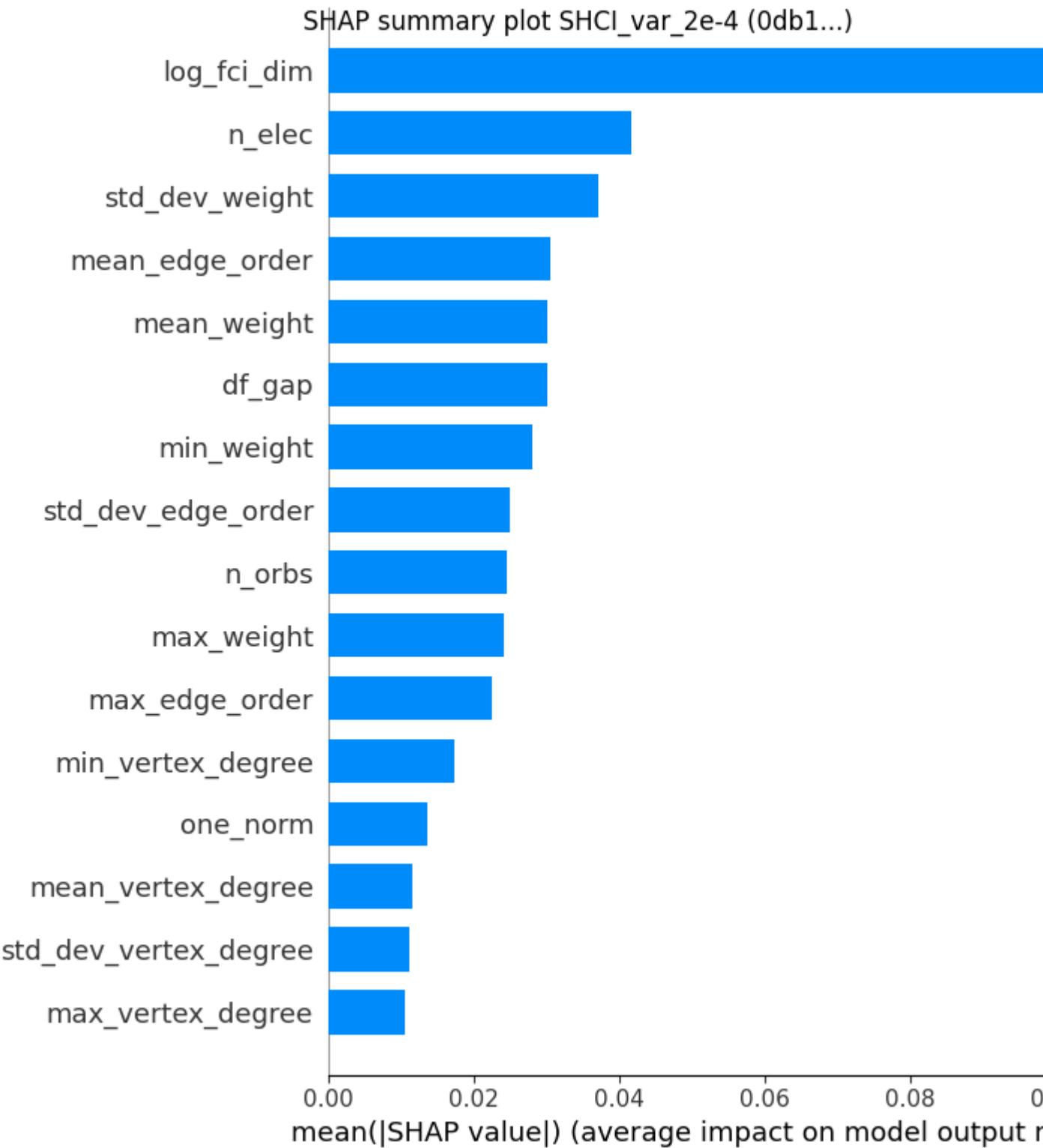
Solver SHCI_var_2e-4 (0db1...)
Embedding: PCA



Solver SHCI_var_2e-4 (0db1...)
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.

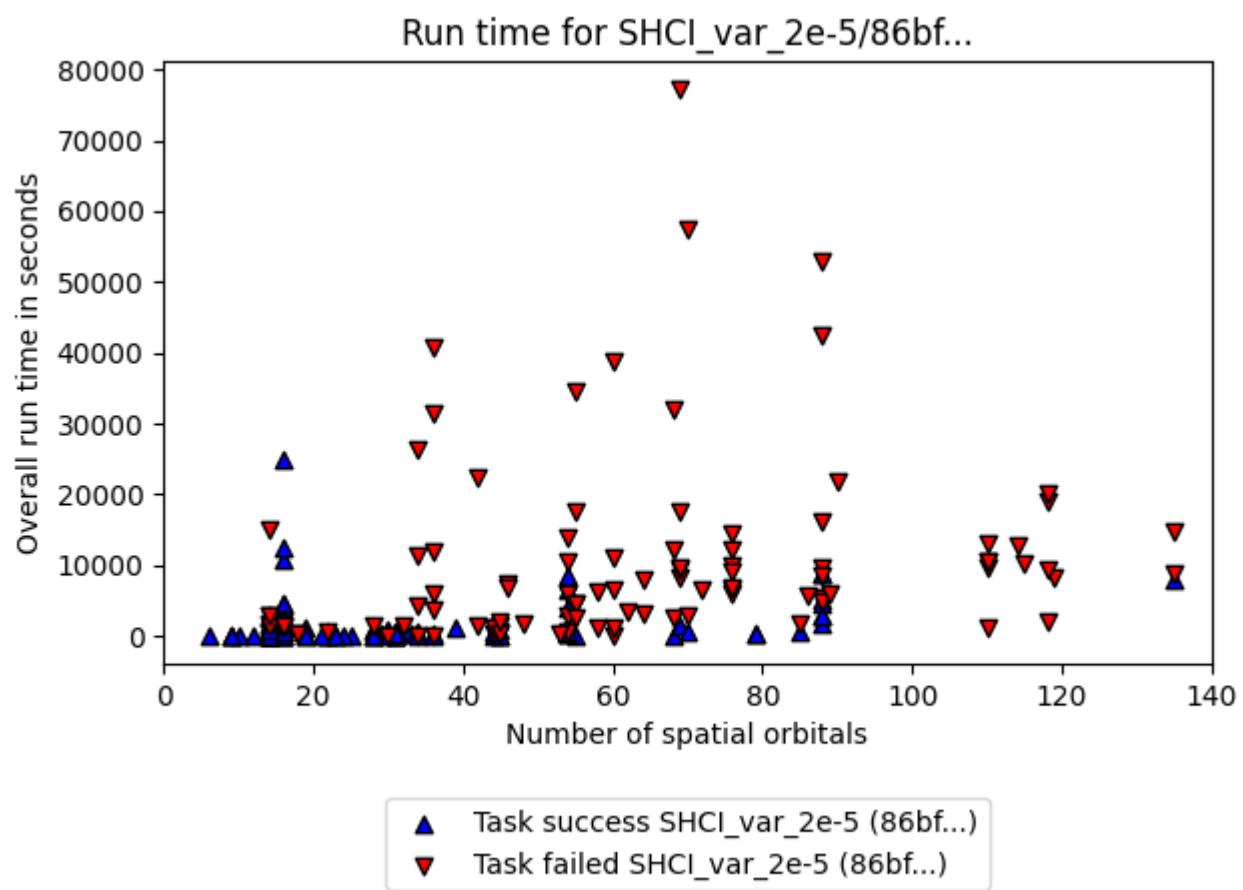


Solver SHCI_var_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688

solver_uuid:86bfe50c-9342-4d54-bb68-abc8abd95688

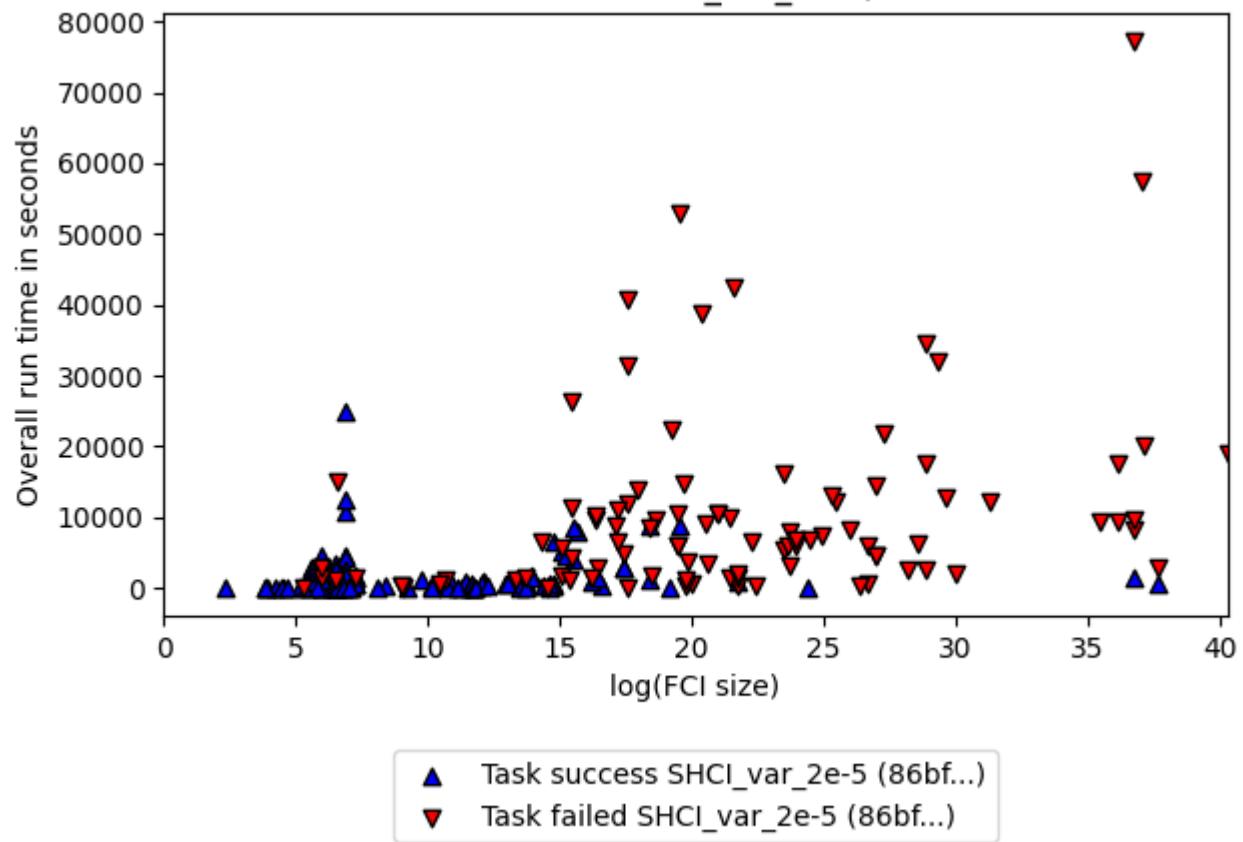
solver_short_name:SHCI_var_2e-5

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: 9e54ad24-0fc1-4e4c-b4bd-c26eca0471c7
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.819672131147541, 0.9551020408163265]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

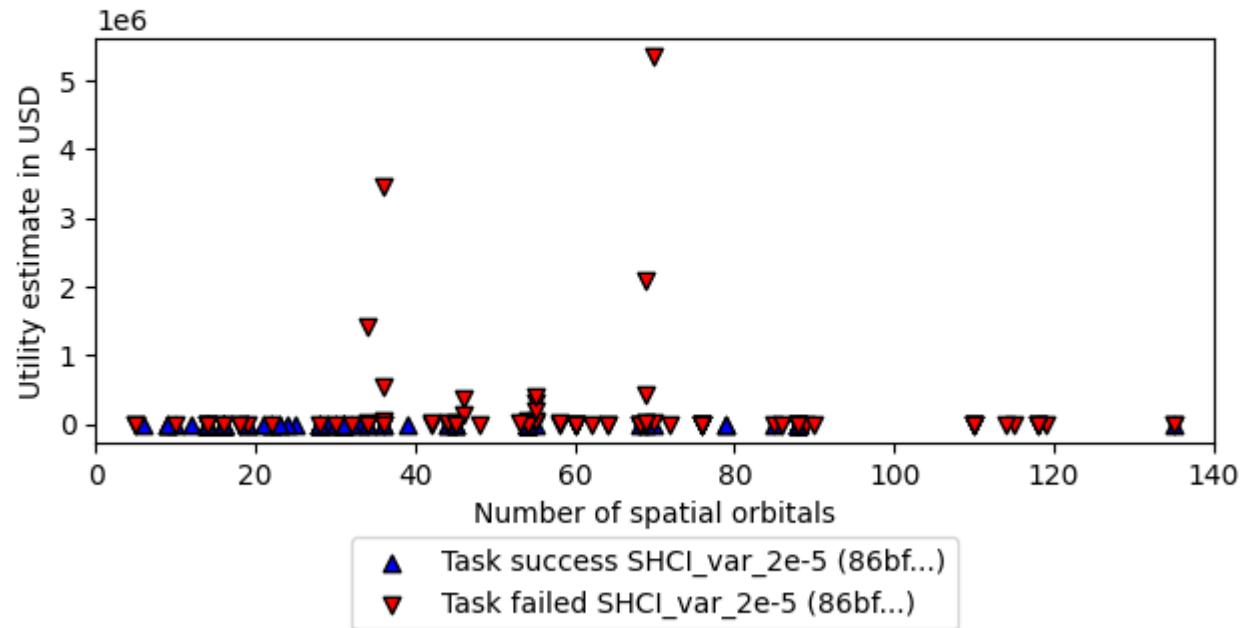
Run time for SHCI_var_2e-5/86bf...



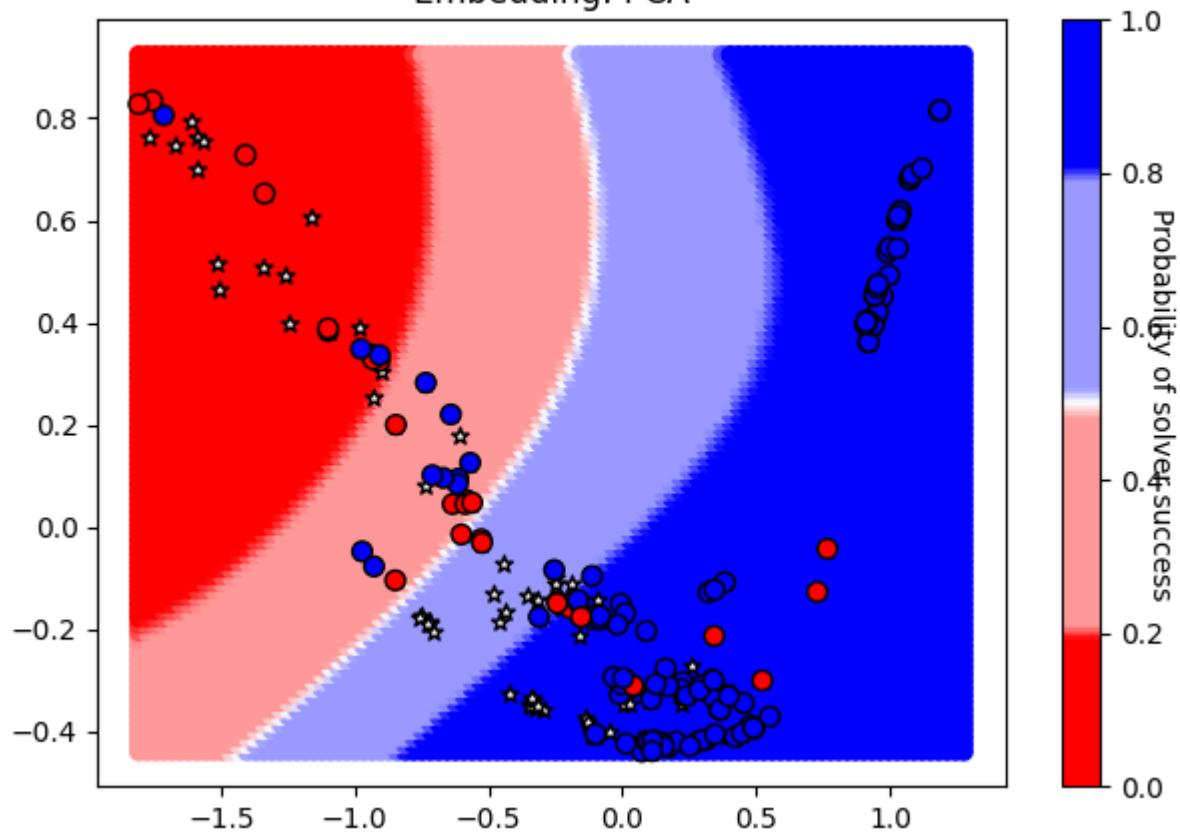
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_2e-5/86bf...

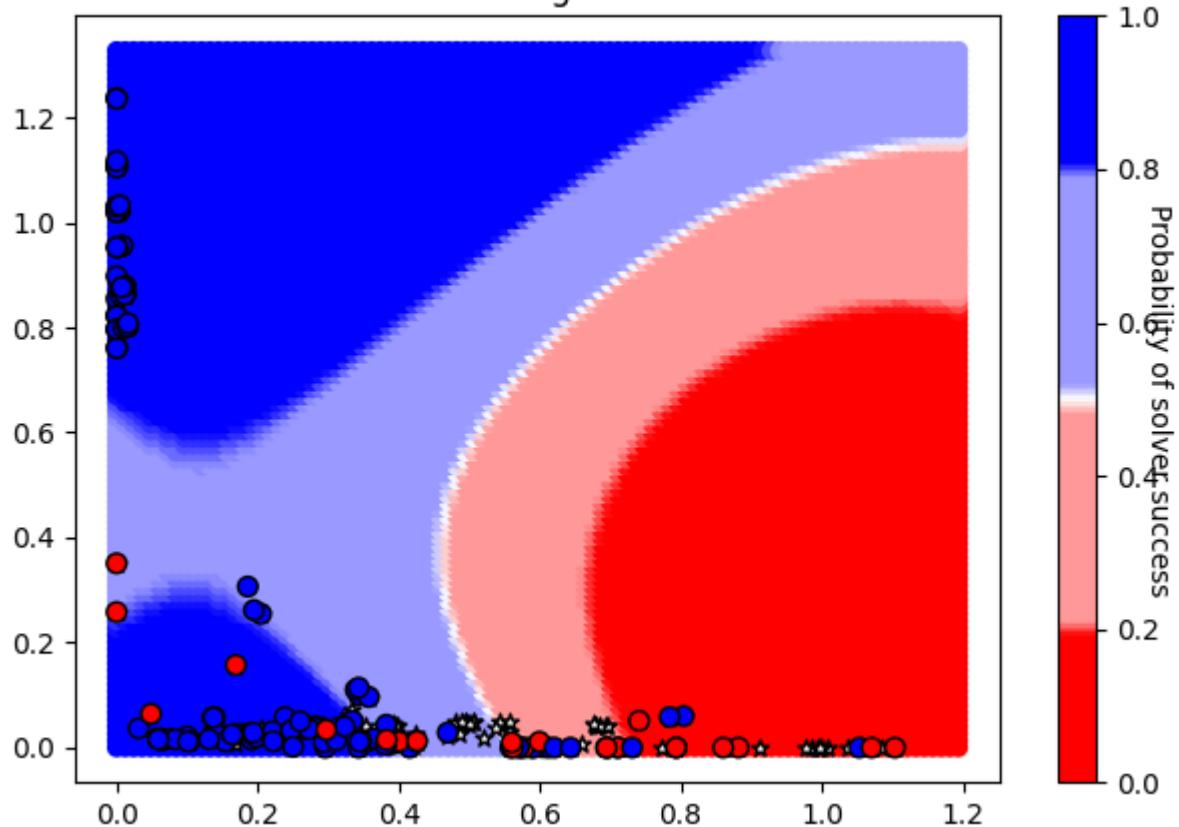
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



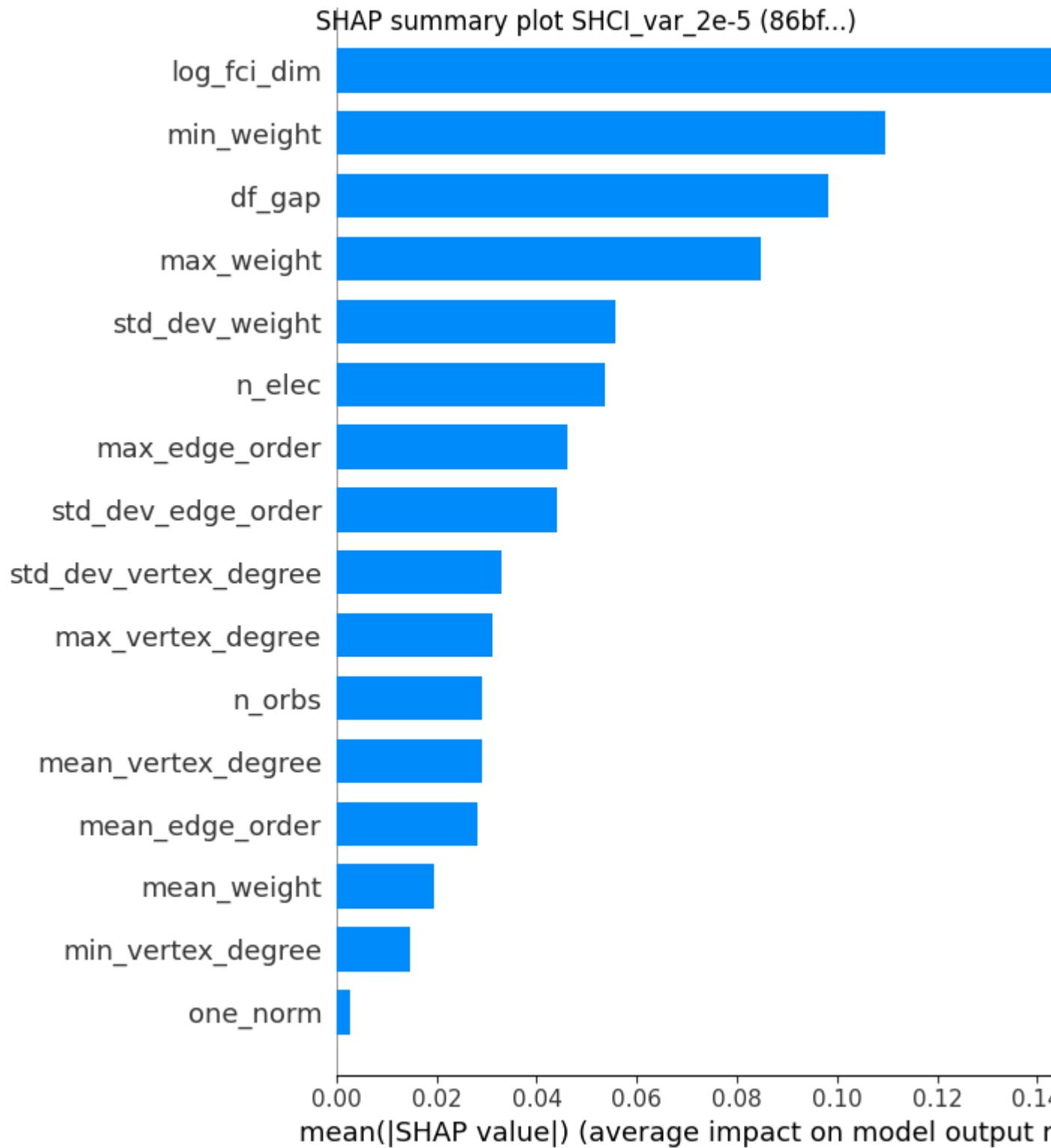
Solver SHCI_var_2e-5 (86bf...)
Embedding: PCA



Solver SHCI_var_2e-5 (86bf...)
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.

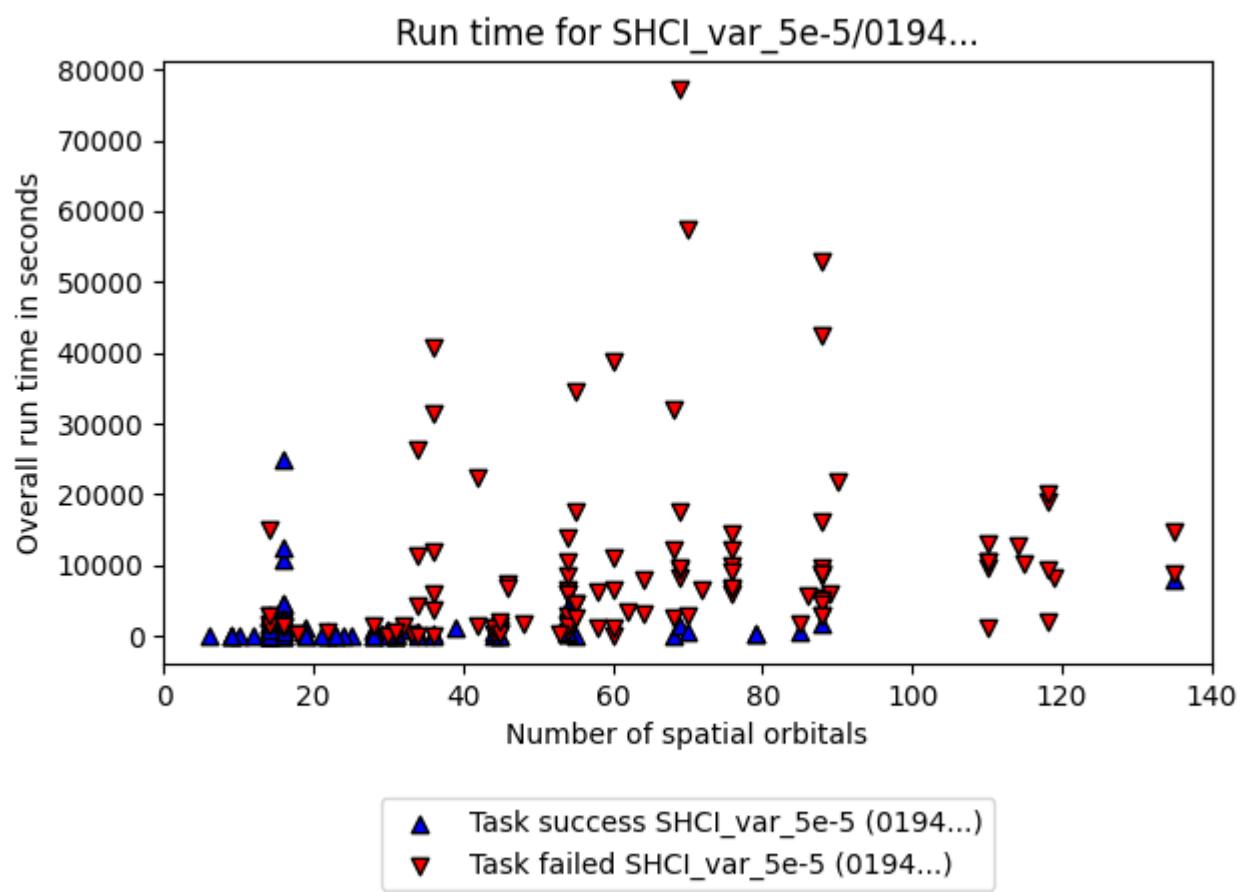


Solver SHCI_var_5e-5, 01949b95-c427-4693-9134-01f47f688c09

solver_uuid:01949b95-c427-4693-9134-01f47f688c09

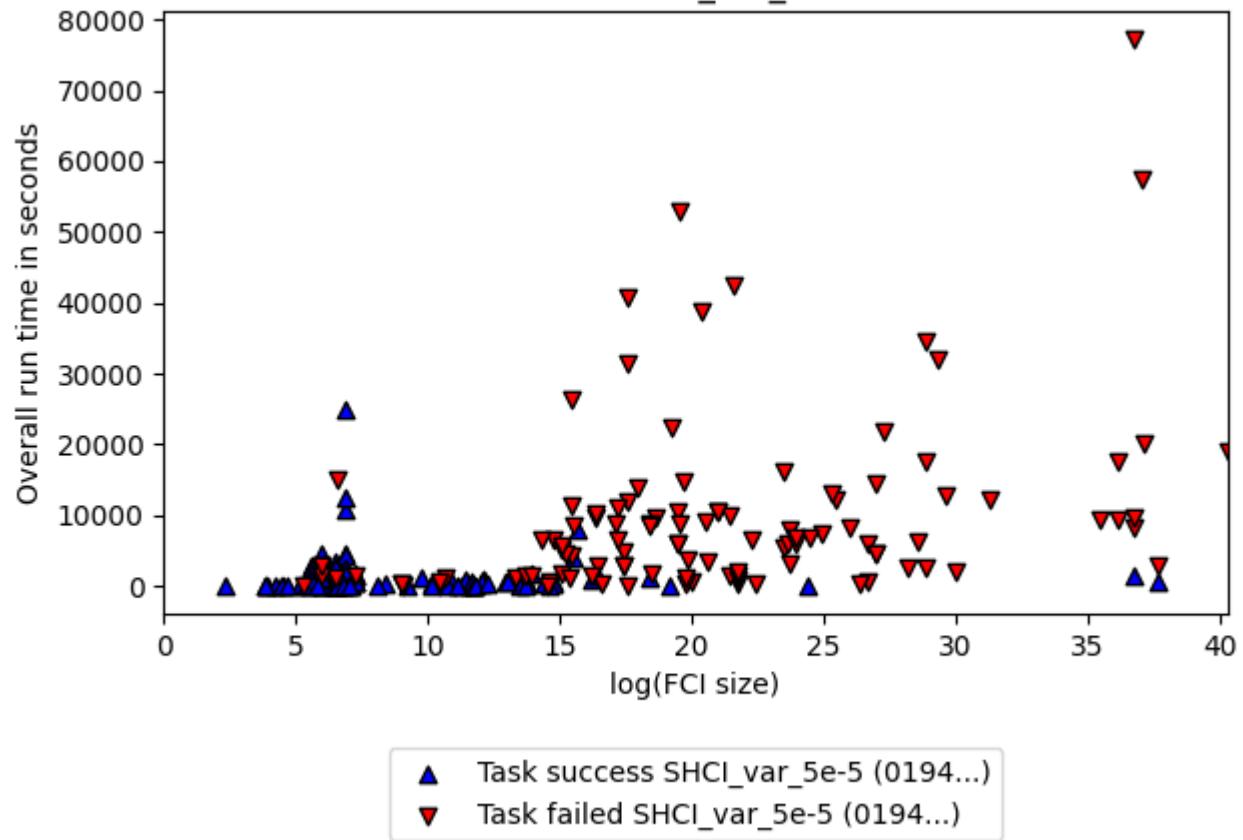
solver_short_name:SHCI_var_5e-5

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: e358ea63-9007-4322-ab6f-0c8b7df21d80
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9545454545454546, 0.981651376146789]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

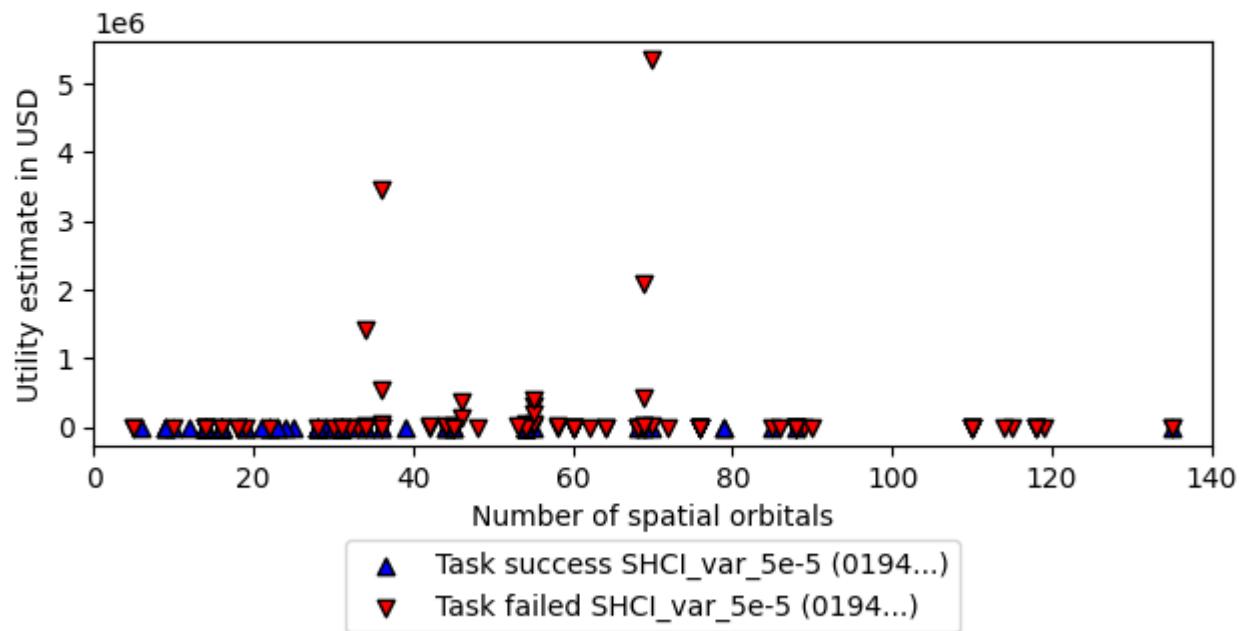
Run time for SHCI_var_5e-5/0194...



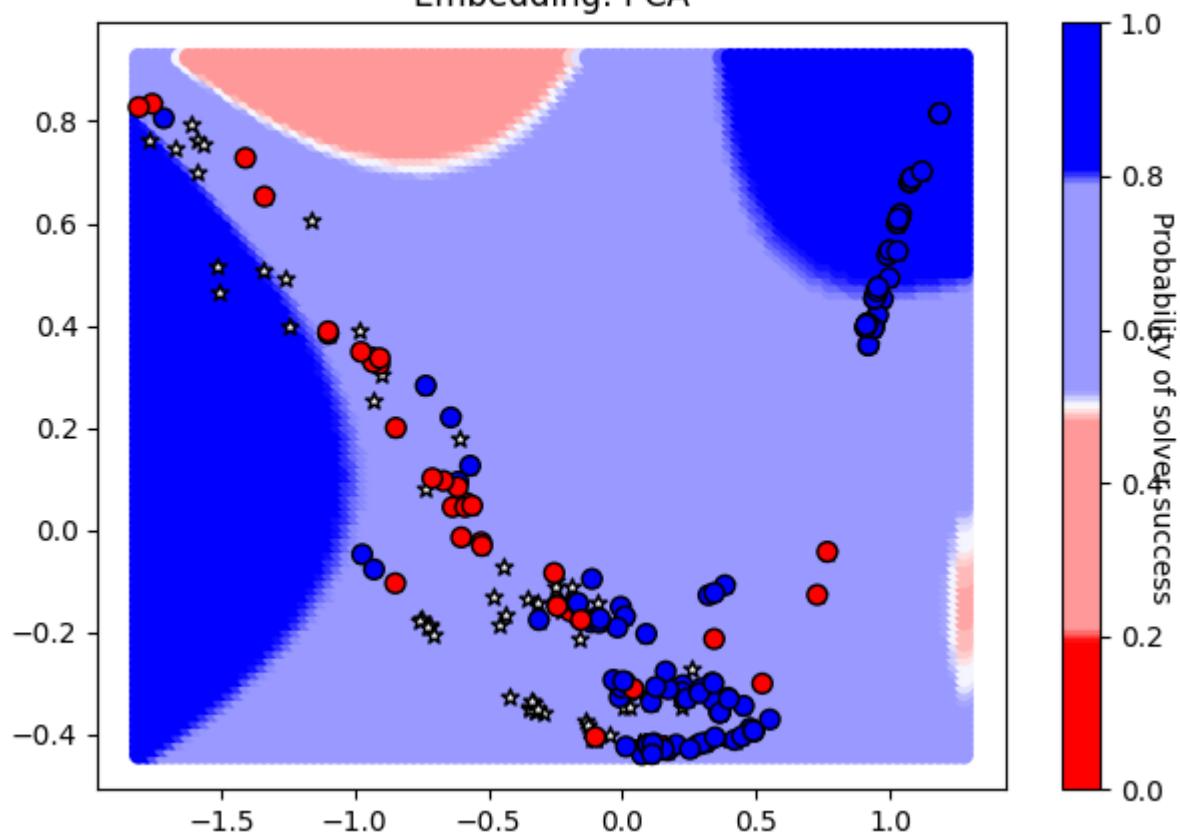
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_5e-5/0194...

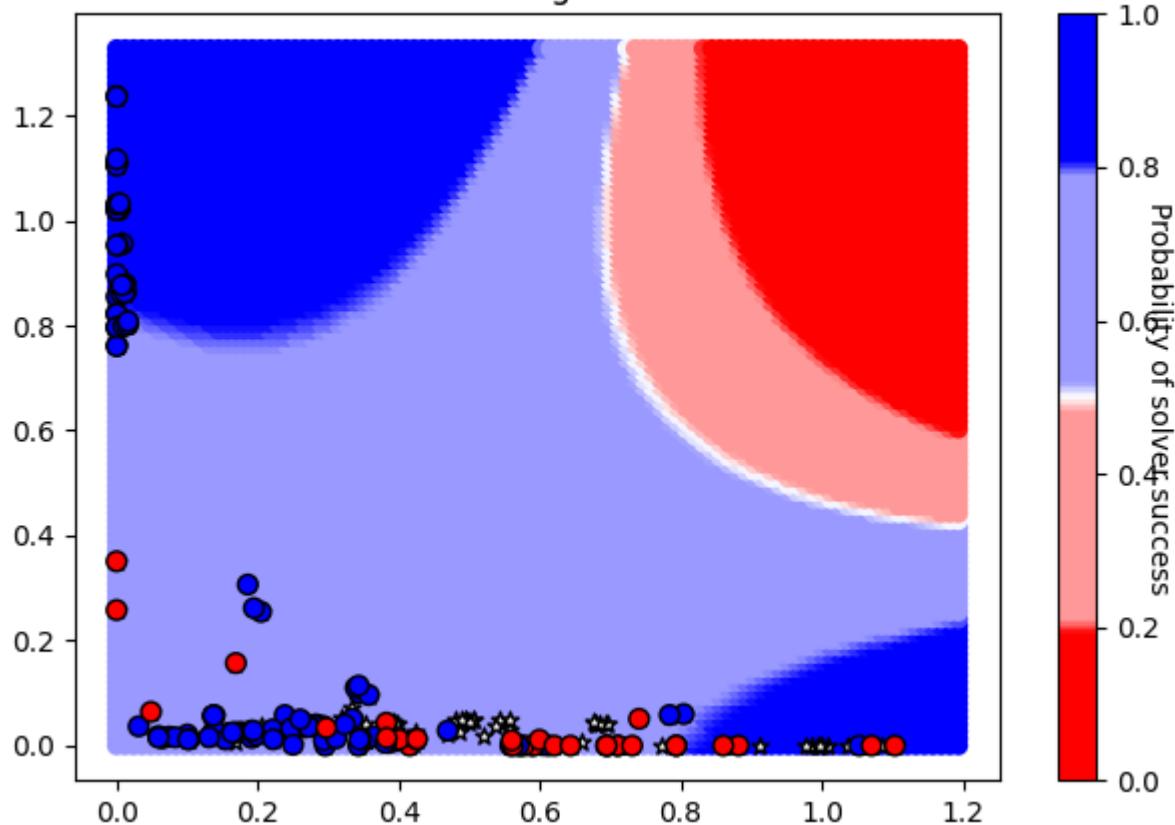
(captured: $\$4.5\text{e+}02/1.5\text{e+}07$, approximately $3.0\text{e-}03\%$)



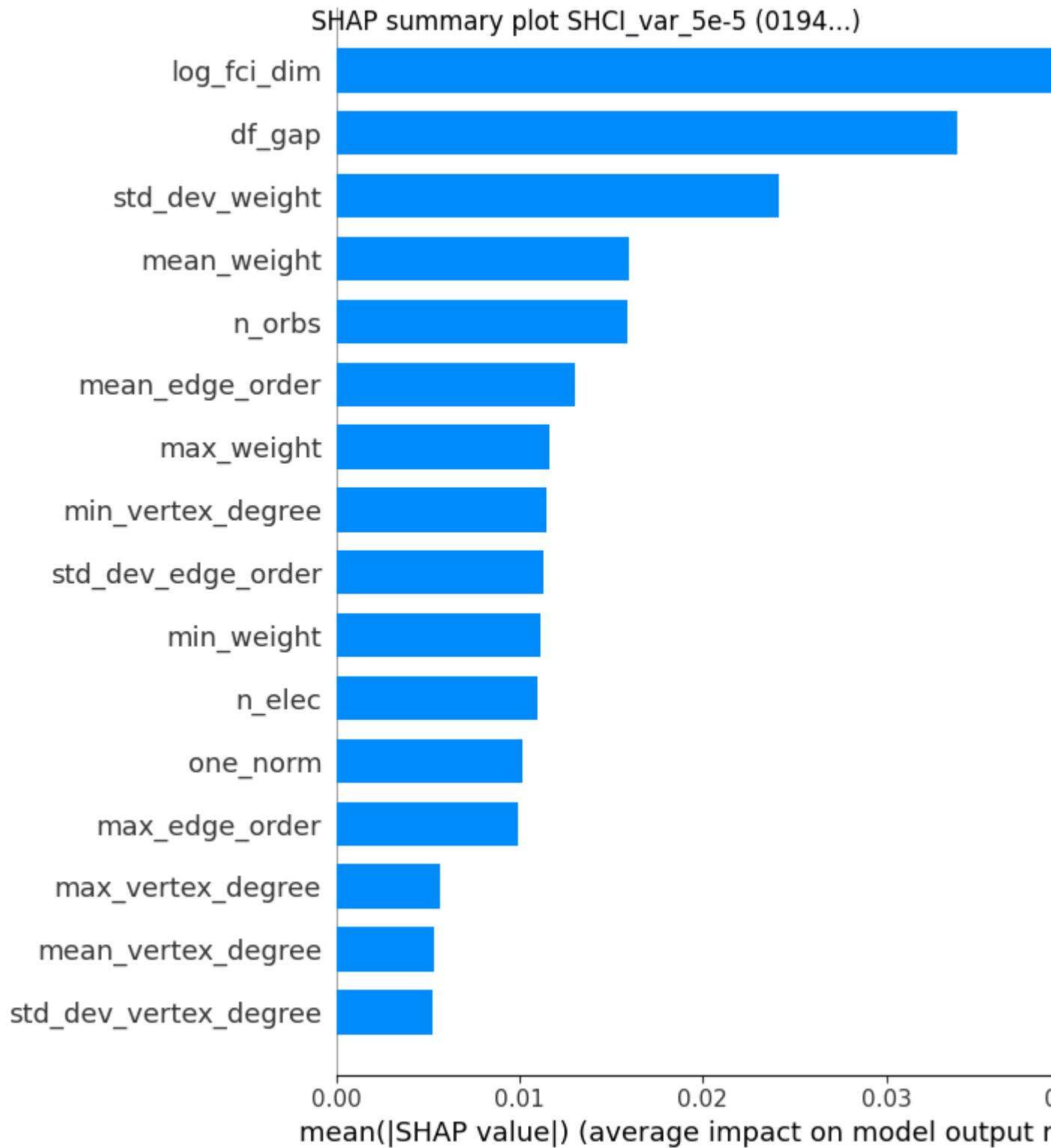
Solver SHCI_var_5e-5 (0194...)
Embedding: PCA



Solver SHCI_var_5e-5 (0194...)
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, 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, 'parallelize_shots': False}}

logical_resource_estimate_solution_uuid:21b3da35-cc33-454b-bd67-8b2f50953c9a

logical_resource_estimate_solver_uuid:f2d73e1f-3058-43c4-a634-b6c267c84ff1

performance_metrics_uuid: e545f69c-ef6b-4378-8054-208d91536cae

creation_timestamp: 2025-03-06T19:54:13.195807+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: 1394068547267.4111

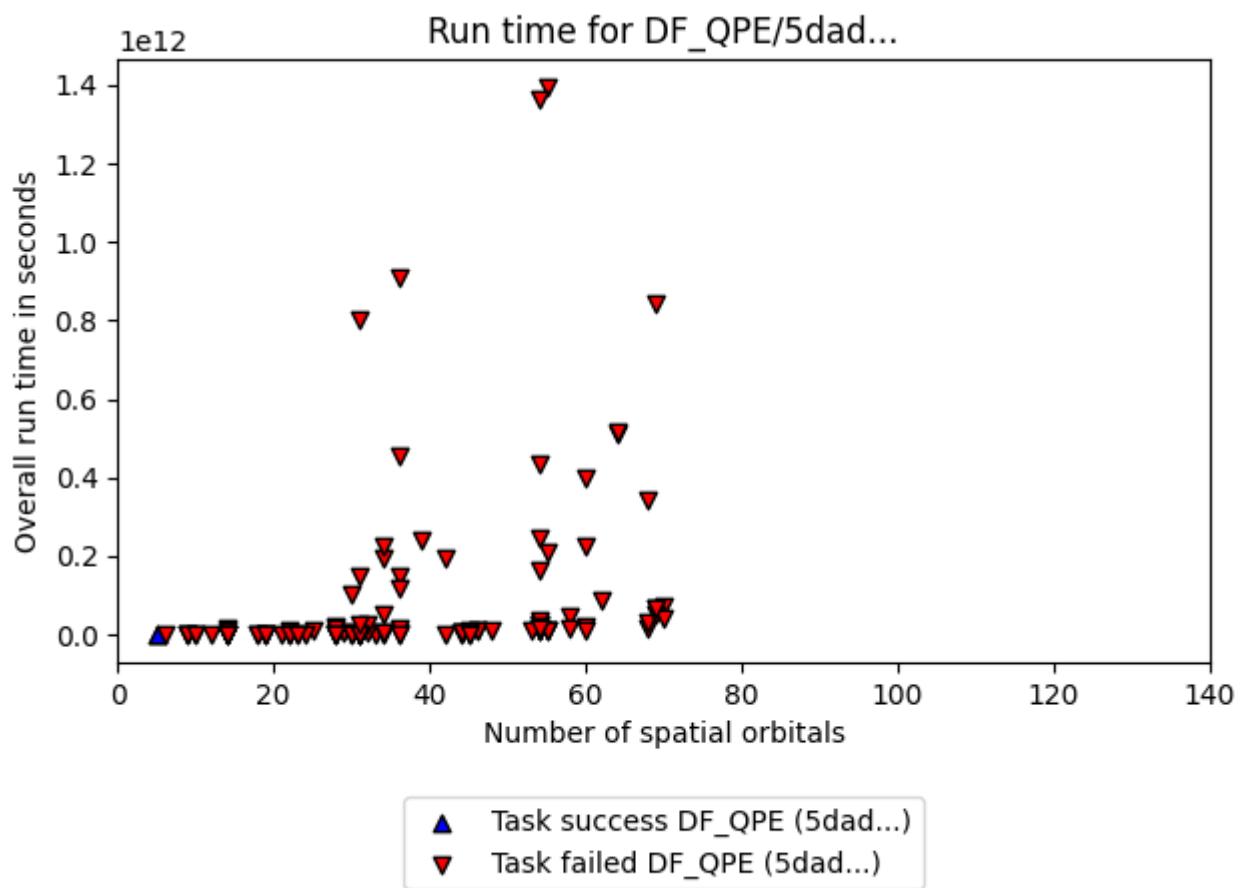
sum_of_run_time_of_attempted_tasks: 11314745416246.352

solvability_ratio: 0.0394

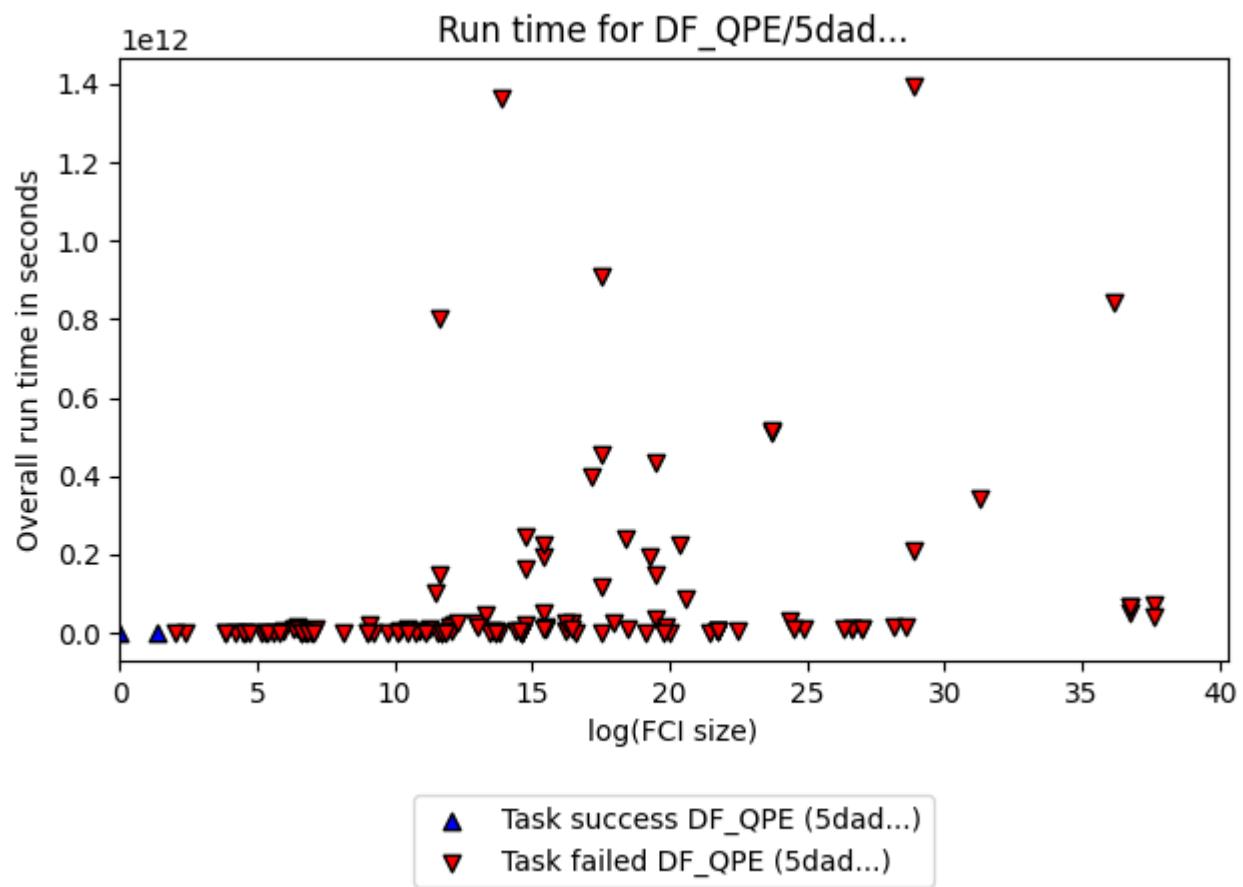
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



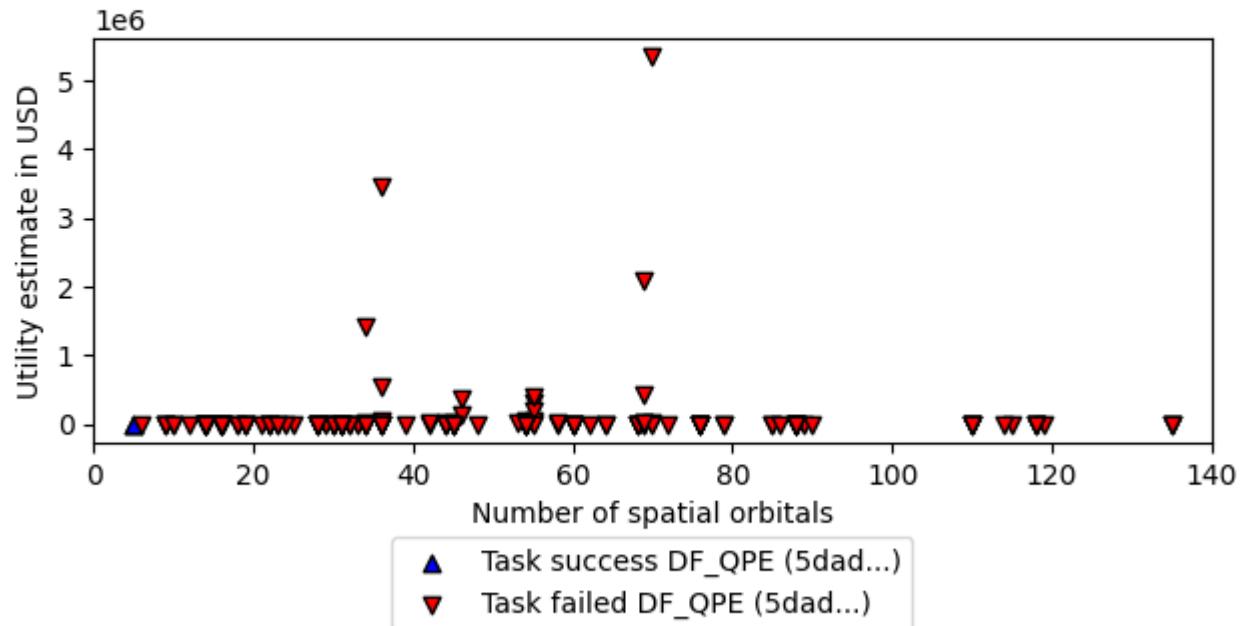
Note: plot only contains attempted tasks.



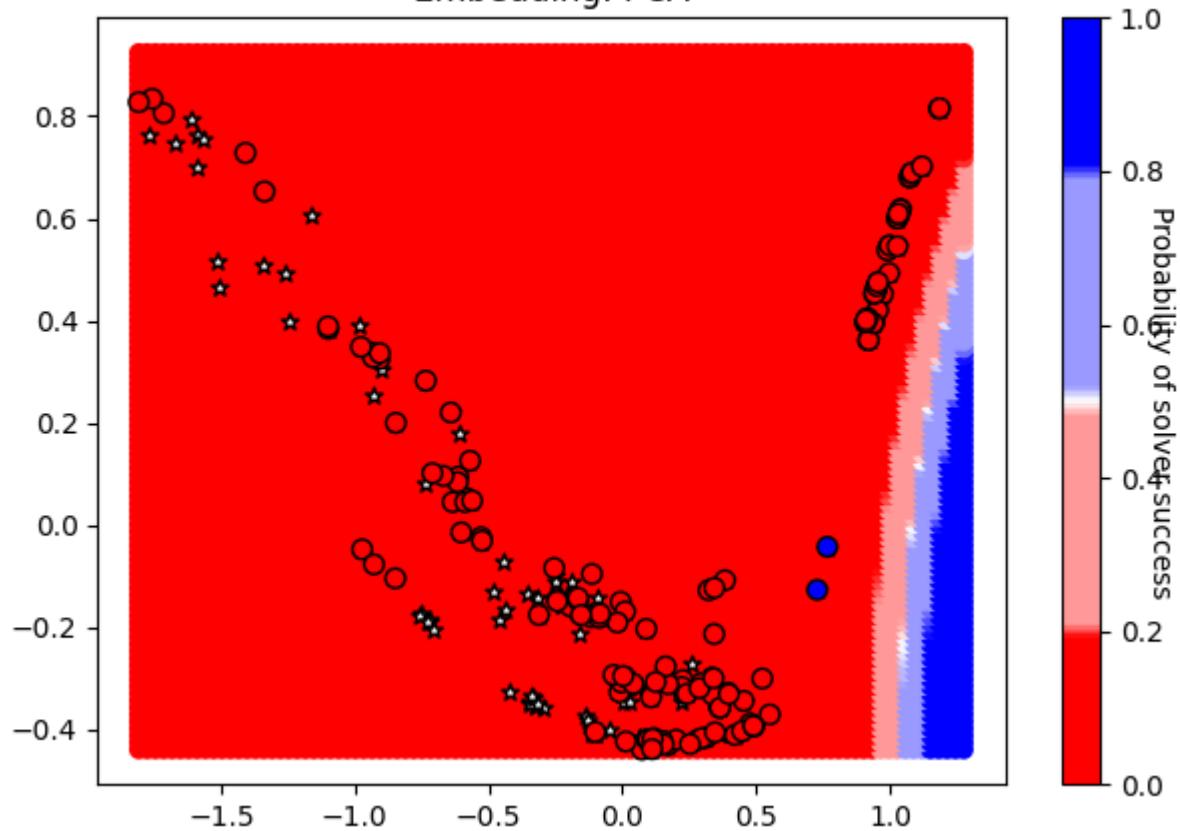
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5dad...

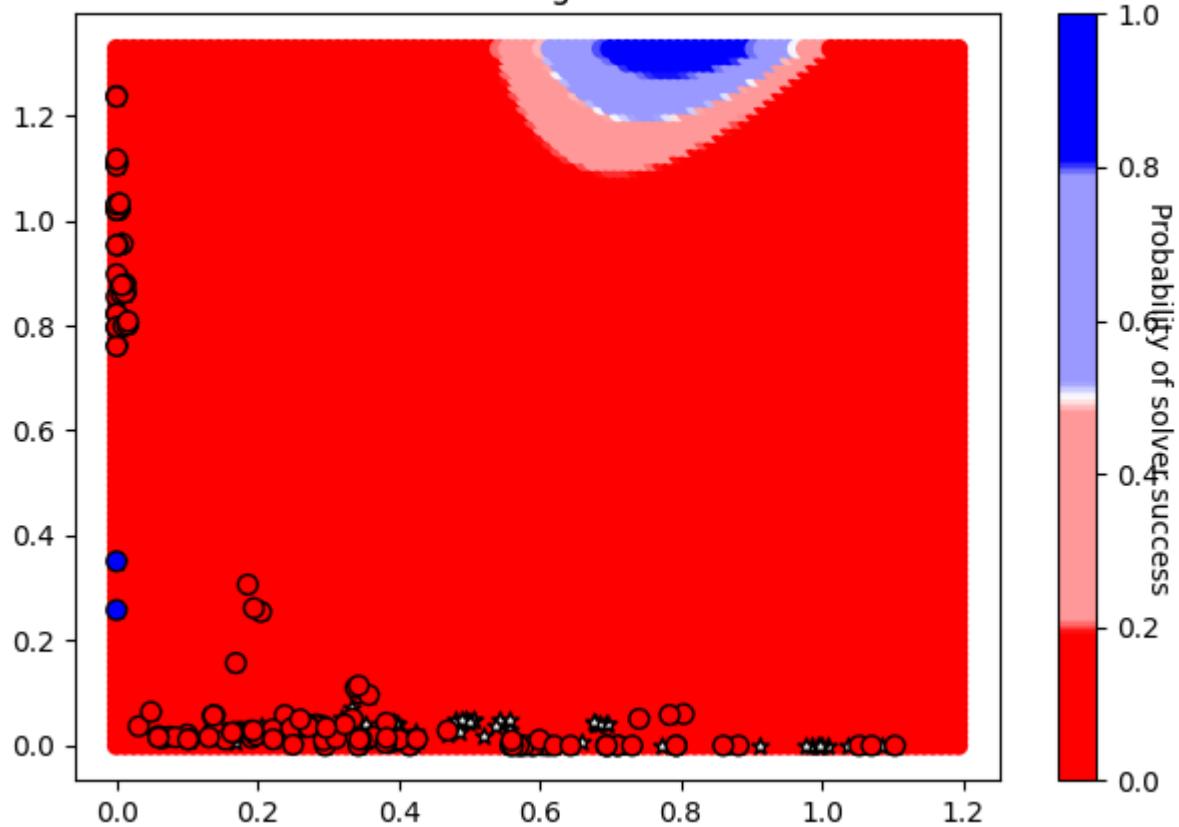
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



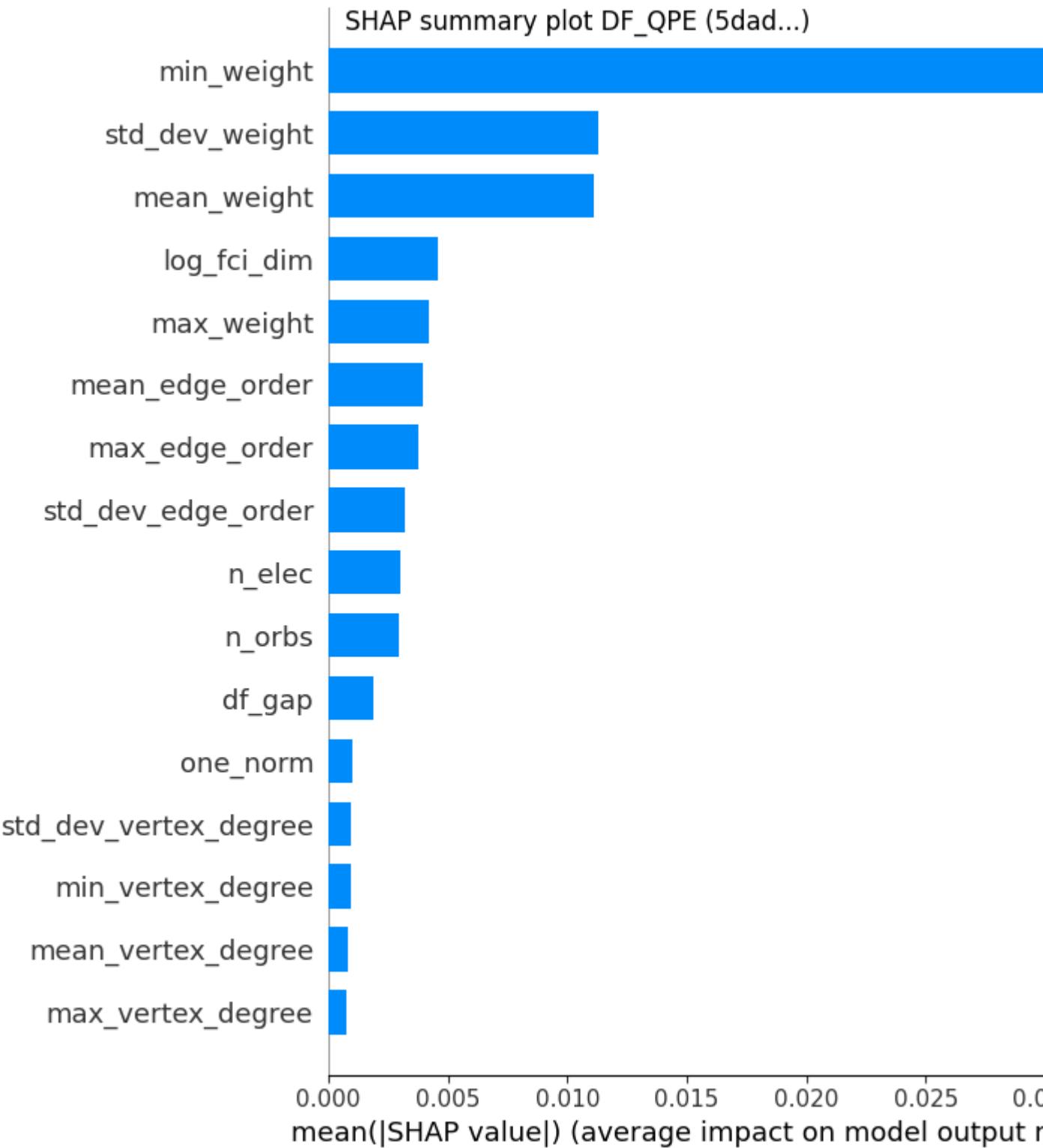
Solver DF_QPE (5dad...)
Embedding: PCA



Solver DF_QPE (5dad...)
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.



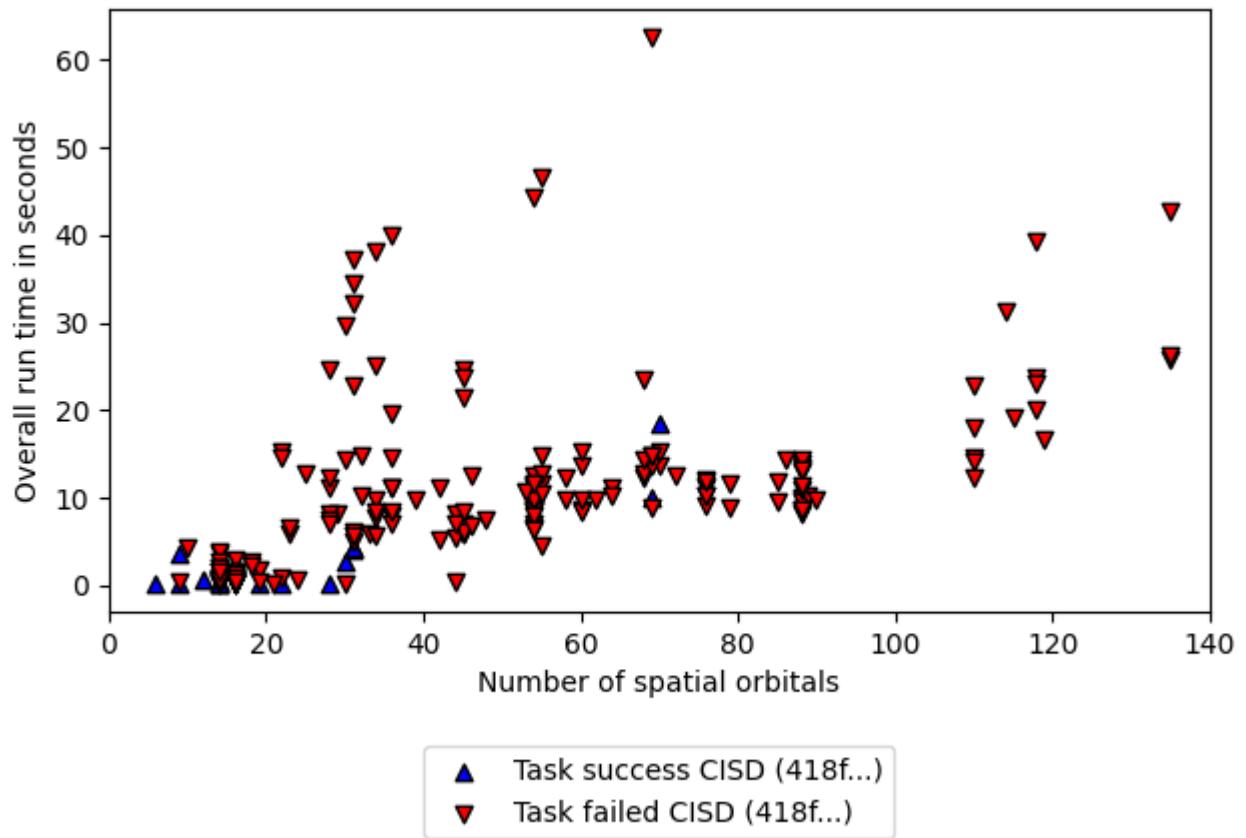
Solver CISD, 418f060e-496b-4024-8d2d-9b1f8791e76d

solver_uuid:418f060e-496b-4024-8d2d-9b1f8791e76d

solver_short_name:CISD

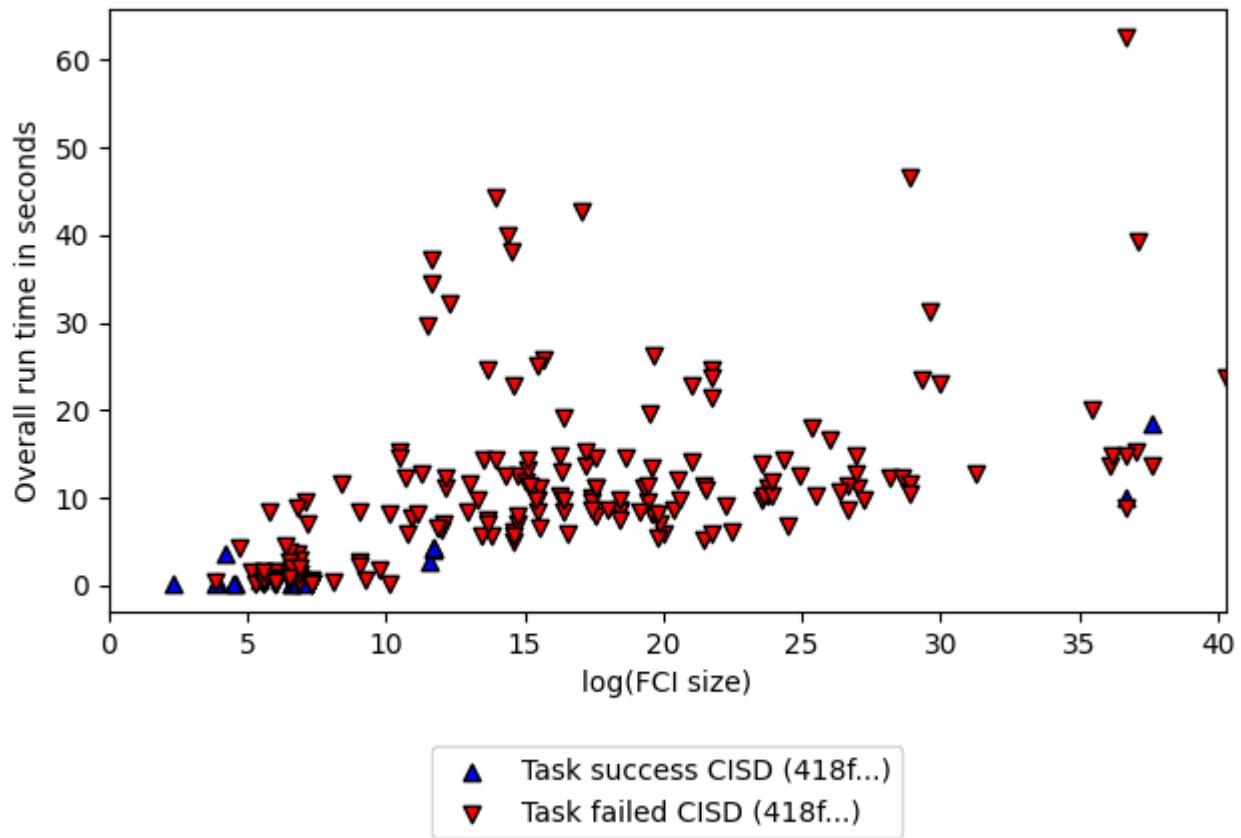
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CISD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: eb043c83-8394-4d84-abc7-c2067240b558
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9774436090225563, 0.85]
ml_metrics_calculator_version: 1

Run time for CISD/418f...



Note: plot only contains attempted tasks.

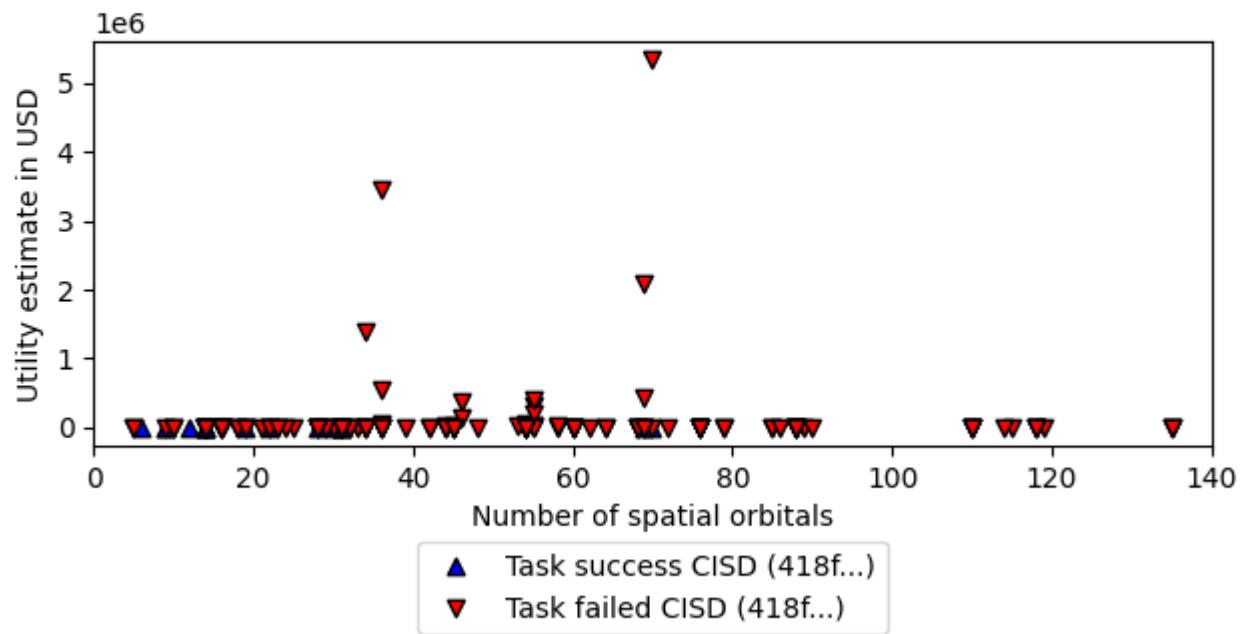
Run time for CISD/418f...



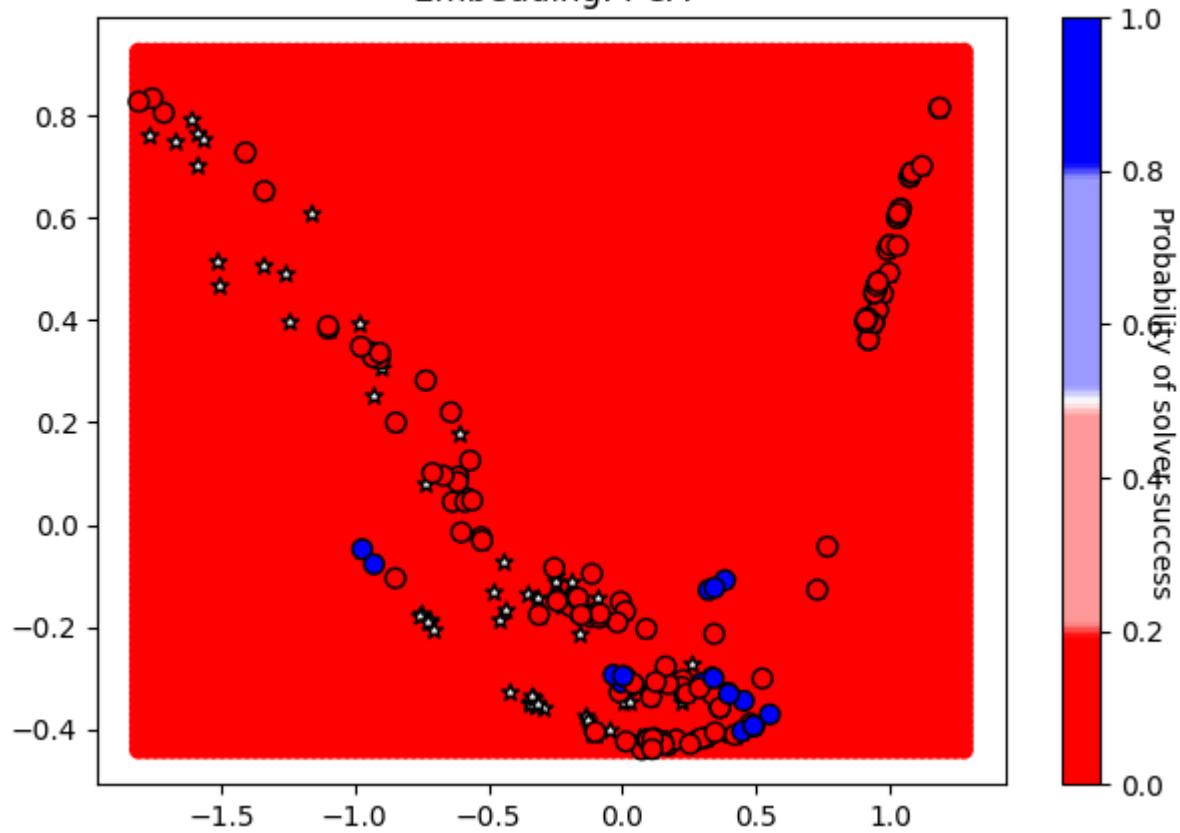
Note: plot only contains attempted tasks.

Utility capture from CISD/418f...

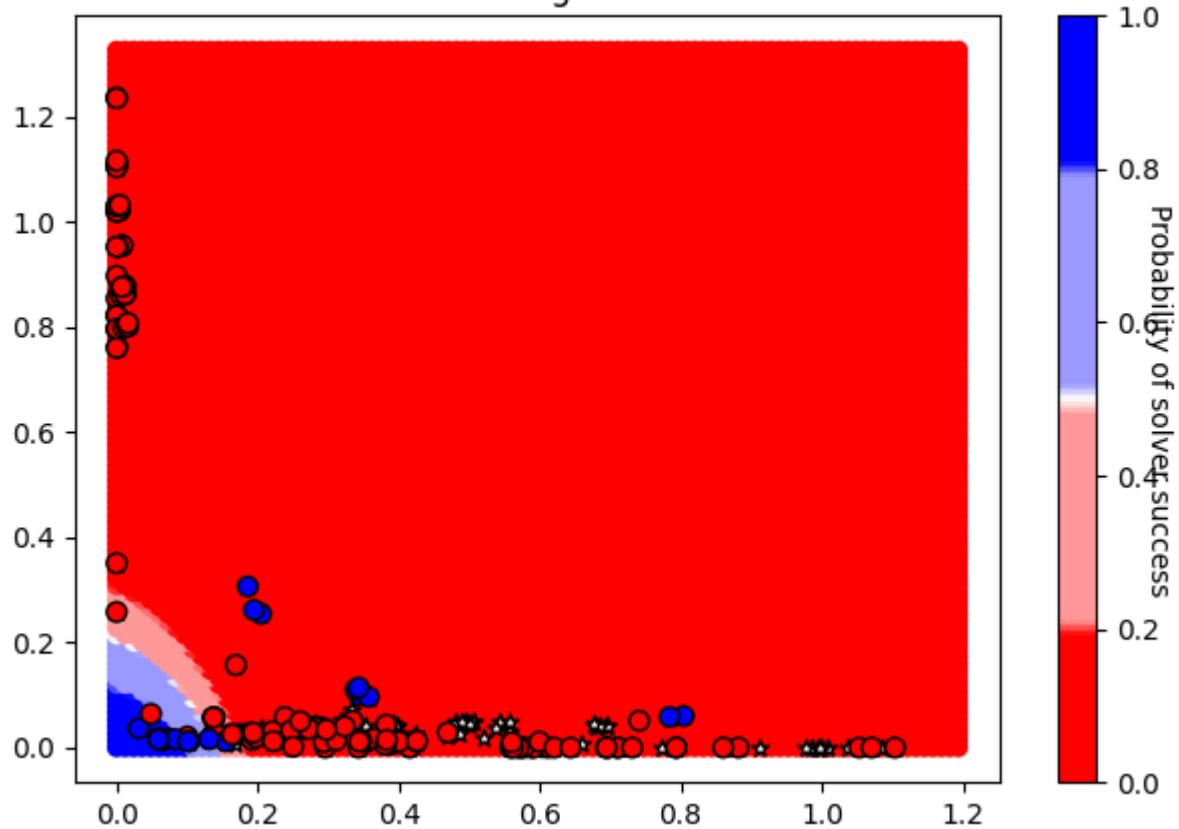
(captured: \$4.8e-03/1.5e+07, approximately 3.2e-08%)



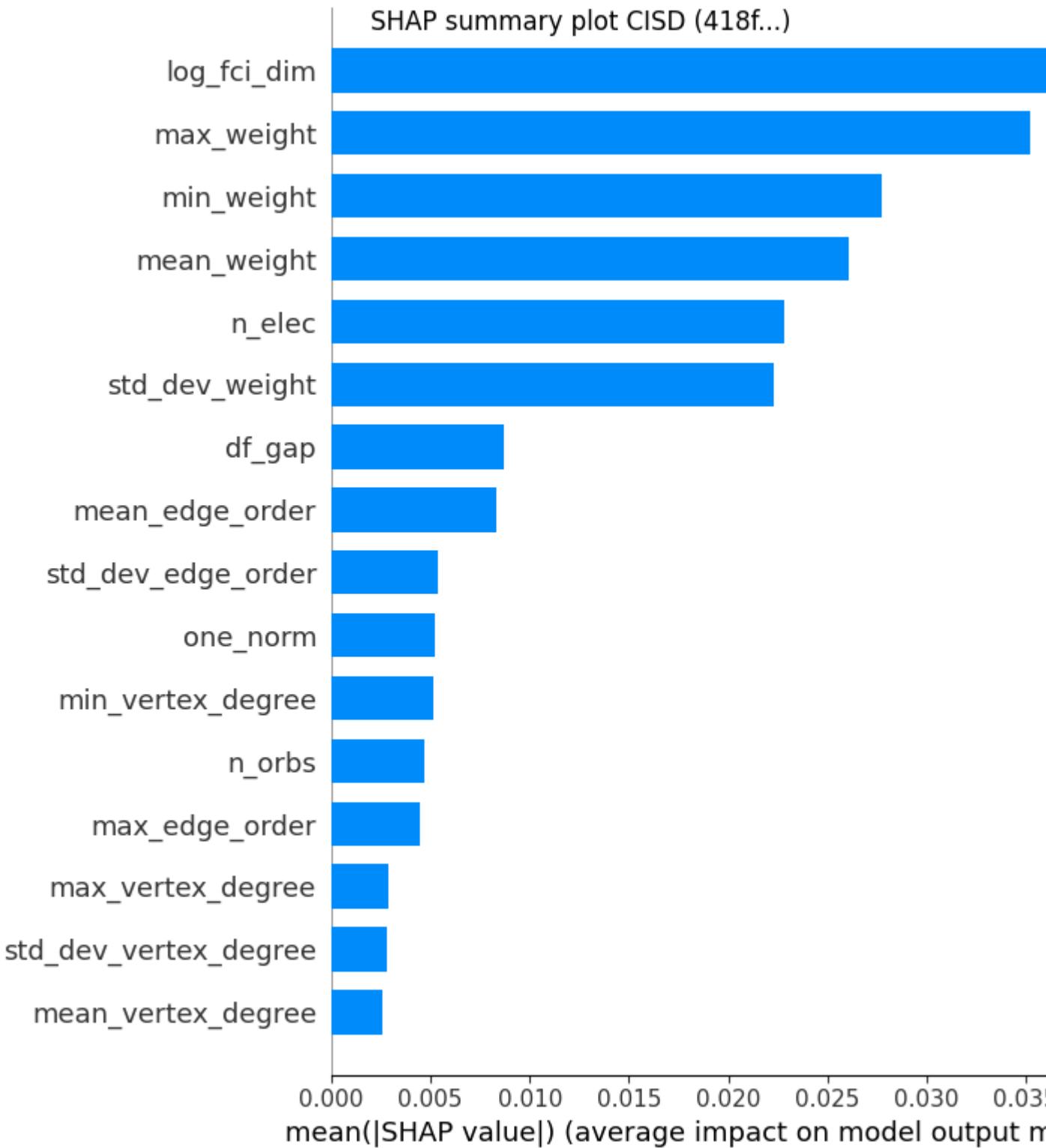
Solver CISD (418f...)
Embedding: PCA



Solver CISD (418f...)
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.



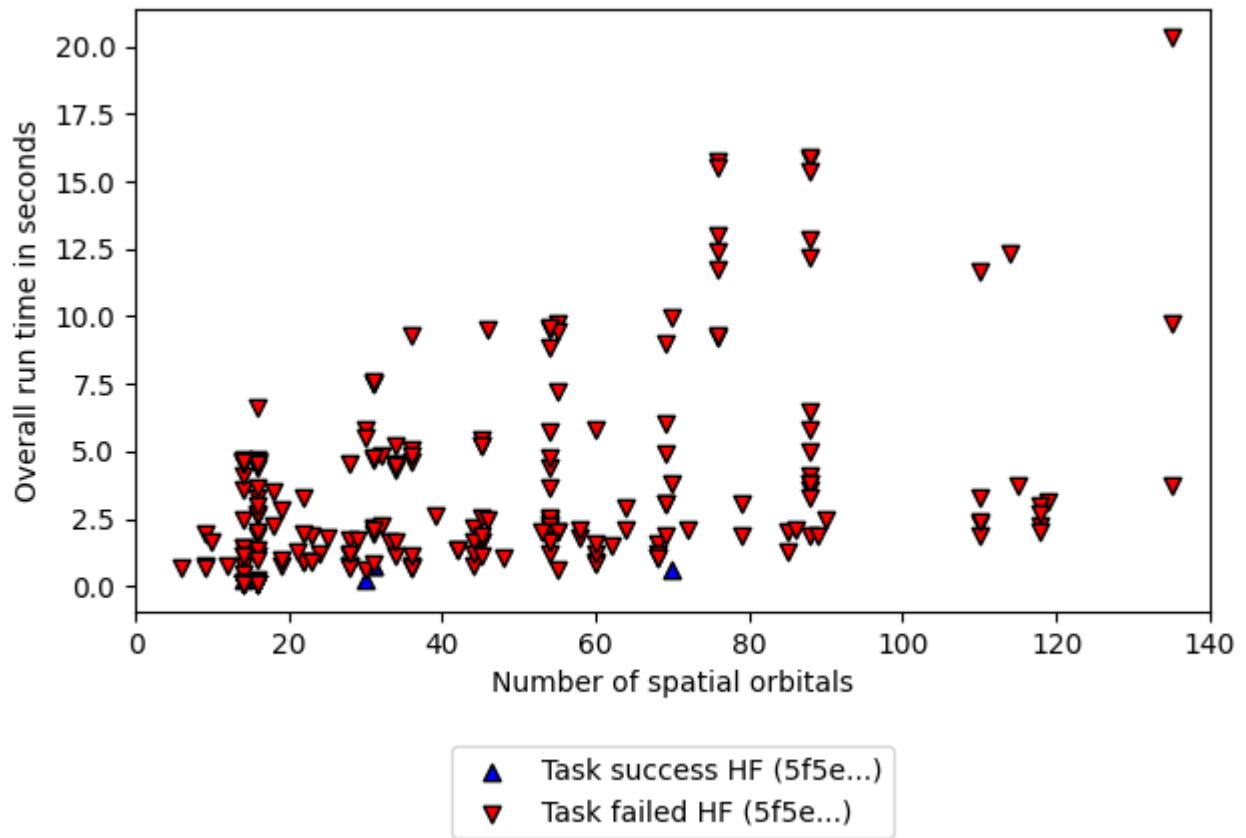
Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

solver_uuid:5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

solver_short_name:HF

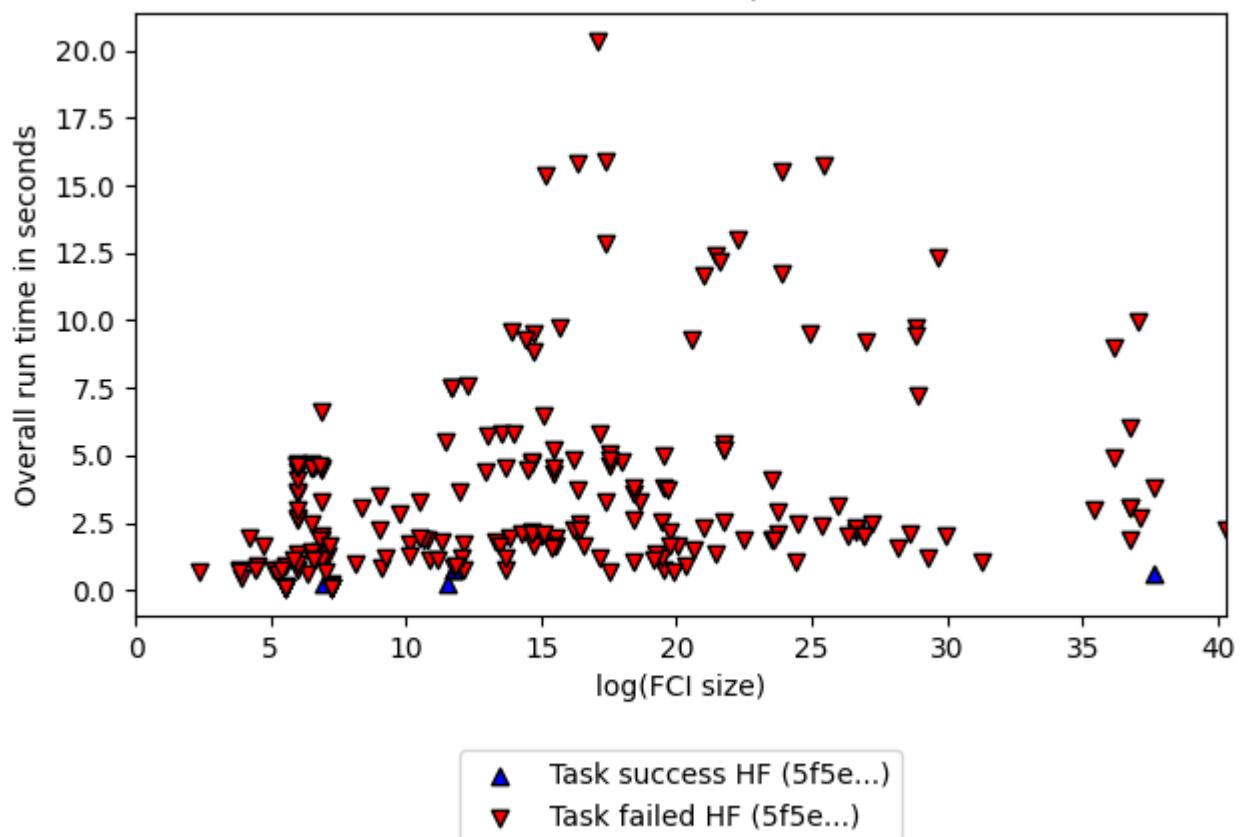
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:Hartree Fock
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: fb56b355-c8a9-4c1d-9623-153c7f61edc3
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9863013698630136, 0.7142857142857143]
ml_metrics_calculator_version: 1

Run time for HF/5f5e...



Note: plot only contains attempted tasks.

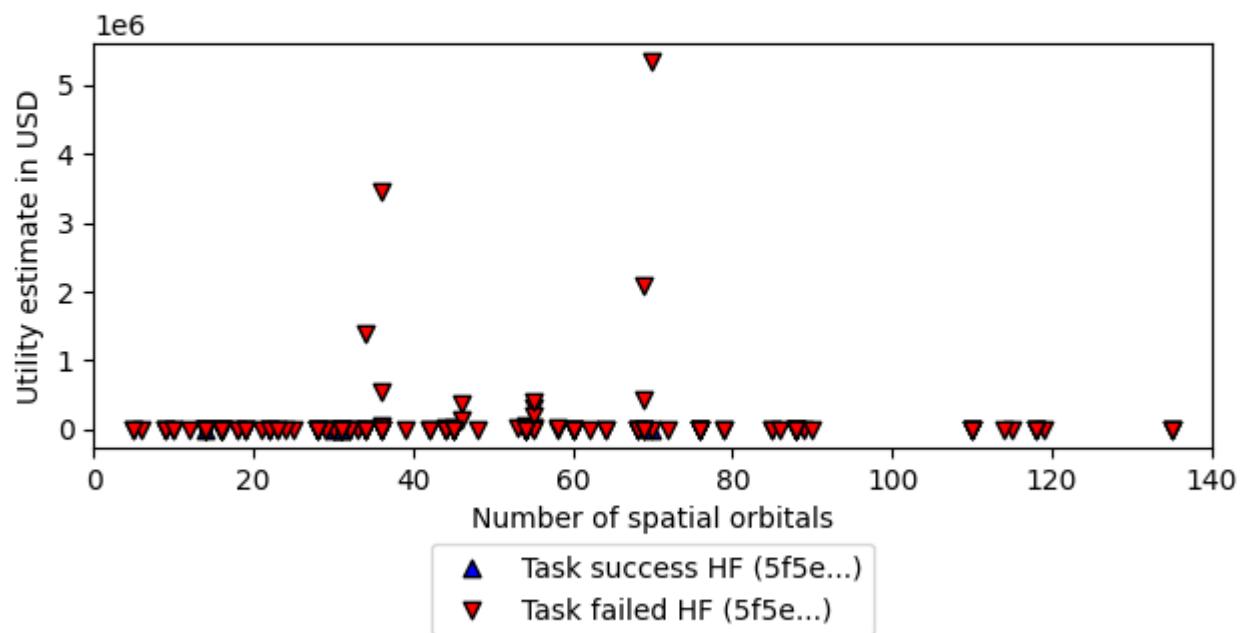
Run time for HF/5f5e...



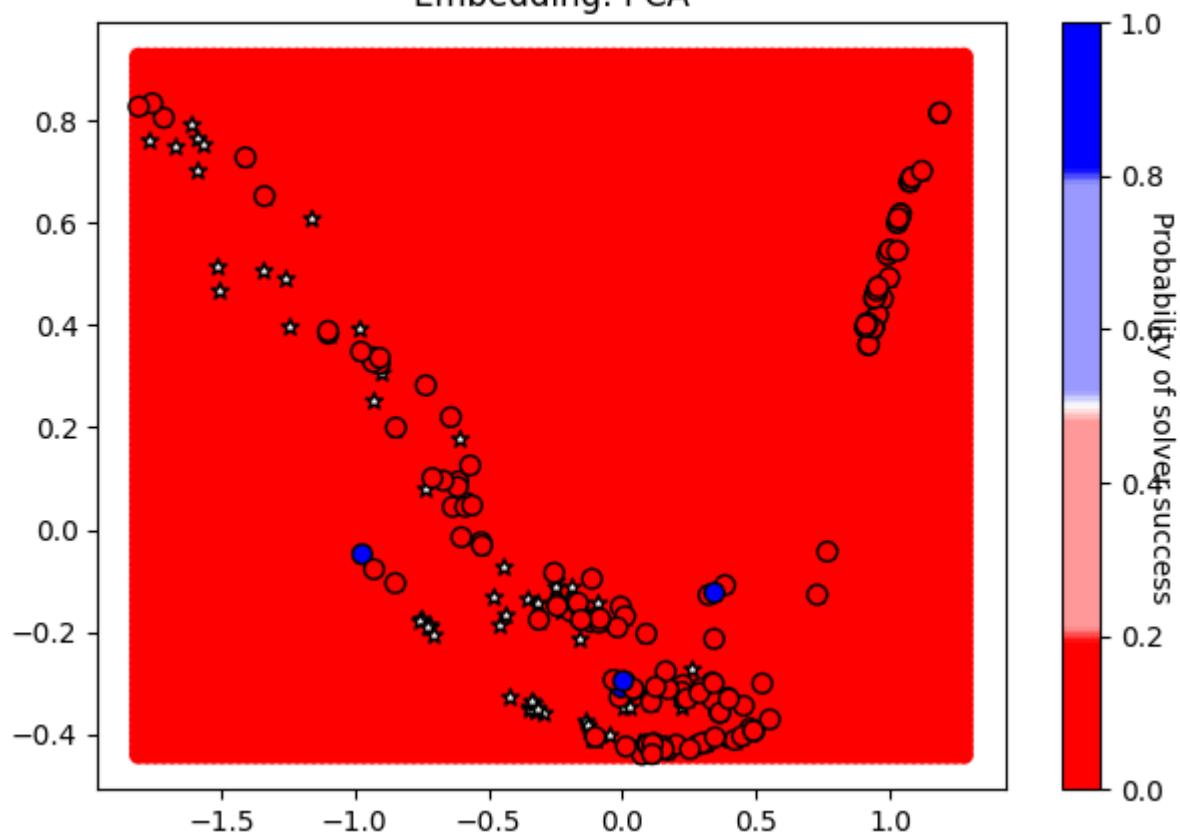
Note: plot only contains attempted tasks.

Utility capture from HF/5f5e...

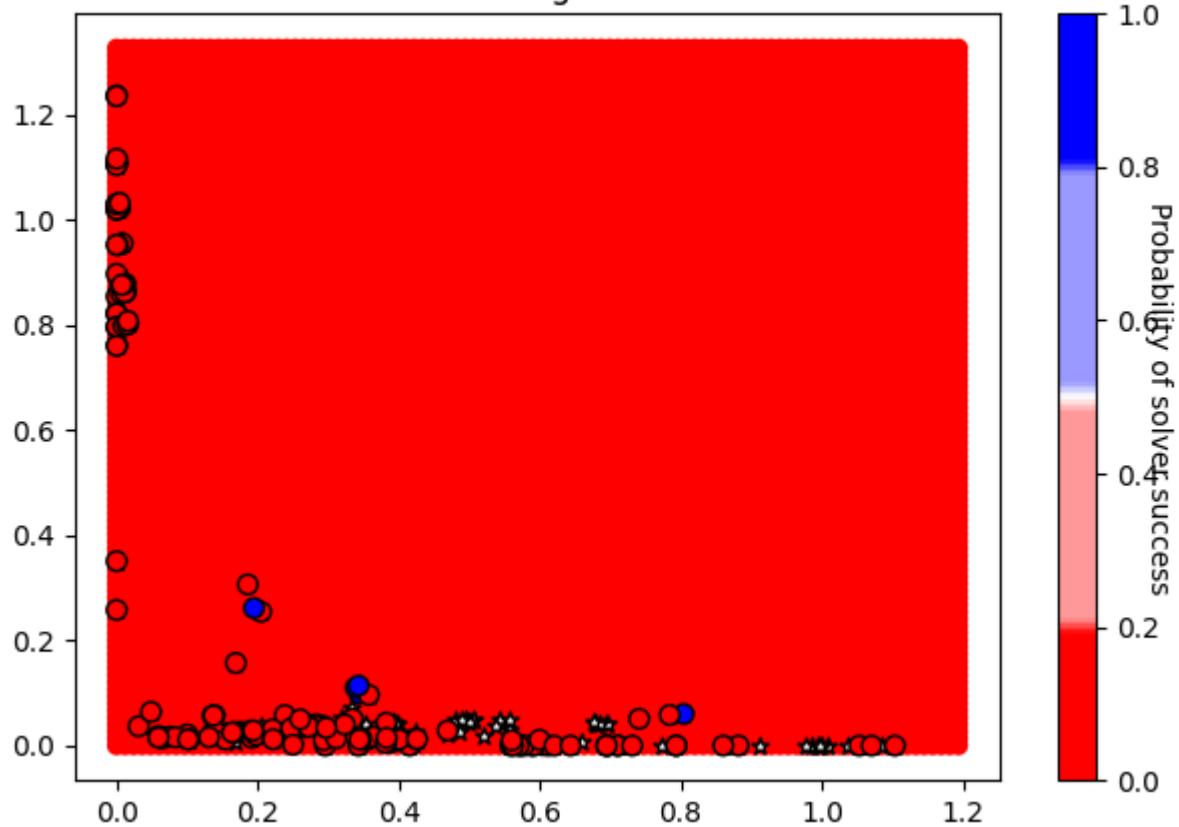
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



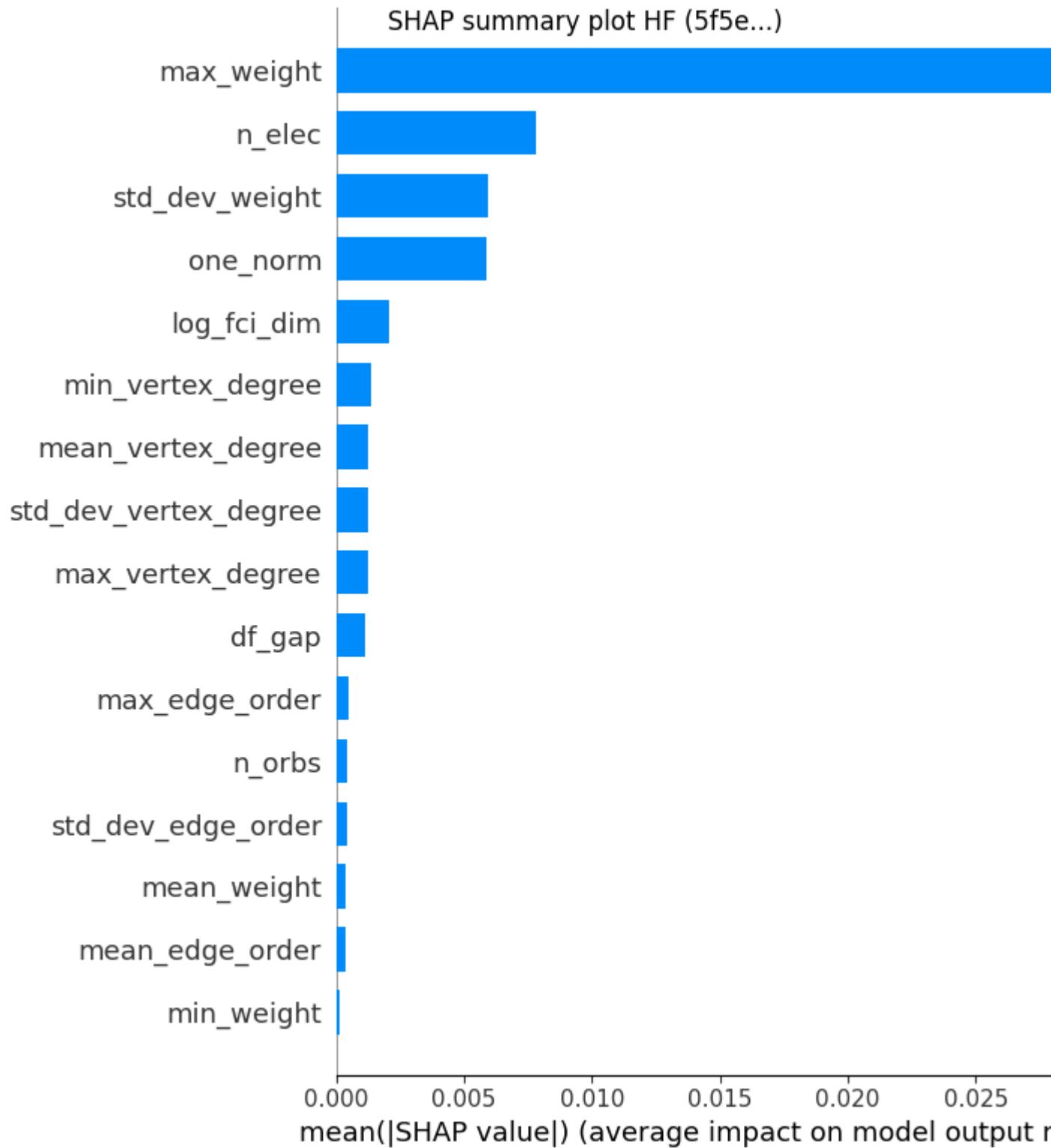
Solver HF (5f5e...)
Embedding: PCA



Solver HF (5f5e...)
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.



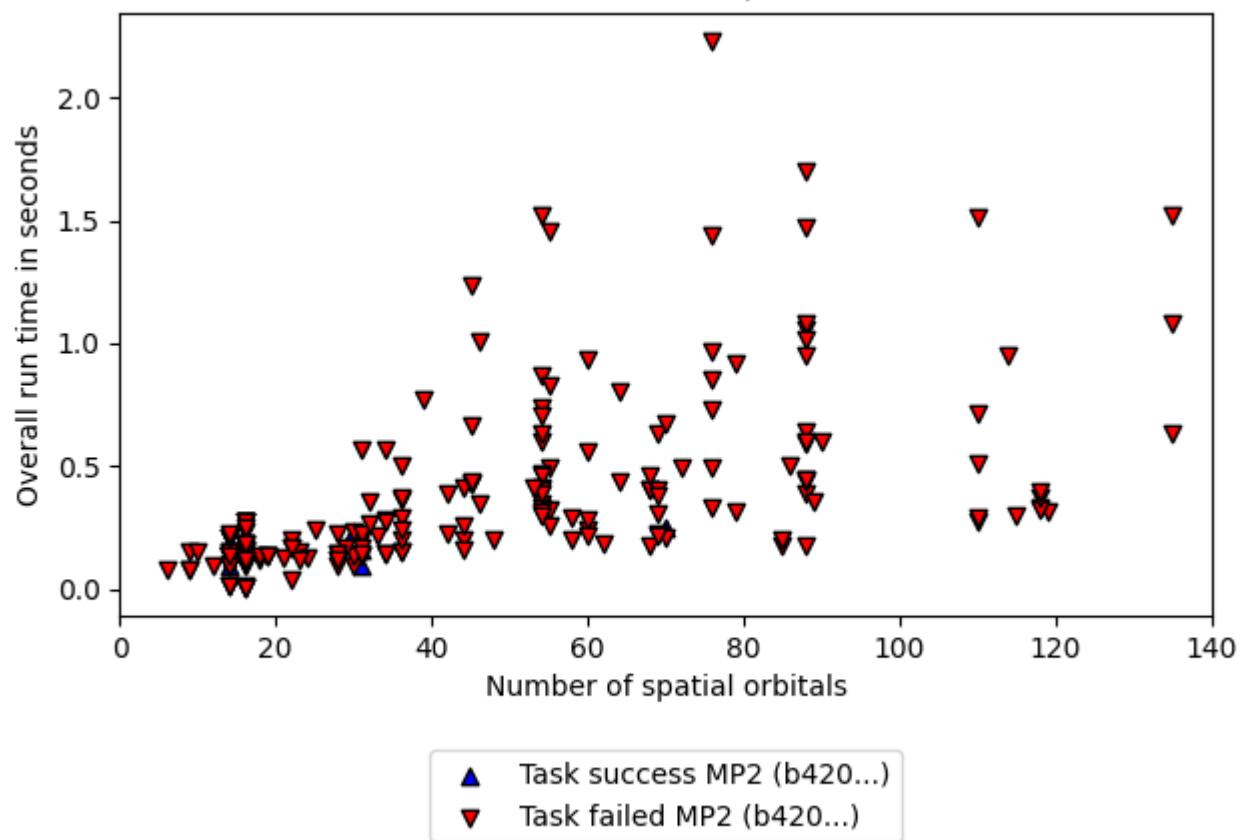
Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aecd2

solver_uuid:b420358b-5def-41e6-8c5d-b9d93b6aecd2

solver_short_name:MP2

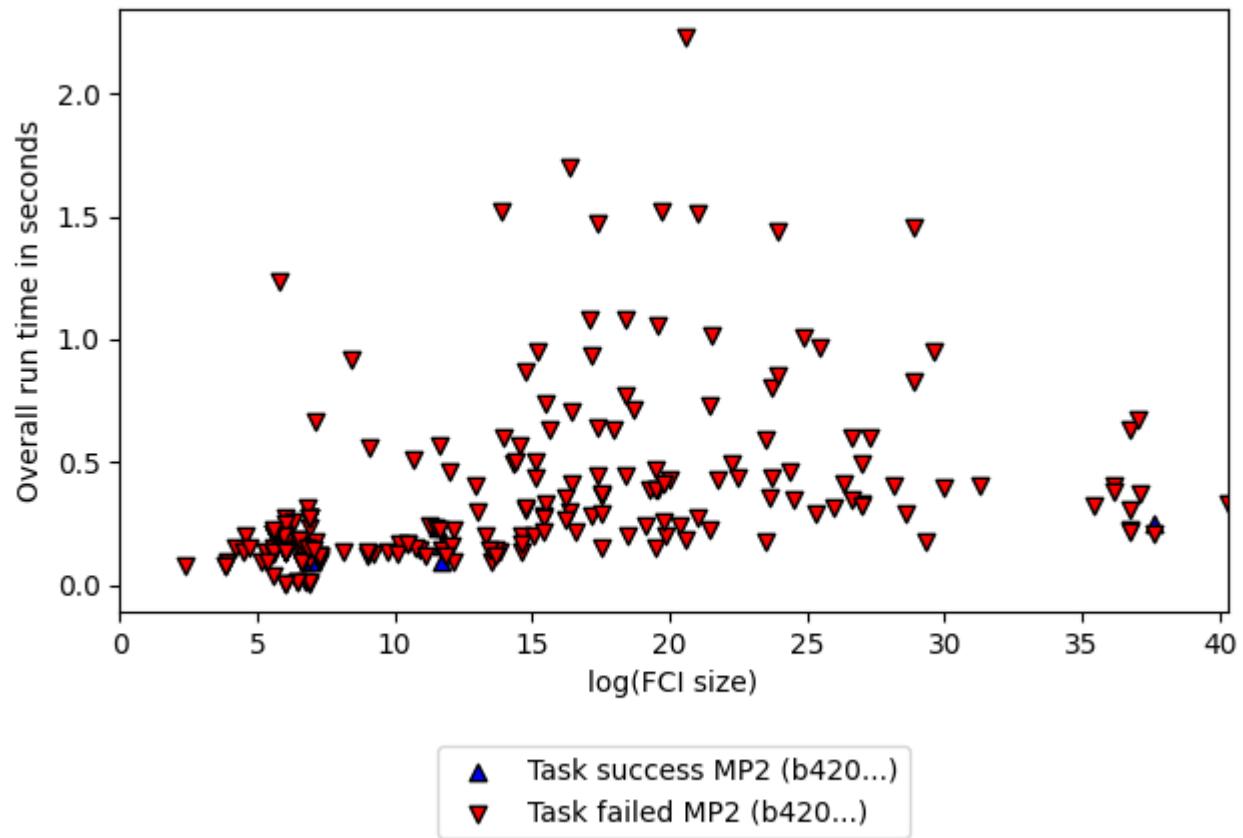
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:MP2
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 59997f05-ee01-4197-87b9-17f327b43ab4
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9863013698630136, 0.7142857142857143]
ml_metrics_calculator_version: 1

Run time for MP2/b420...



Note: plot only contains attempted tasks.

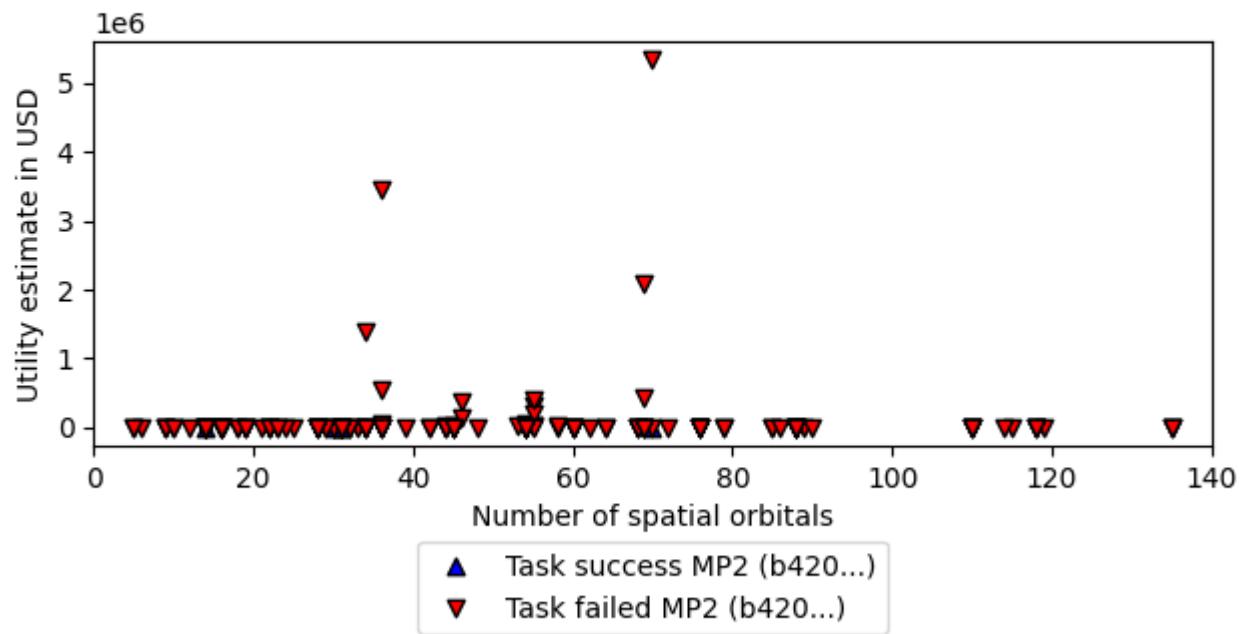
Run time for MP2/b420...



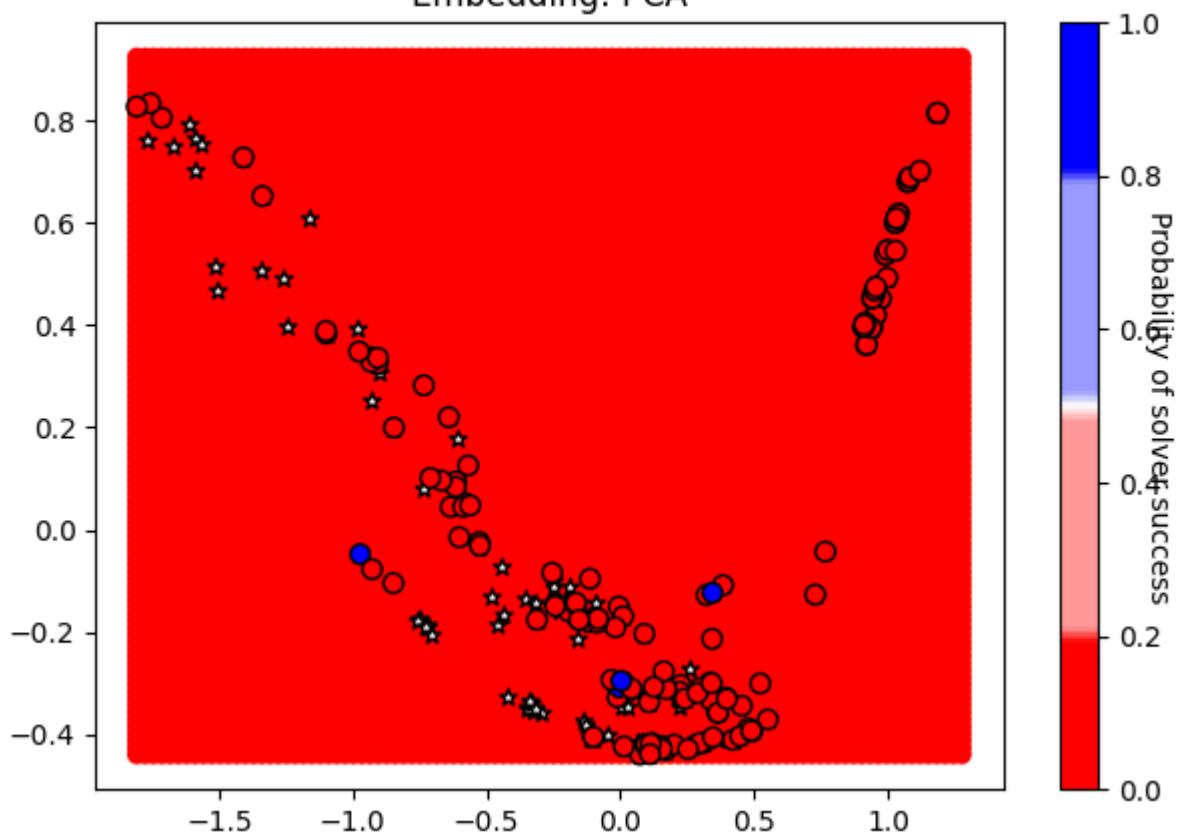
Note: plot only contains attempted tasks.

Utility capture from MP2/b420...

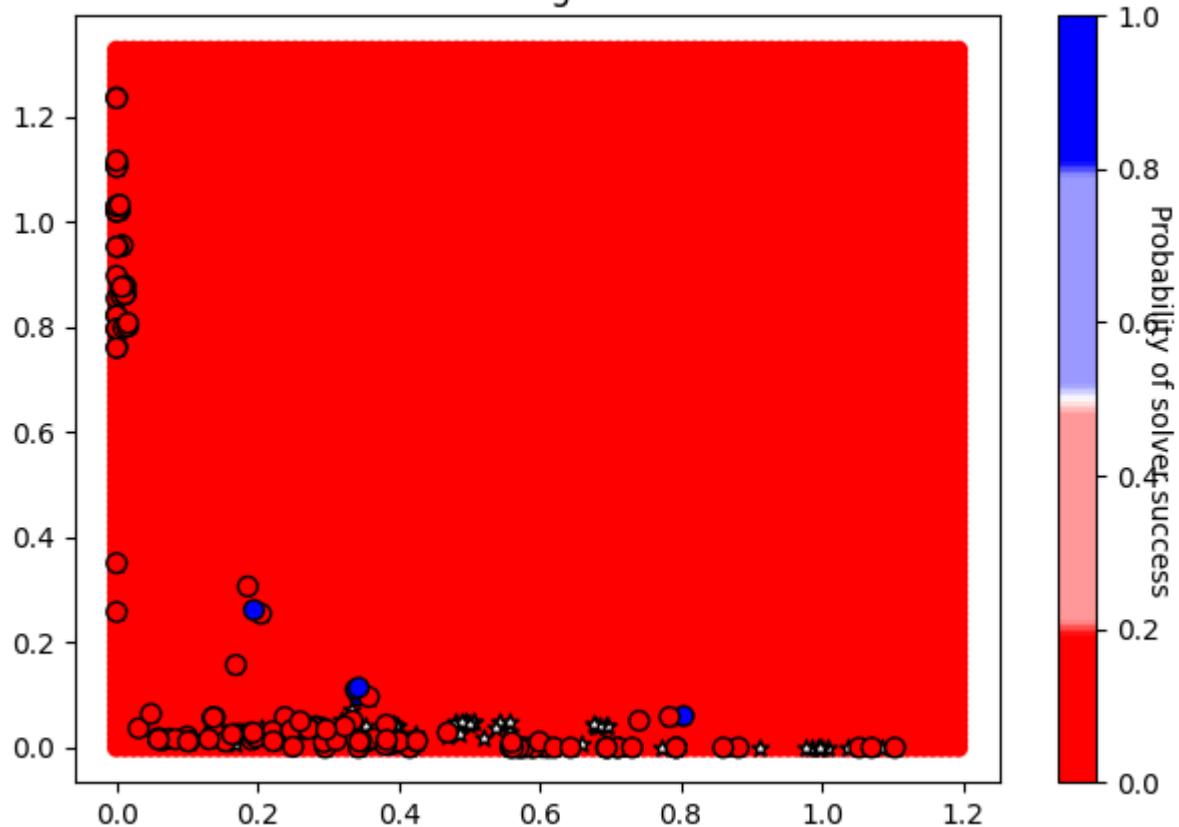
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



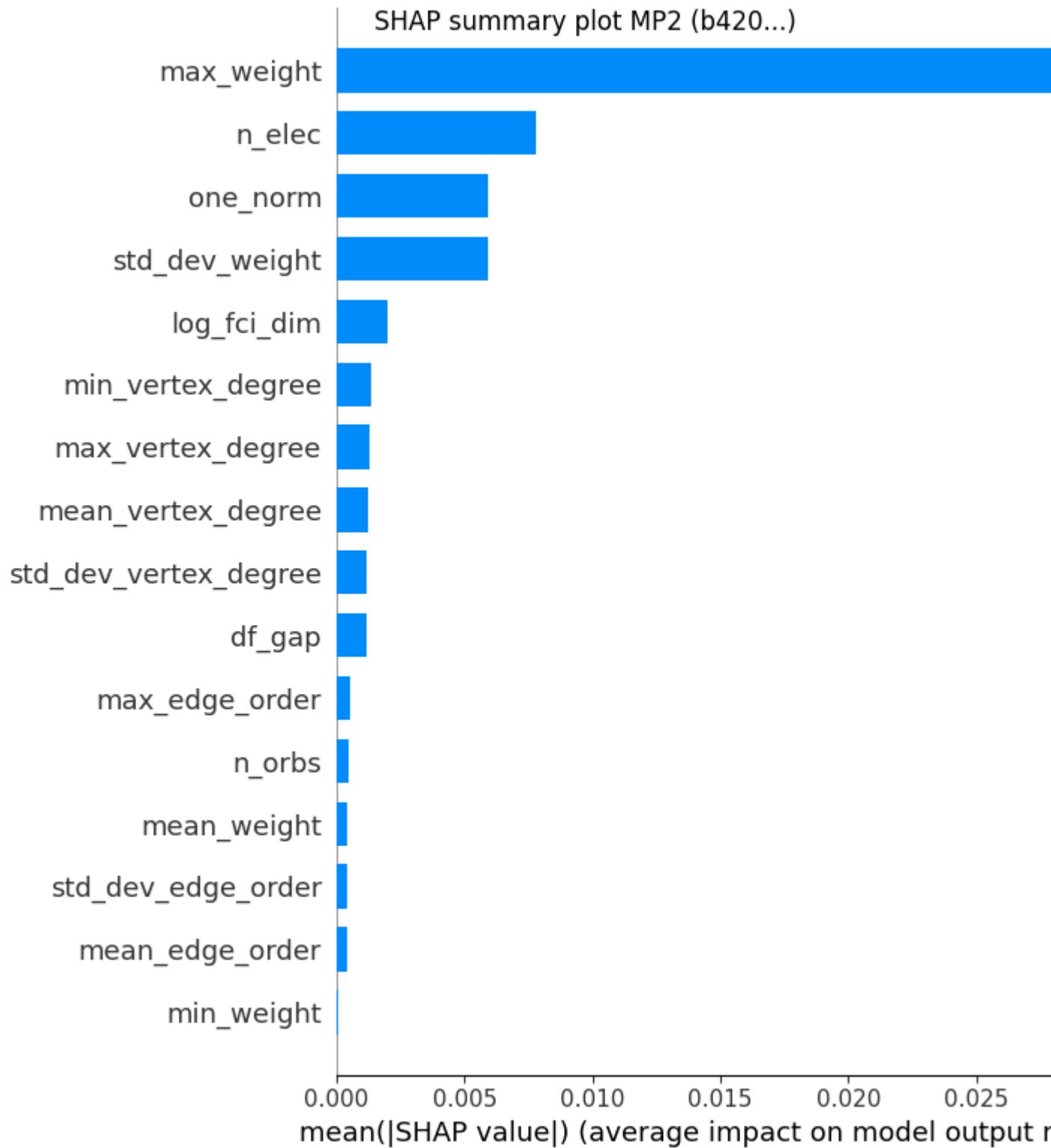
Solver MP2 (b420...)
Embedding: PCA



Solver MP2 (b420...)
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.



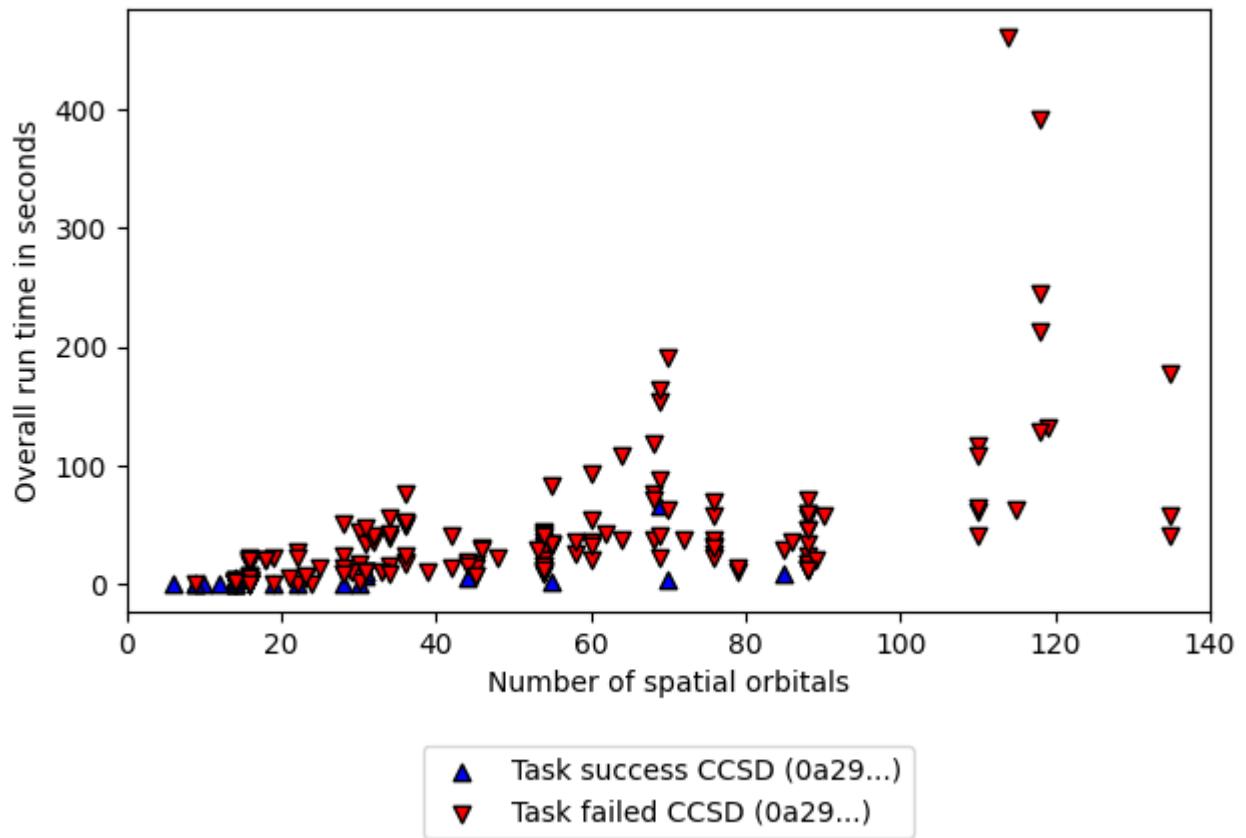
Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

solver_uuid:0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

solver_short_name:CCSD

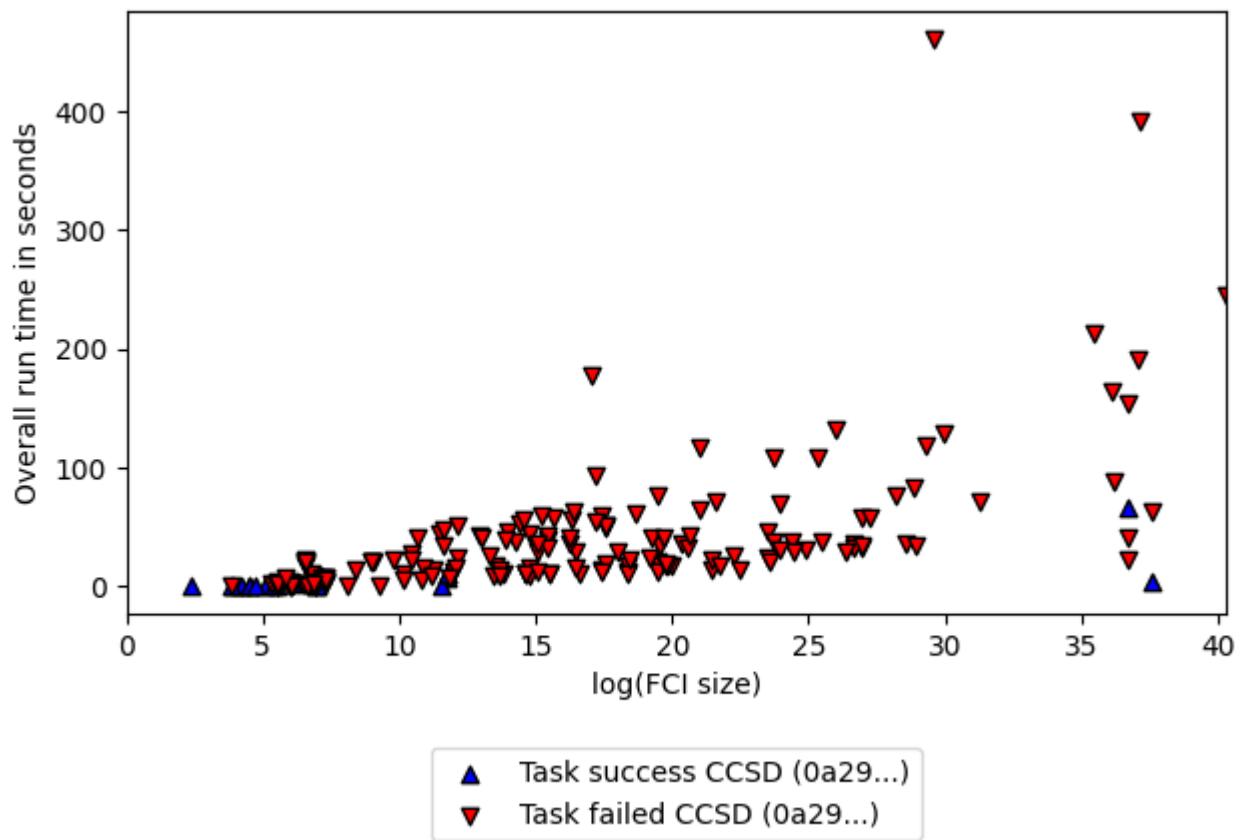
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 4983172b-efbe-43a7-b431-6e2ff2db5ed3
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9763779527559056, 0.8846153846153846]
ml_metrics_calculator_version: 1

Run time for CCSD/0a29...



Note: plot only contains attempted tasks.

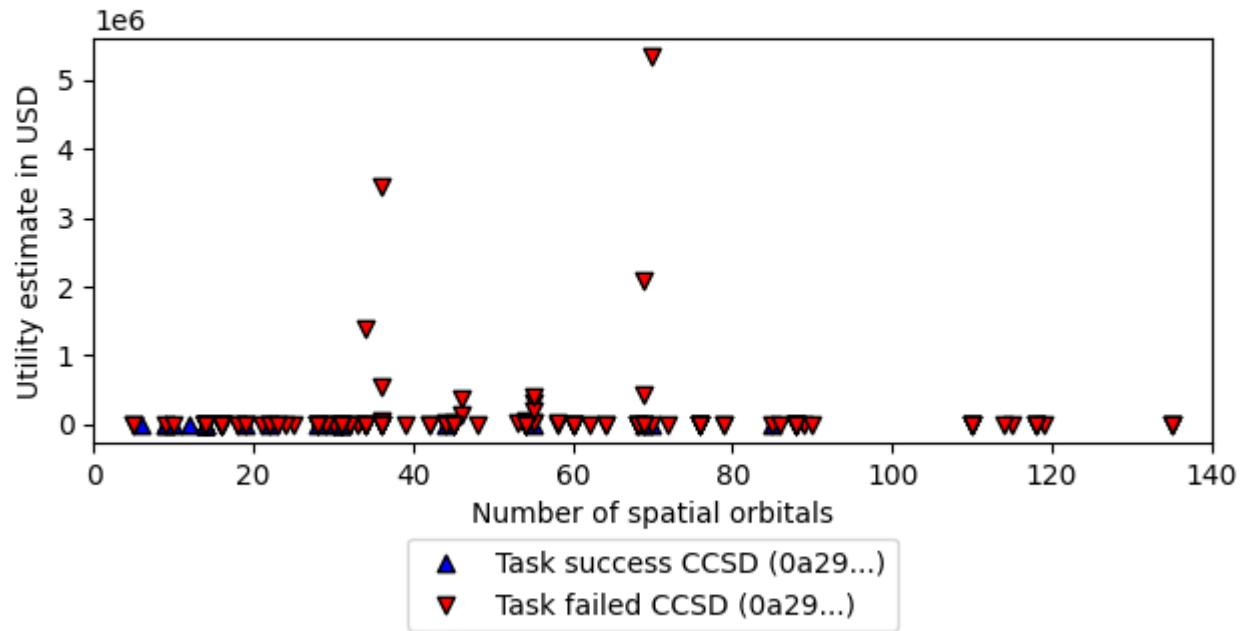
Run time for CCSD/0a29...



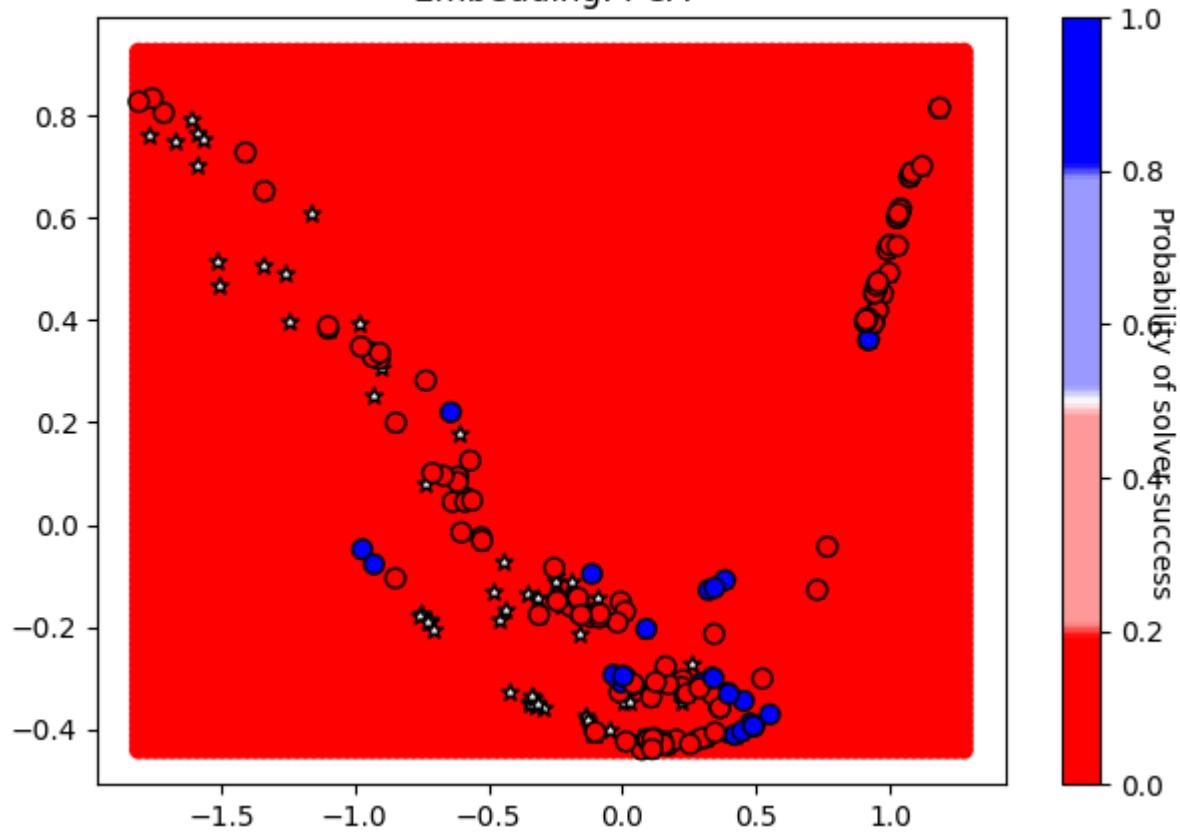
Note: plot only contains attempted tasks.

Utility capture from CCSD/0a29...

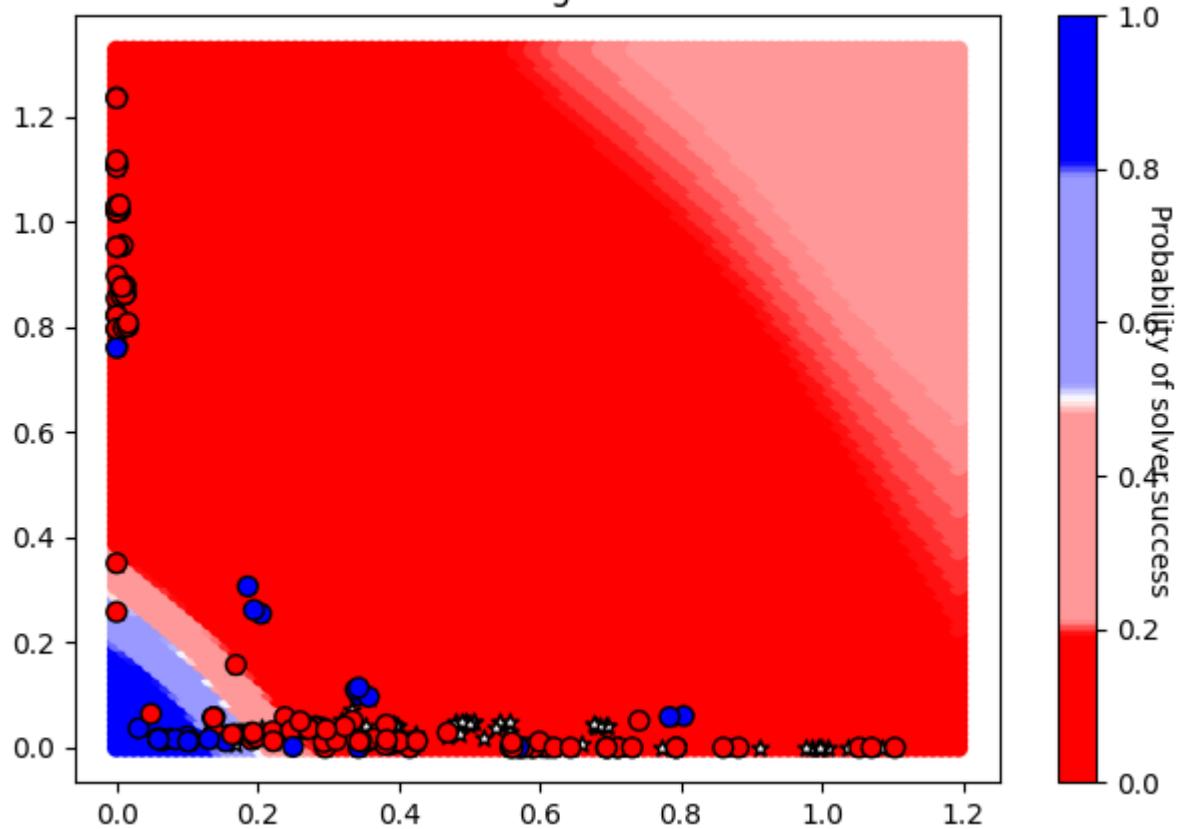
(captured: \$2.1e-02/1.5e+07, approximately 1.4e-07%)



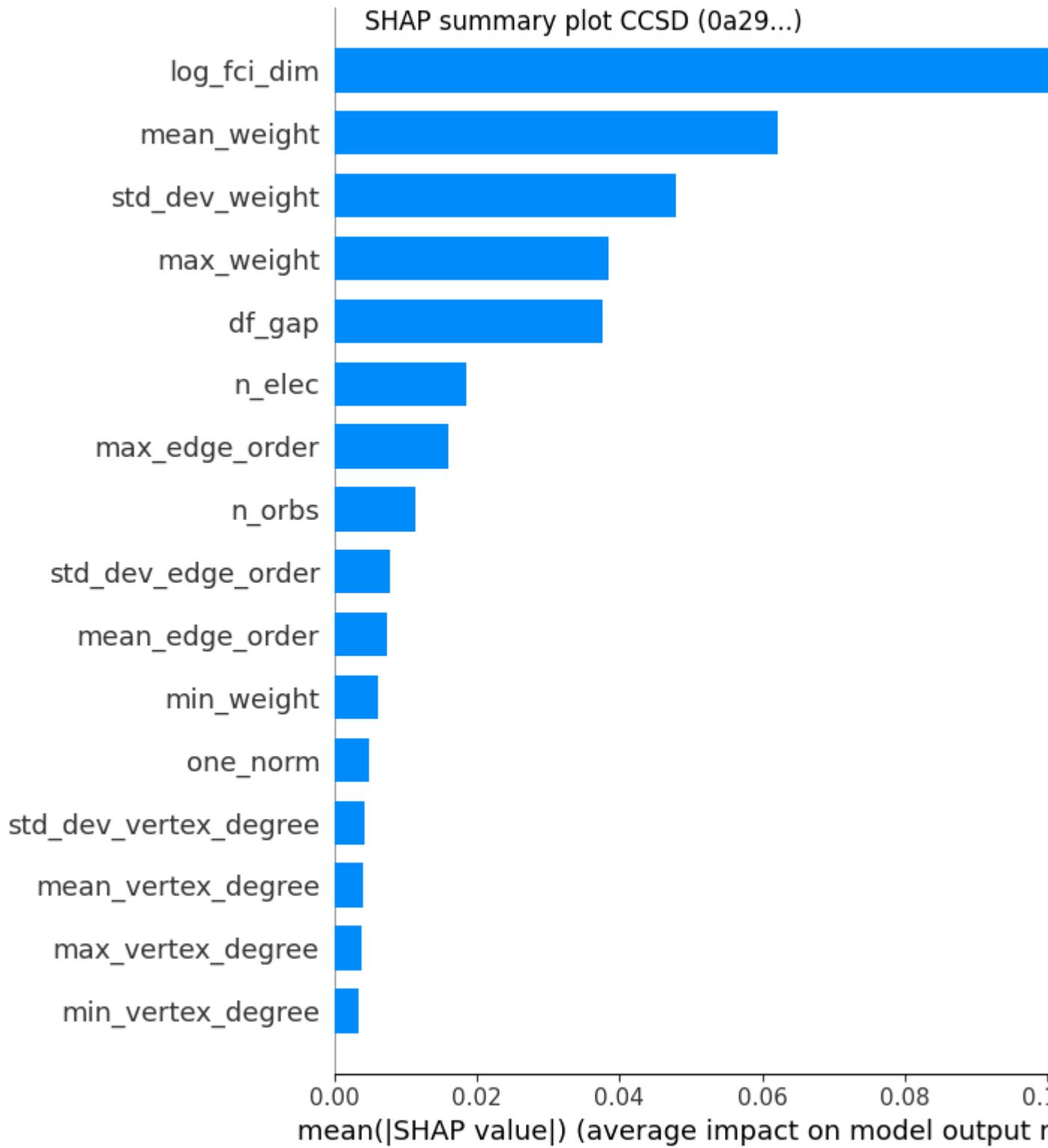
Solver CCSD (0a29...)
Embedding: PCA



Solver CCSD (0a29...)
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.



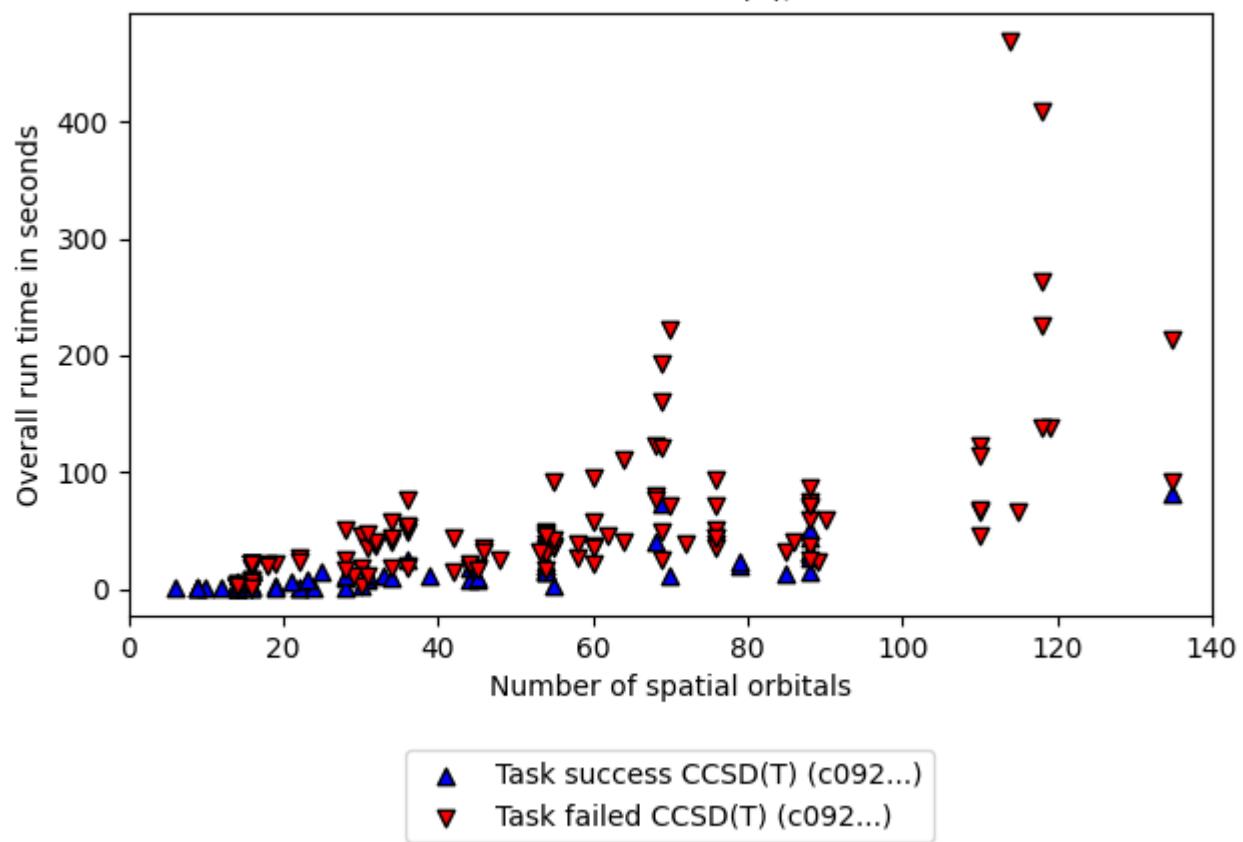
Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878

solver_uuid:c09217e6-d0f7-4b0f-81c4-79210b7ac878

solver_short_name:CCSD(T)

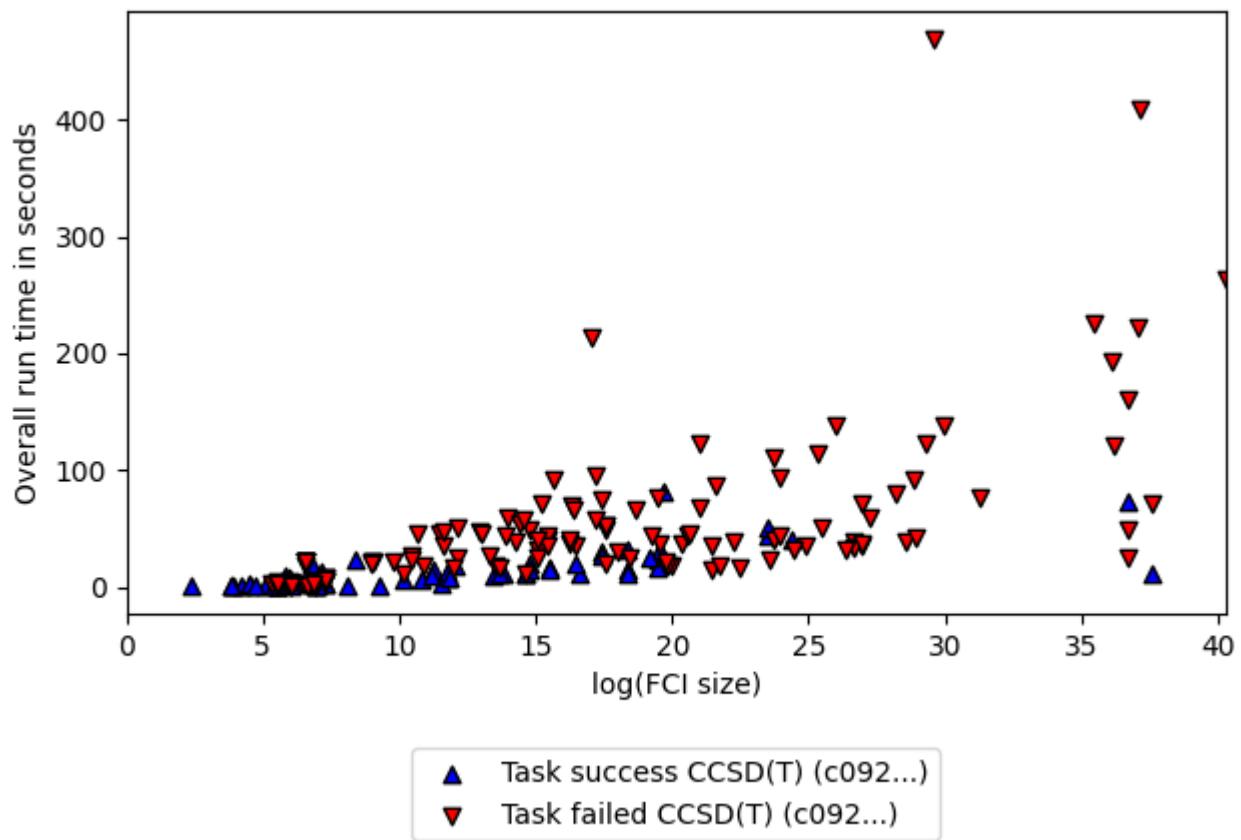
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD(T)
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 54293ef6-1132-4a4e-8fb7-c502af443f4b
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9512195121951219, 0.9436619718309859]
ml_metrics_calculator_version: 1

Run time for CCSD(T)/c092...



Note: plot only contains attempted tasks.

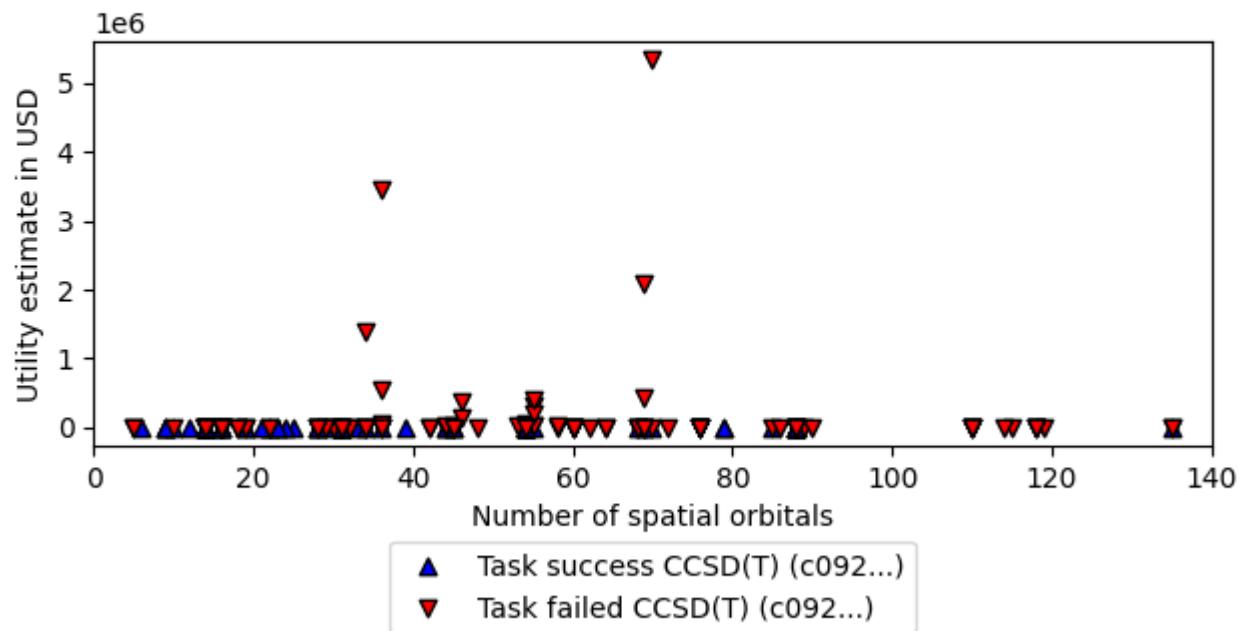
Run time for CCSD(T)/c092...



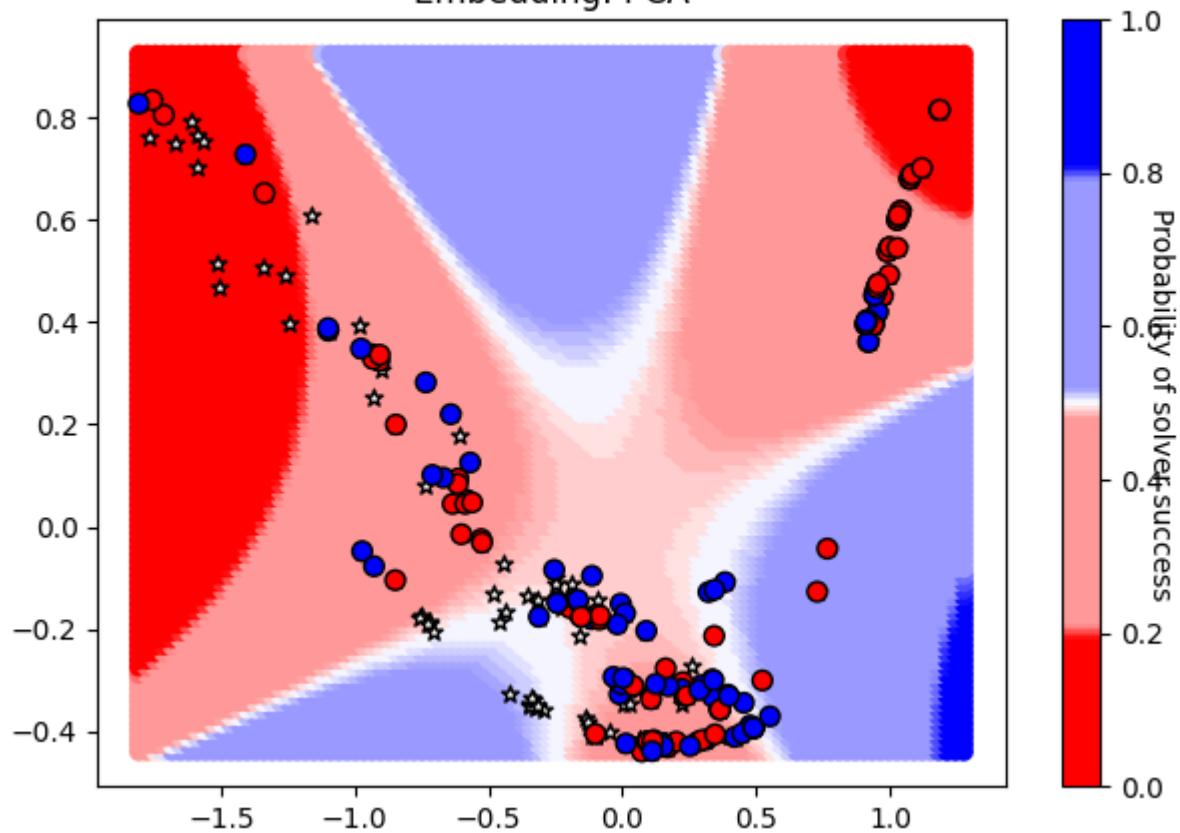
Note: plot only contains attempted tasks.

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

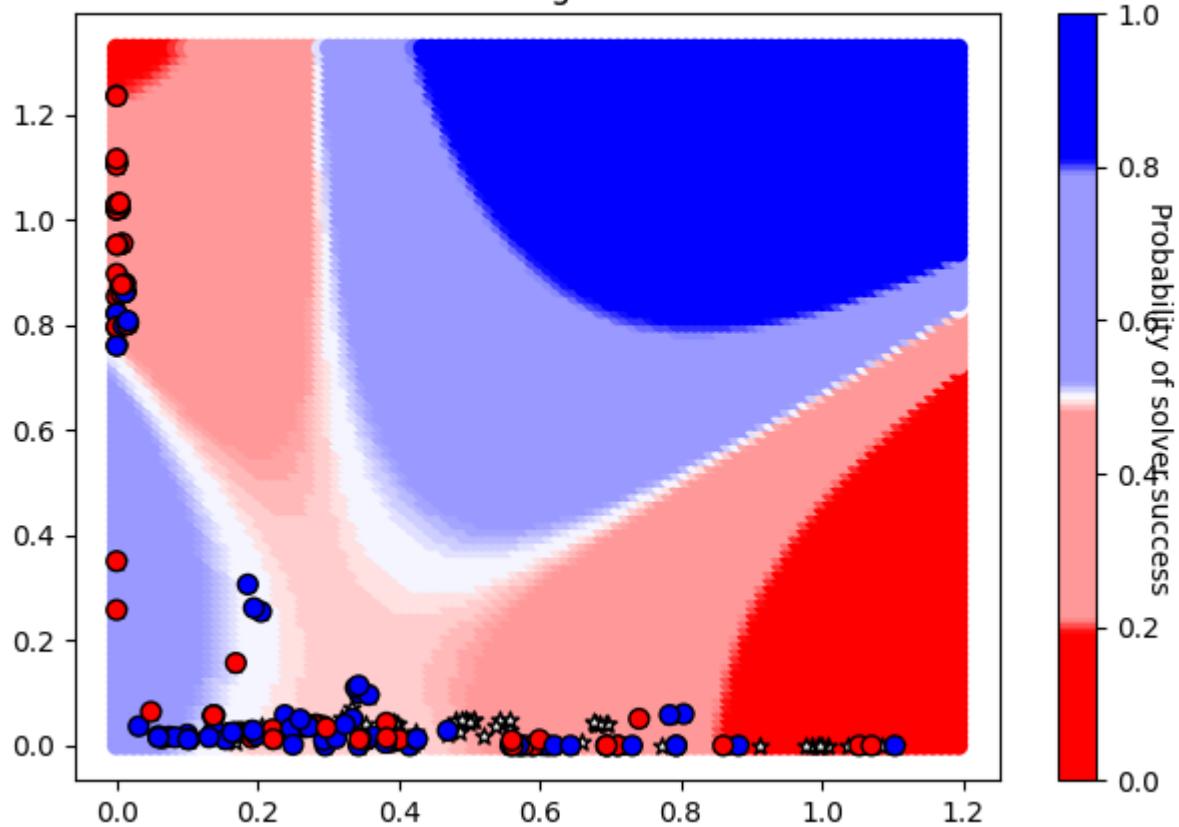
(captured: $\$1.8e+02/1.5e+07$, approximately $1.2e-03\%$)



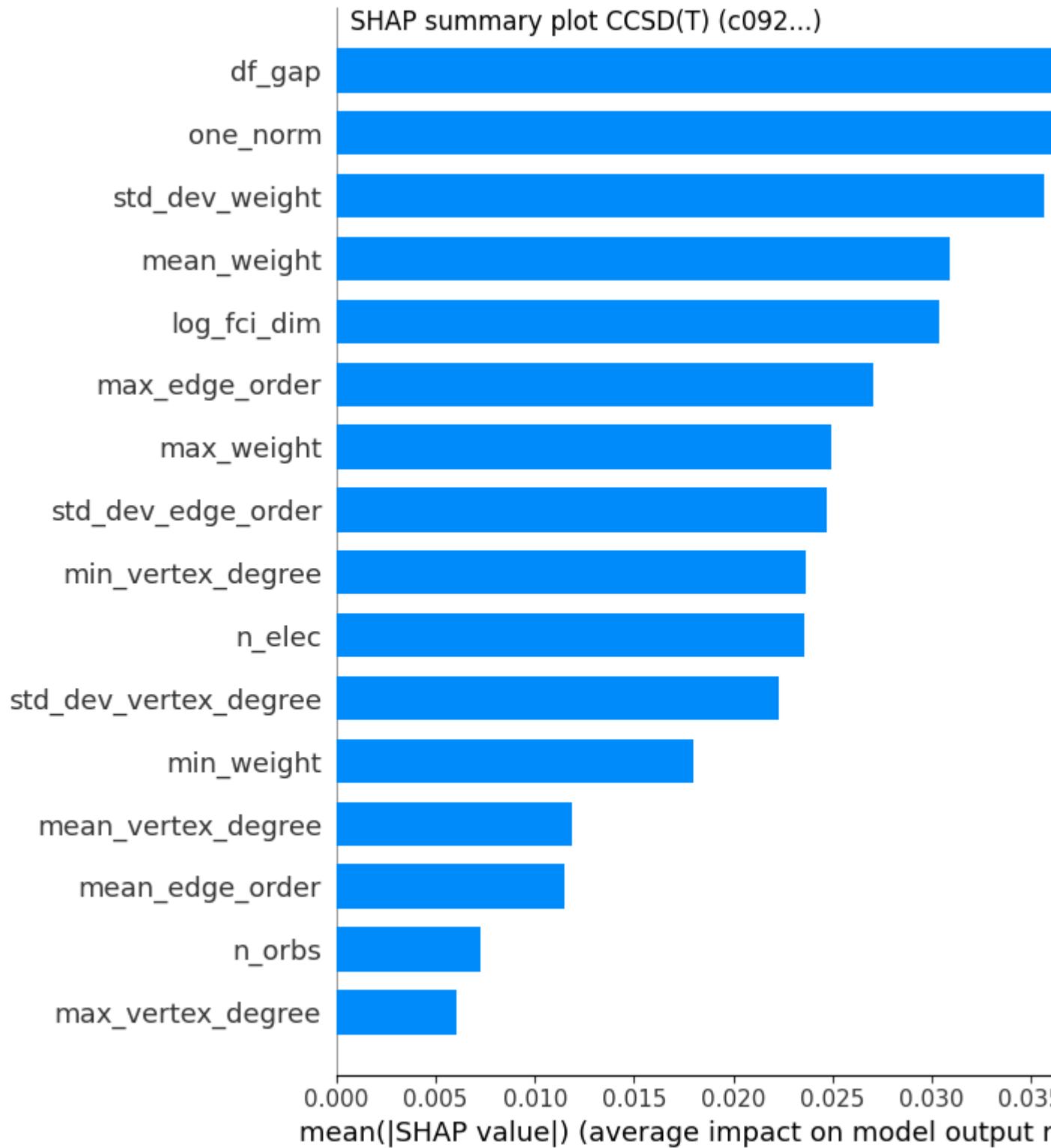
Solver CCSD(T) (c092...)
Embedding: PCA



Solver CCSD(T) (c092...)
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, 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': '1.3.4'}, {'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': '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:6a6781f9-bc5c-4fb6-b21b-268ce527c900

logical_resource_estimate_solver_uuid:f2d73e1f-3058-43c4-a634-b6c267c84ff1

performance_metrics_uuid: b45cb0d8-0ede-4012-ae87-2c088e6f4fbe

creation_timestamp: 2025-03-06T19:54:13.195807+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: 143762960615180.72

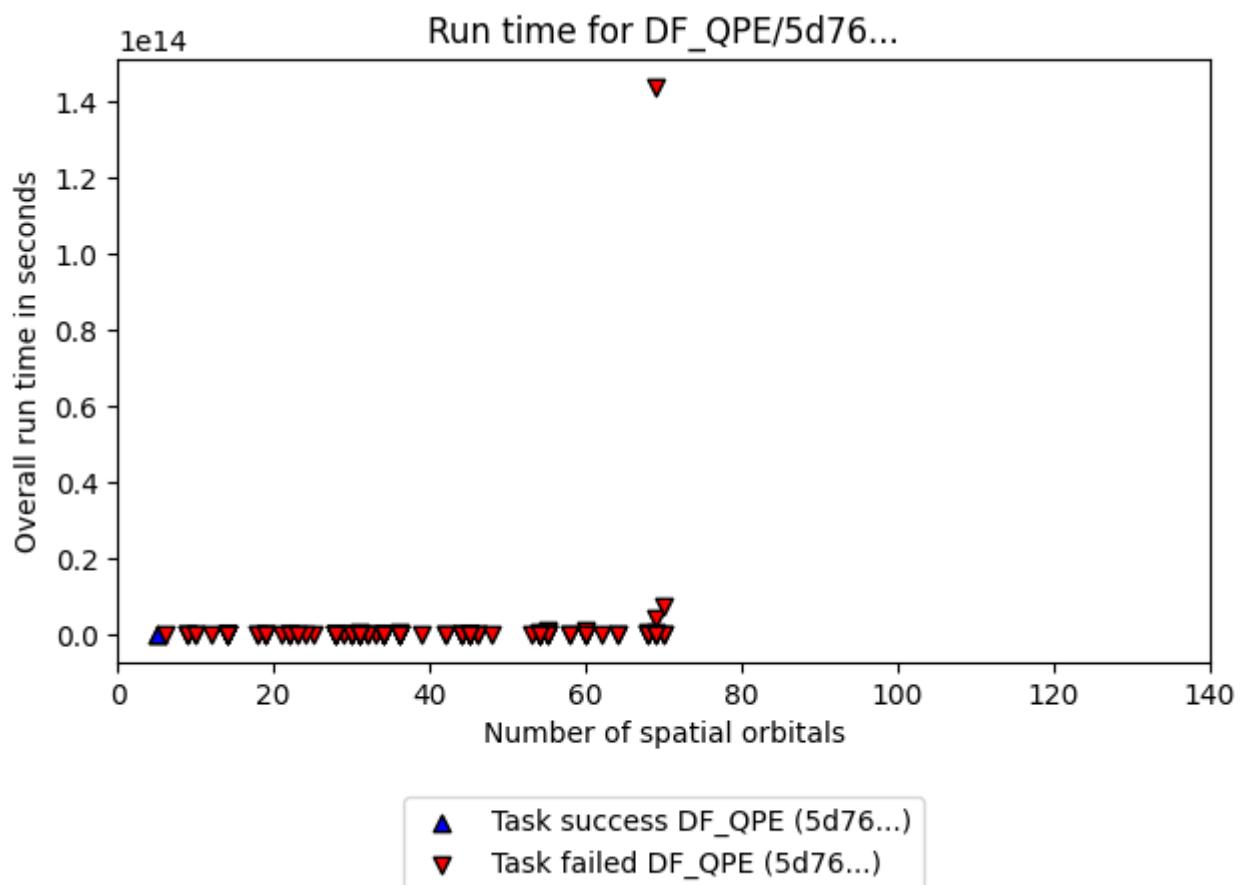
sum_of_run_time_of_attempted_tasks: 164517943847731.3

solvability_ratio: 0.0394

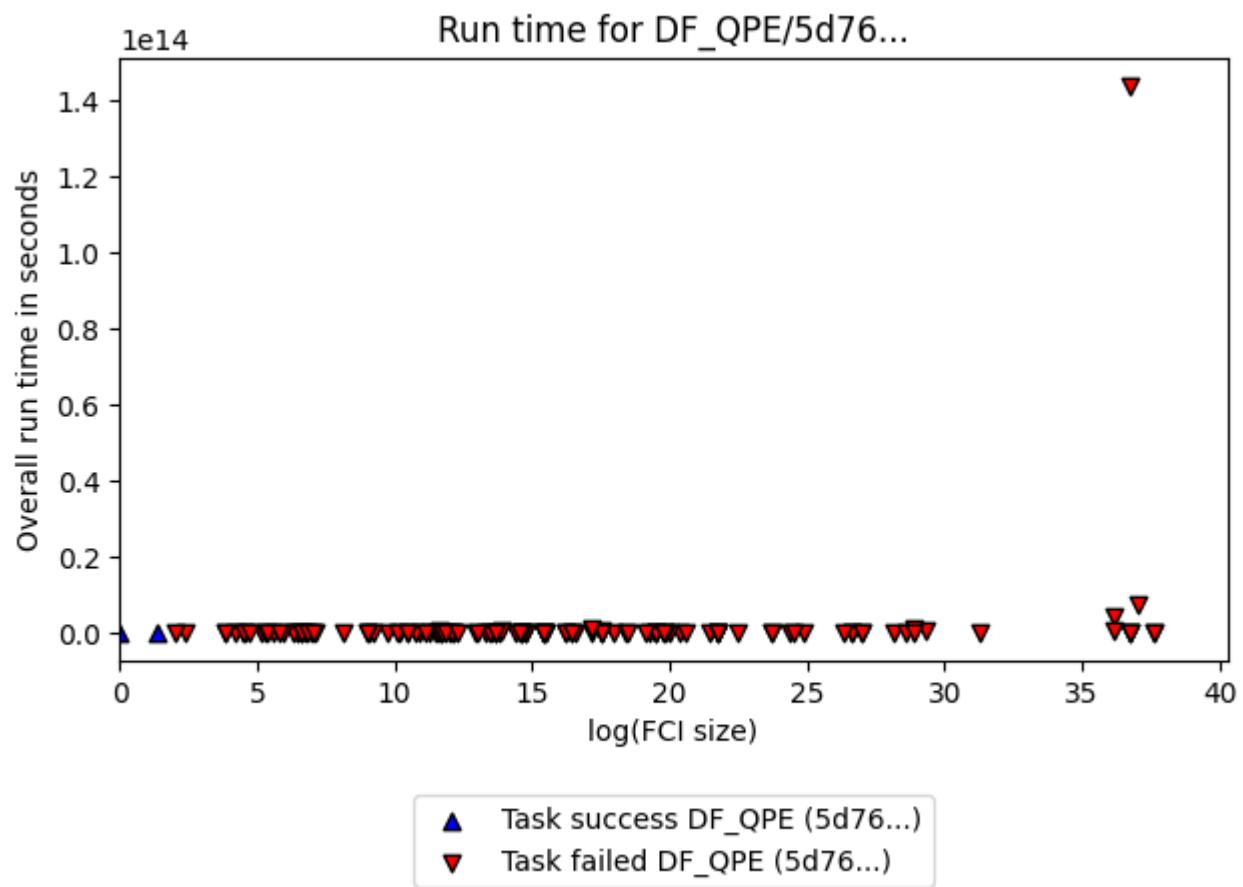
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



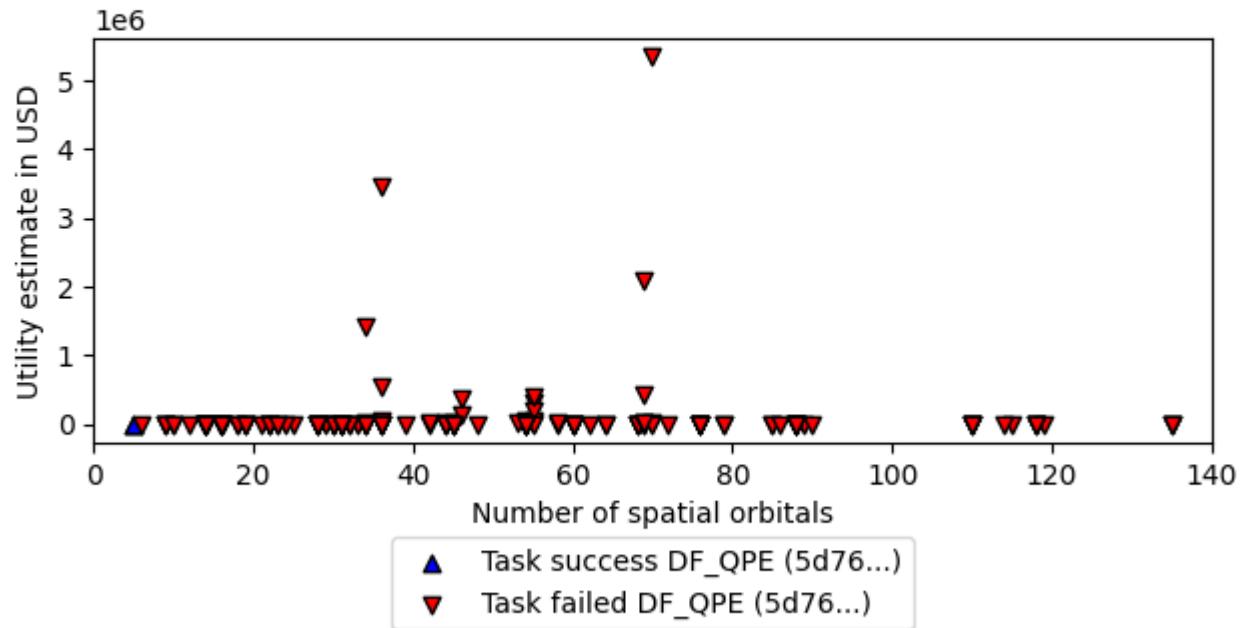
Note: plot only contains attempted tasks.



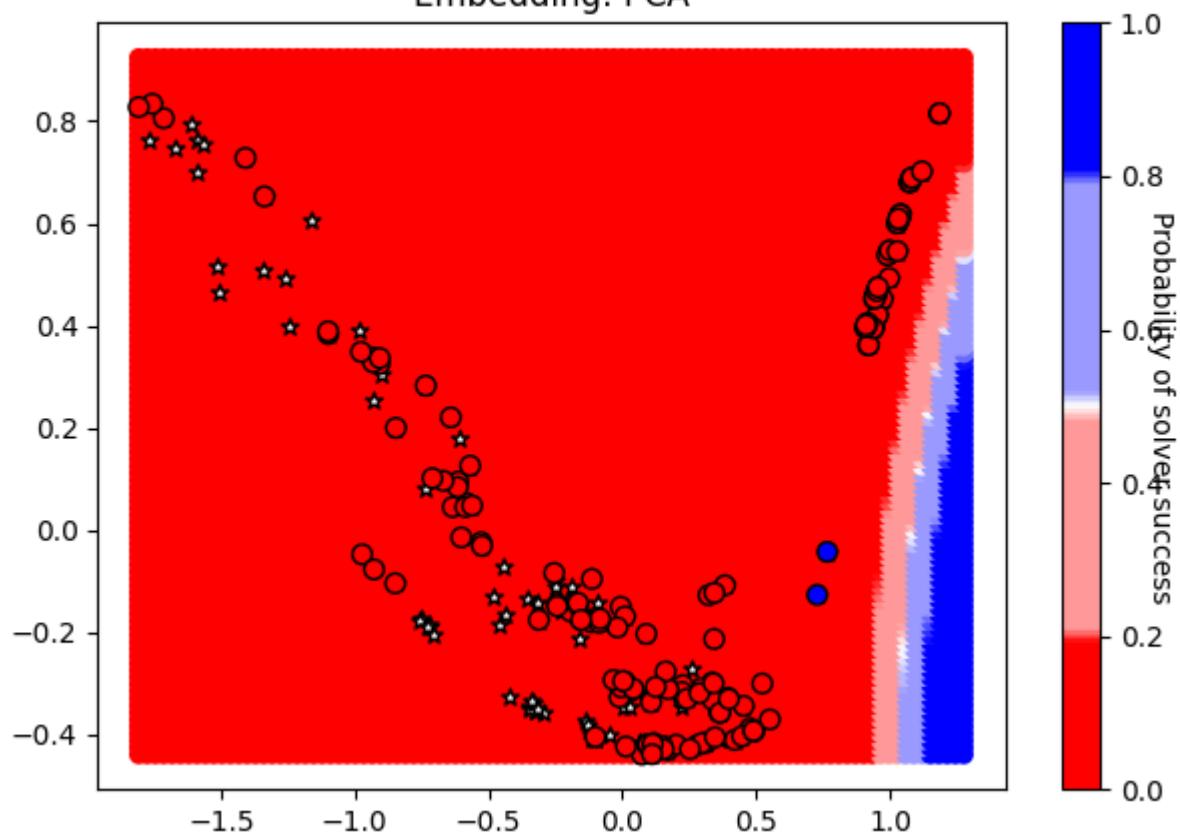
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5d76...

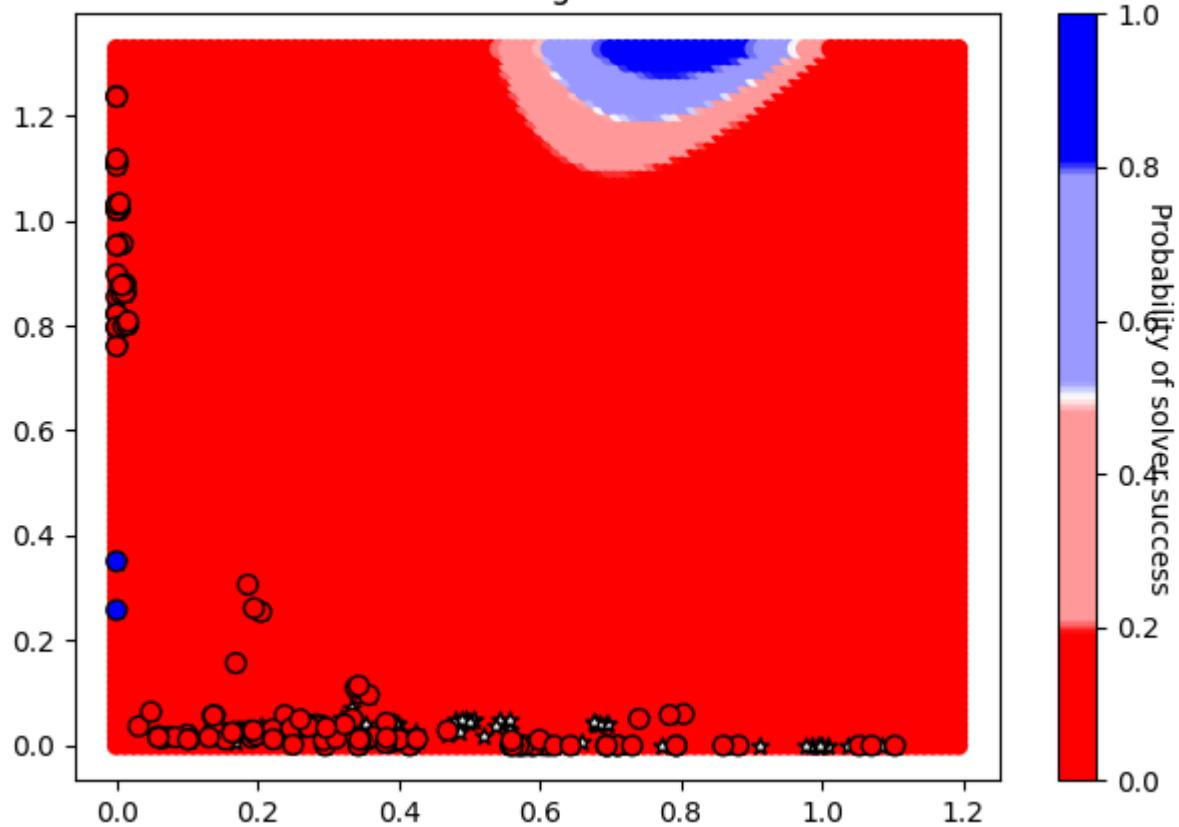
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



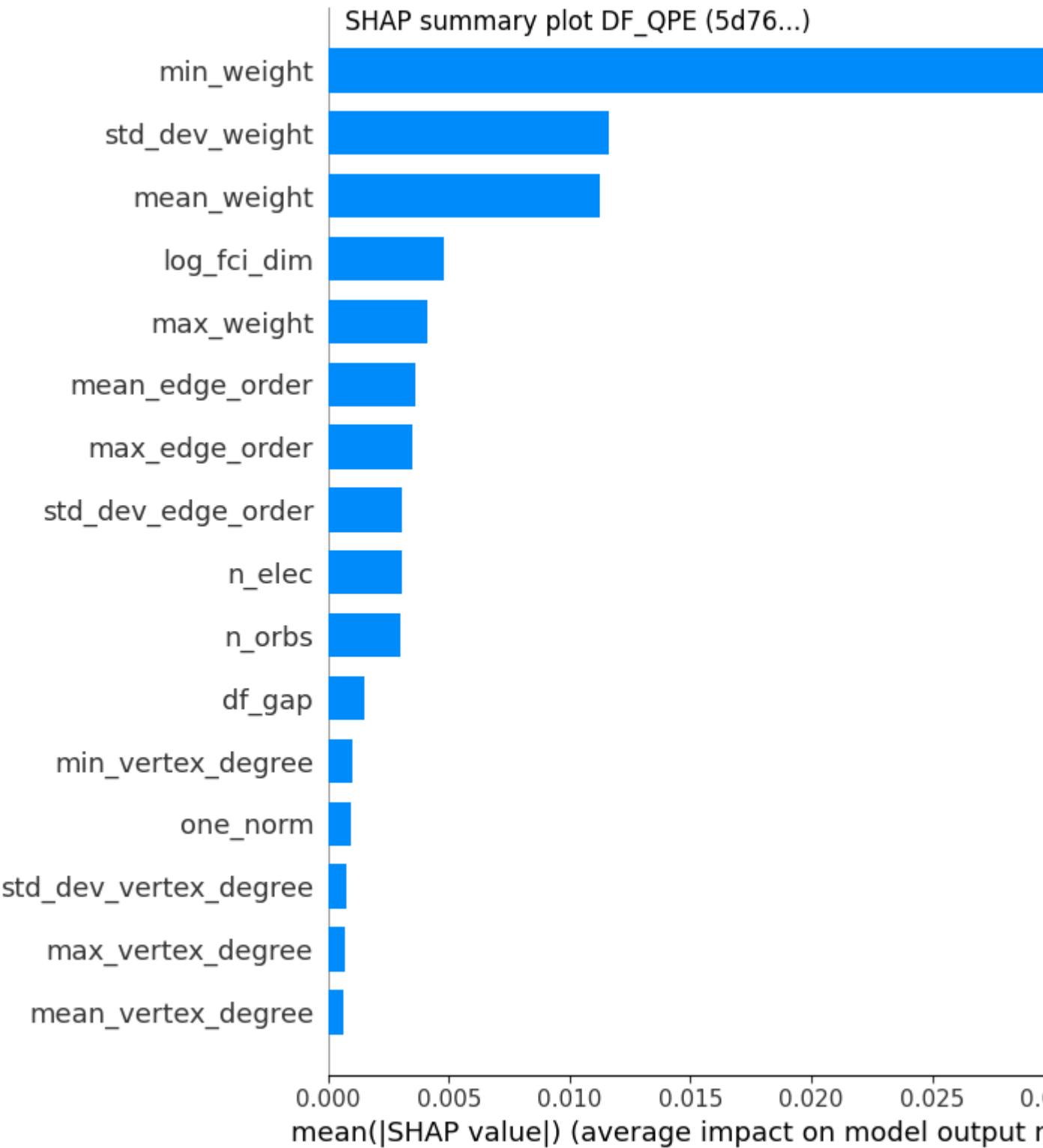
Solver DF_QPE (5d76...)
Embedding: PCA



Solver DF_QPE (5d76...)
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': '1.3.4'}, {'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': '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:d837d3d6-c954-495f-8f87-d93f85f1be21

logical_resource_estimate_solver_uuid:f2d73e1f-3058-43c4-a634-b6c267c84ff1

performance_metrics_uuid: 66a825e9-068a-4e6b-8858-03e7b394b417

creation_timestamp: 2025-03-06T19:54:13.195807+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: 14376296065792.11

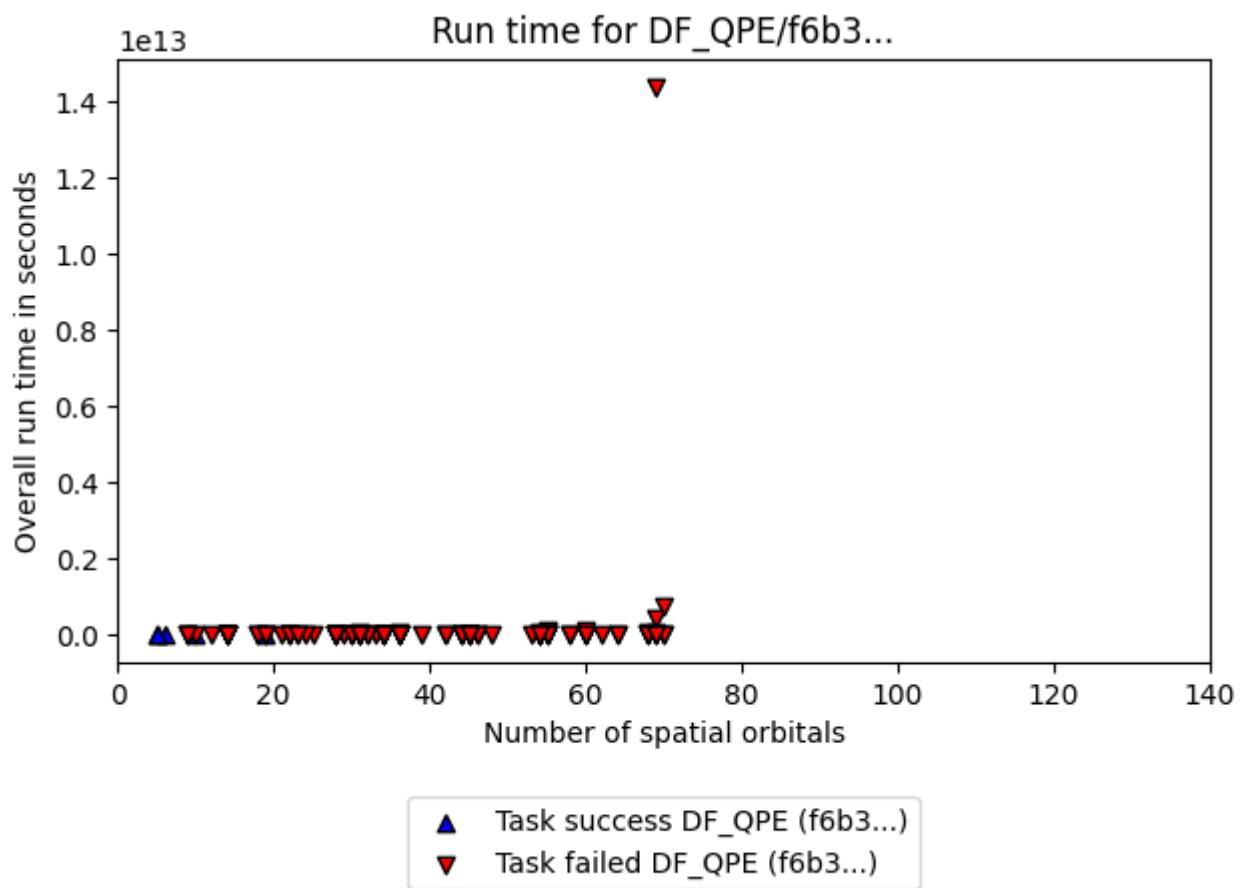
sum_of_run_time_of_attempted_tasks: 16451794516511.004

solvability_ratio: 0.013

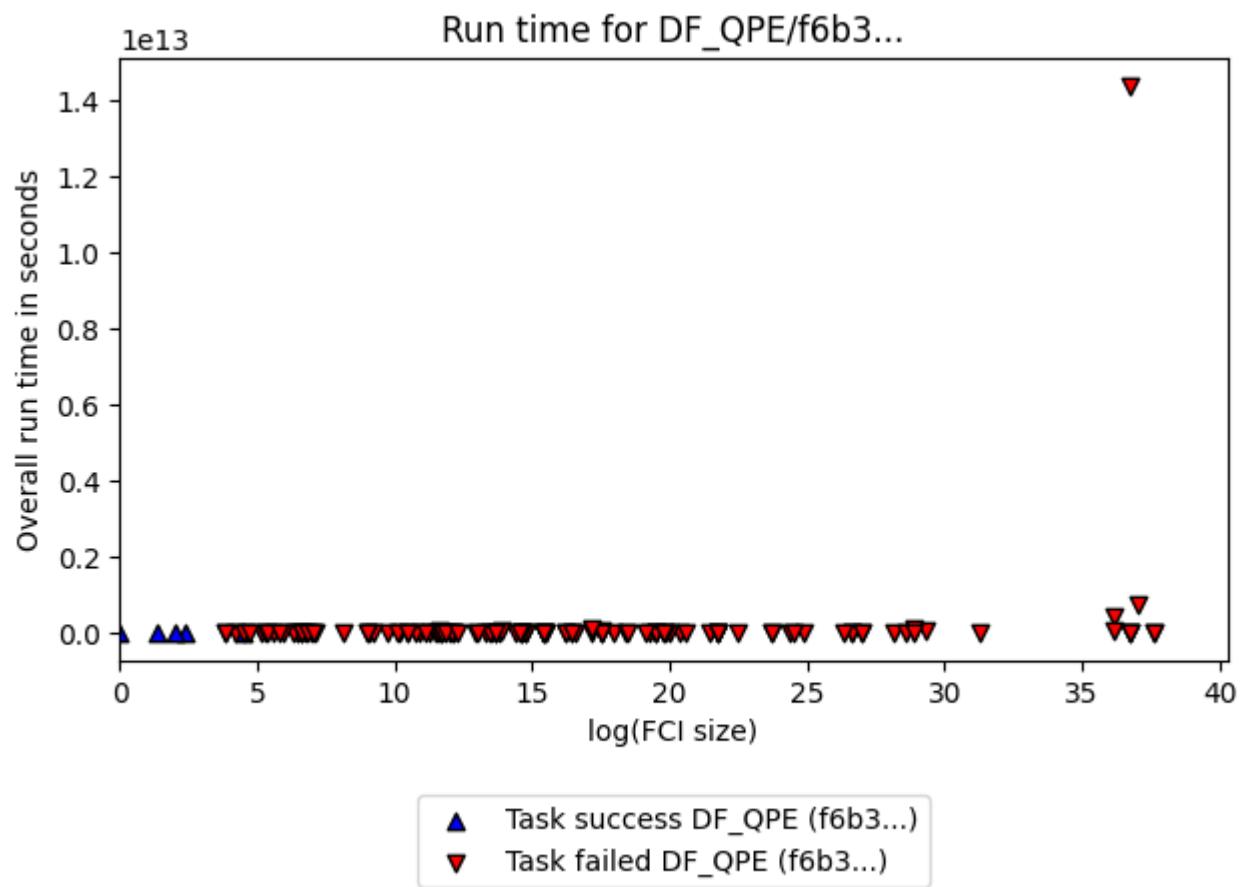
comment: solvability ratio based on PCA embedding.

f1_score: [0.9931972789115646, 0.8333333333333334]

ml_metrics_calculator_version: 1



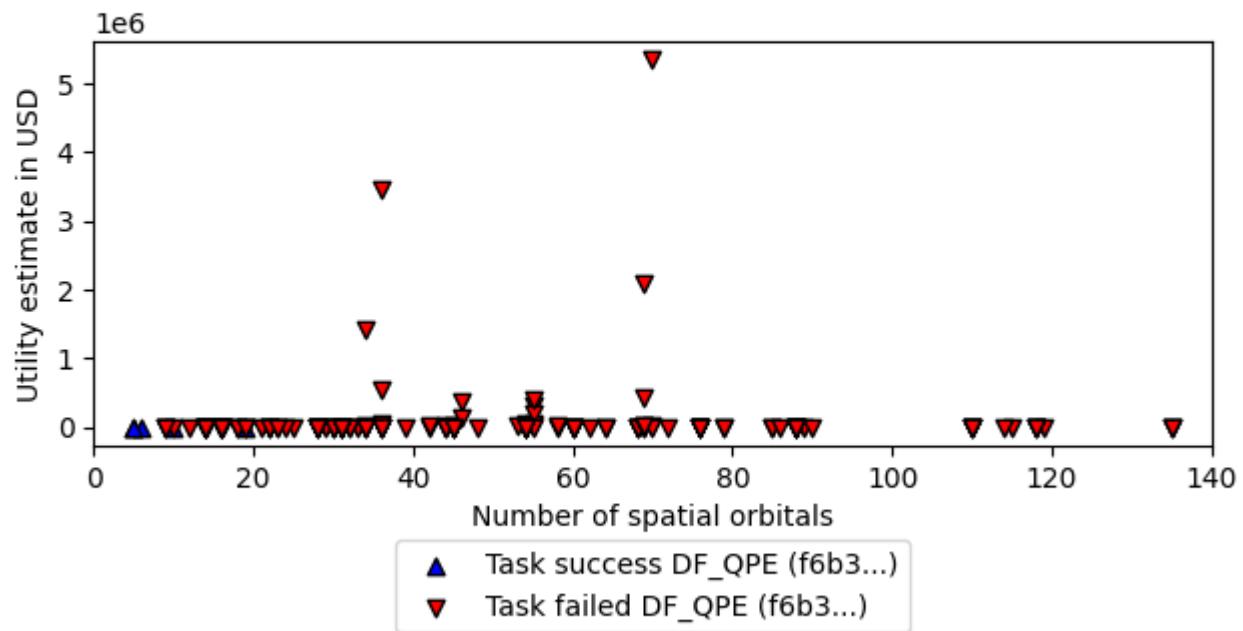
Note: plot only contains attempted tasks.



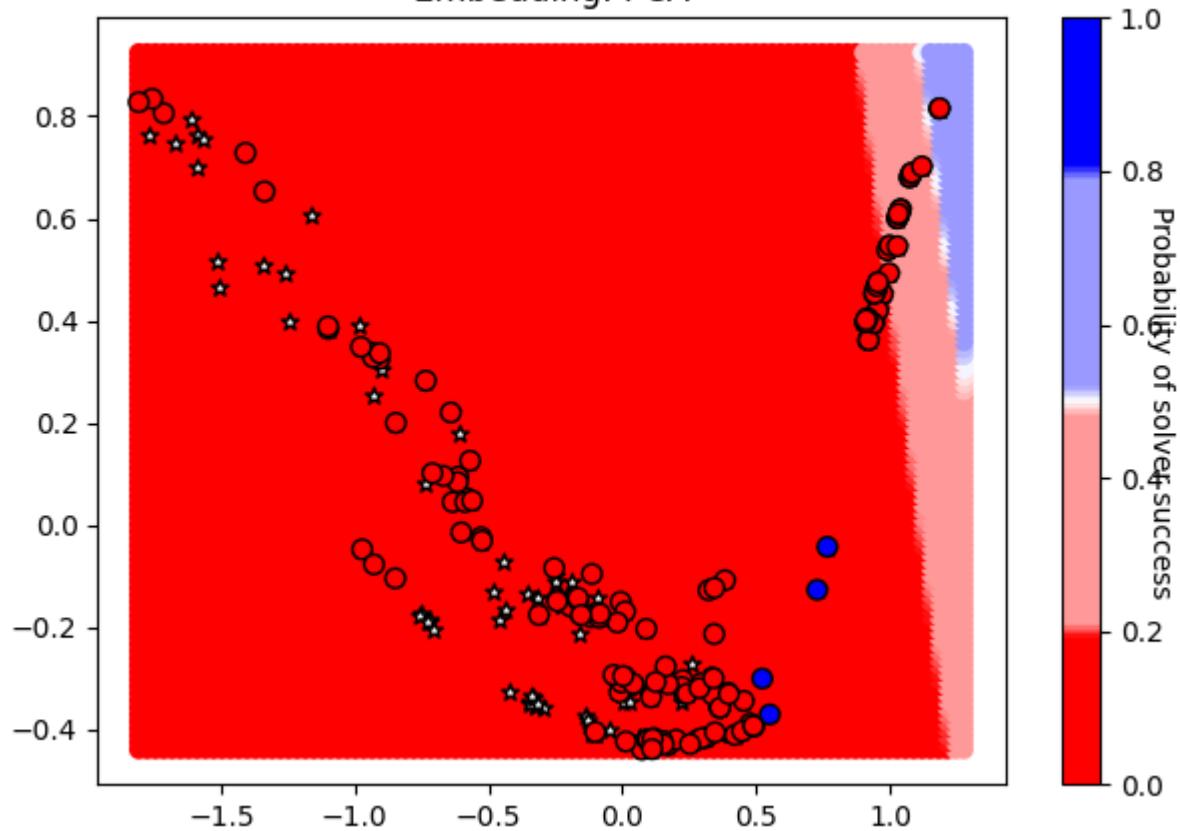
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/f6b3...

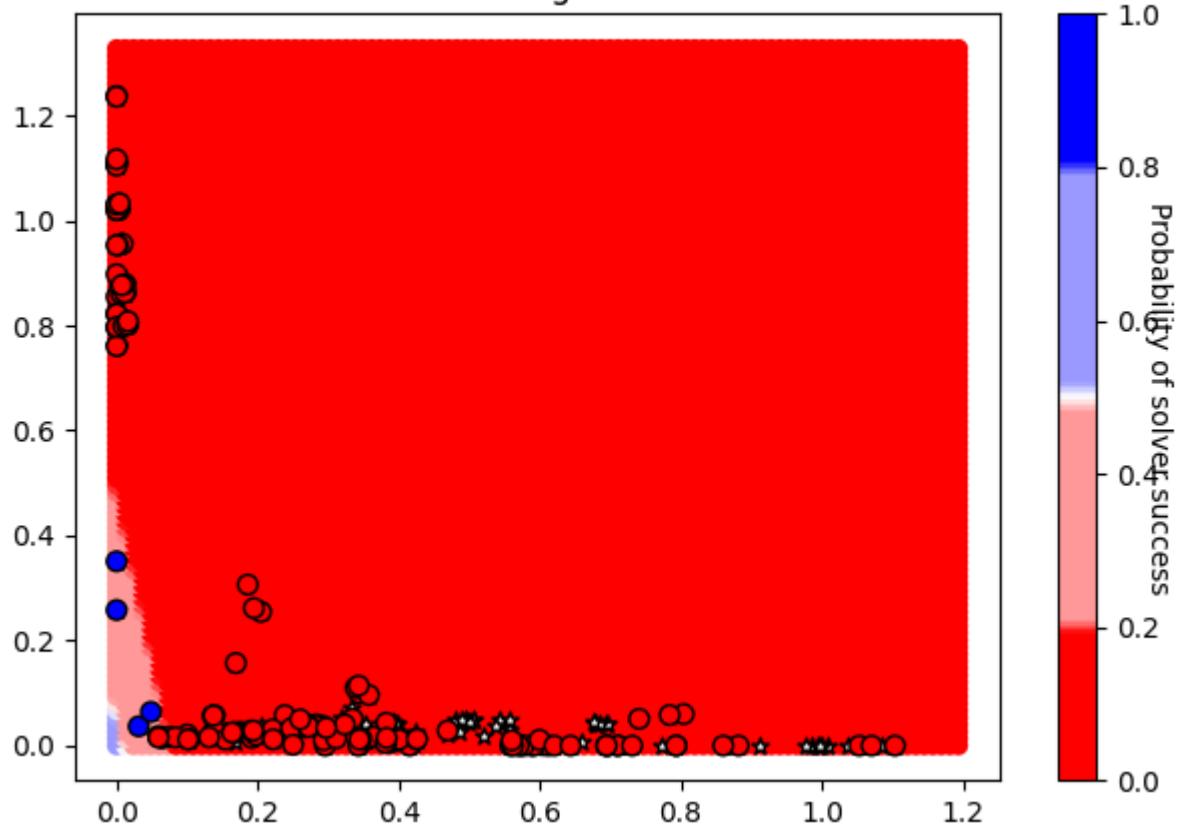
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



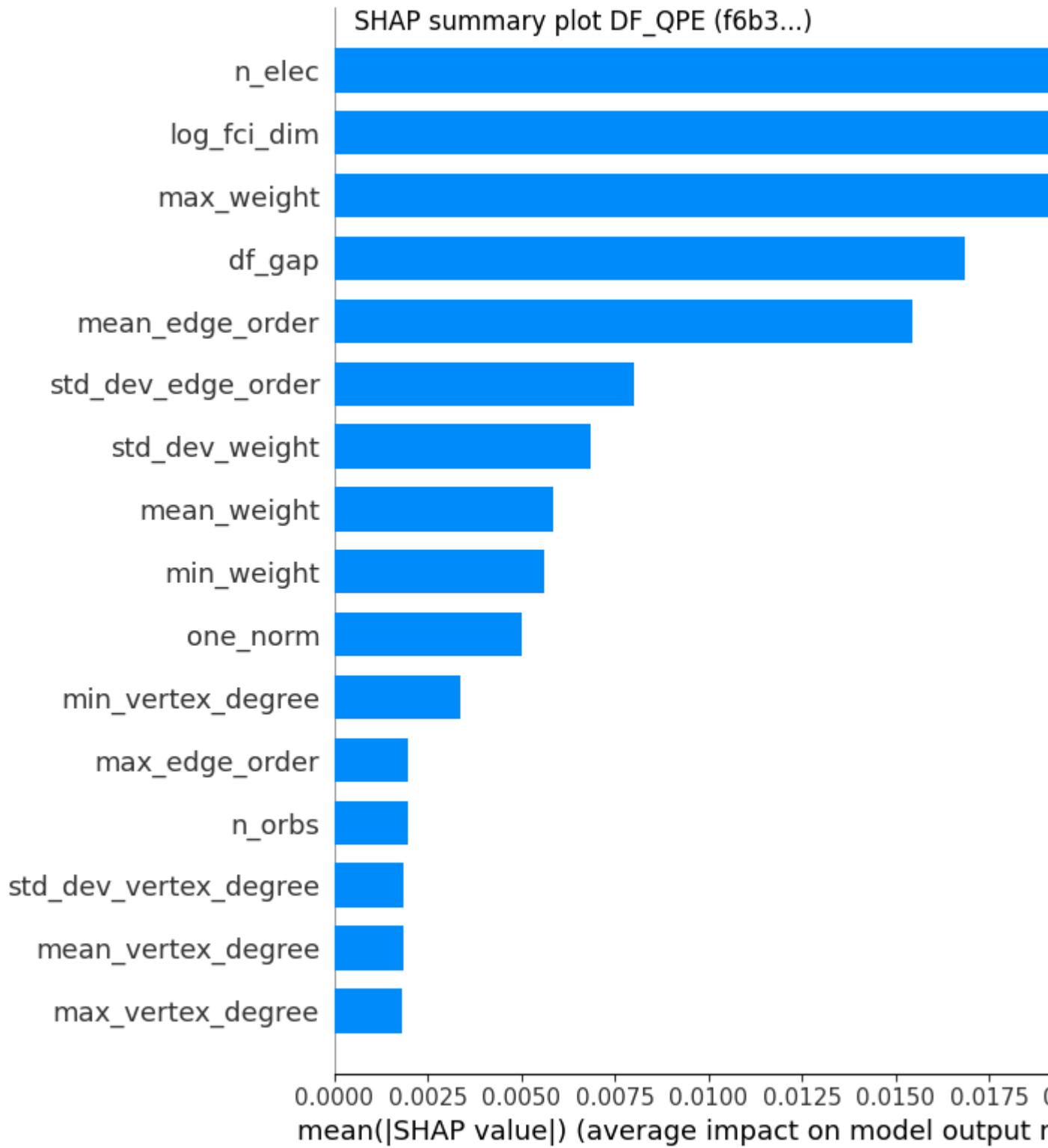
Solver DF_QPE (f6b3...)
Embedding: PCA



Solver DF_QPE (f6b3...)
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, 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': '1.3.4'}, {'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. 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:94b387a7-0256-4b81-aff5-d0f69eb5656c

logical_resource_estimate_solver_uuid:f2d73e1f-3058-43c4-a634-b6c267c84ff1

performance_metrics_uuid: 3510f73b-bf61-45b5-9bff-2ee82ce84c94

creation_timestamp: 2025-03-06T19:54:13.195807+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: 28597112908.874496

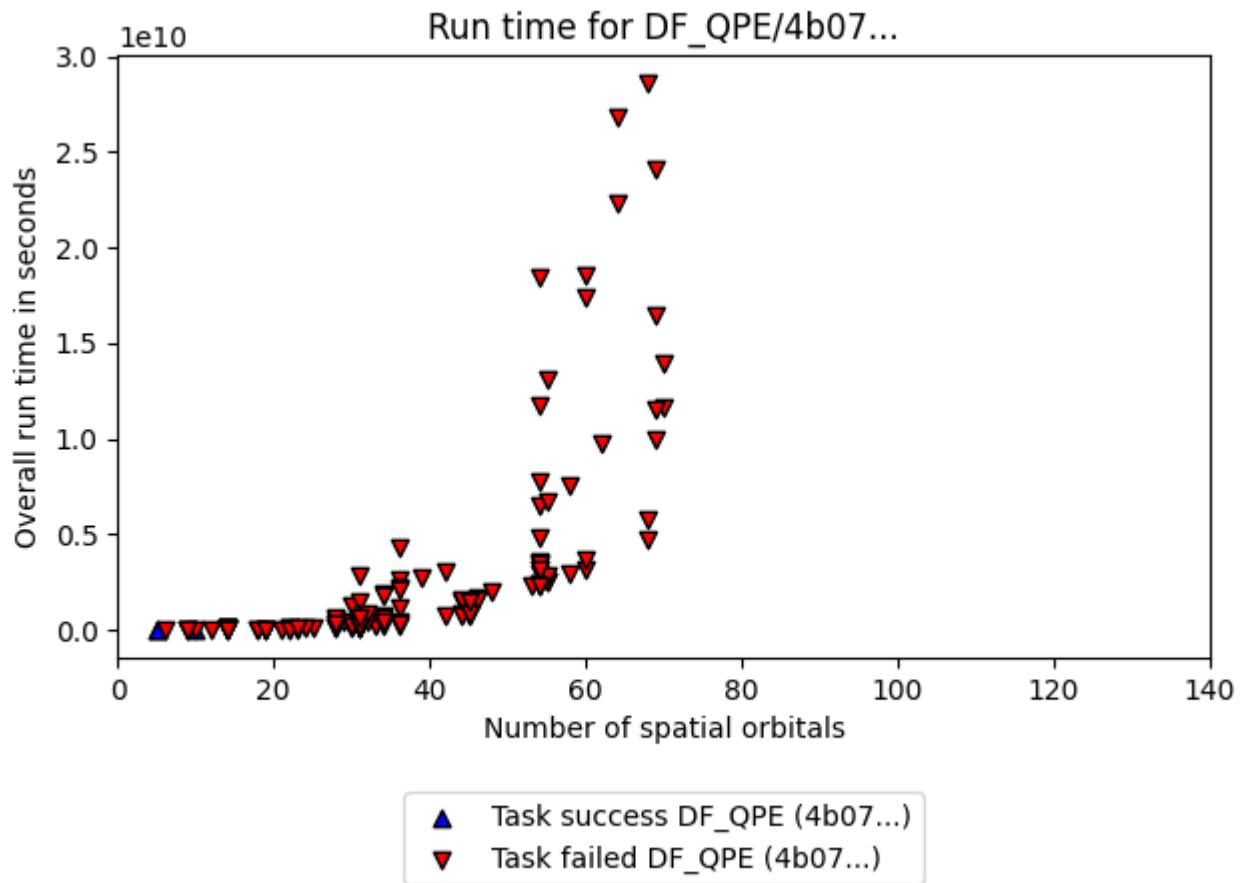
sum_of_run_time_of_attempted_tasks: 407899131893.85156

solvability_ratio: 0.0

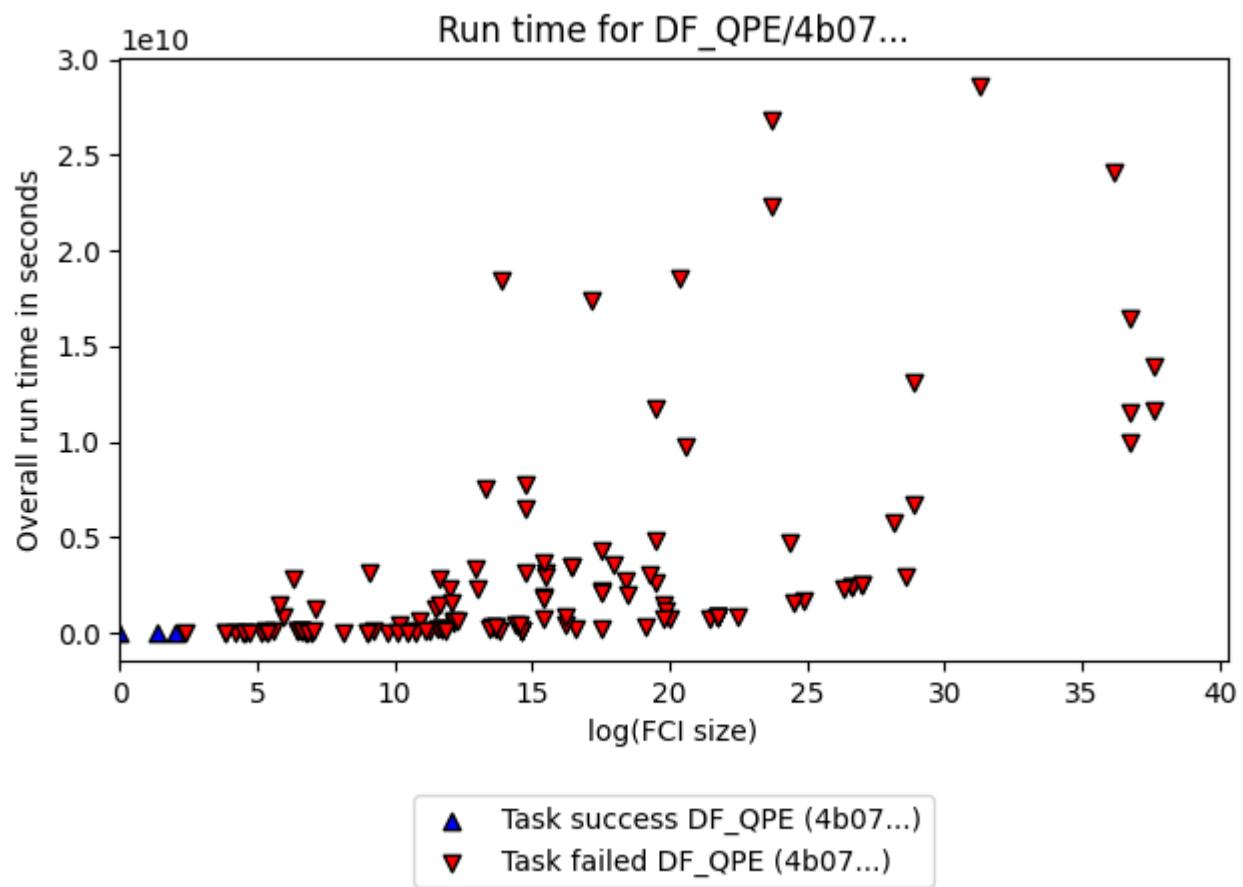
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



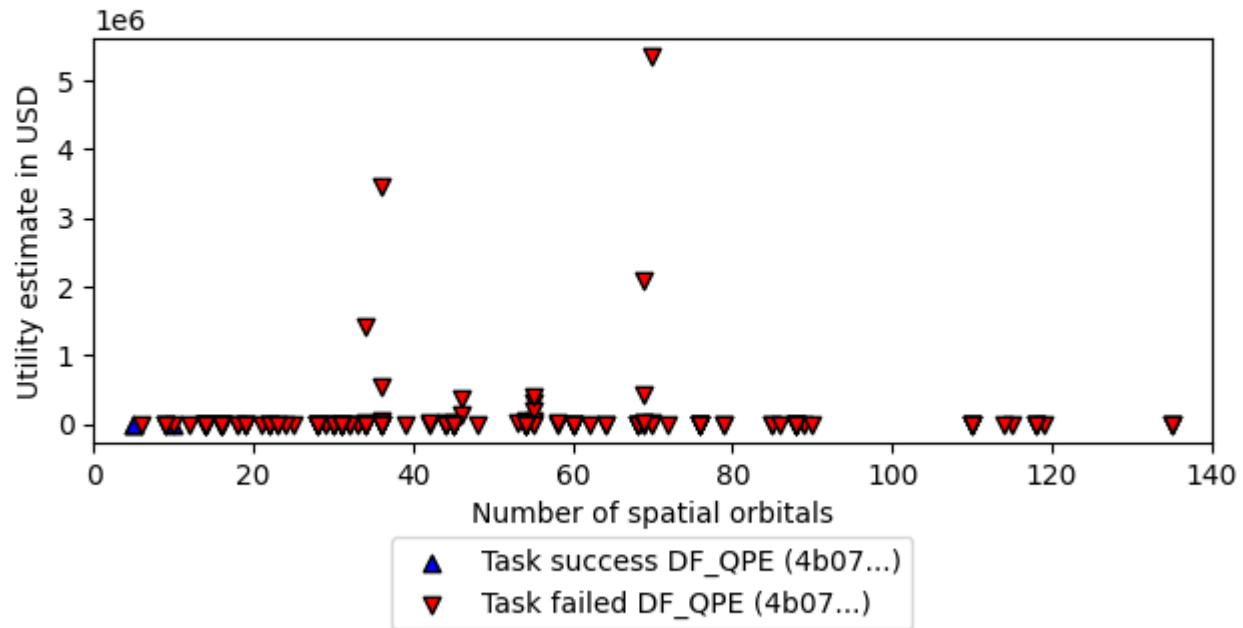
Note: plot only contains attempted tasks.



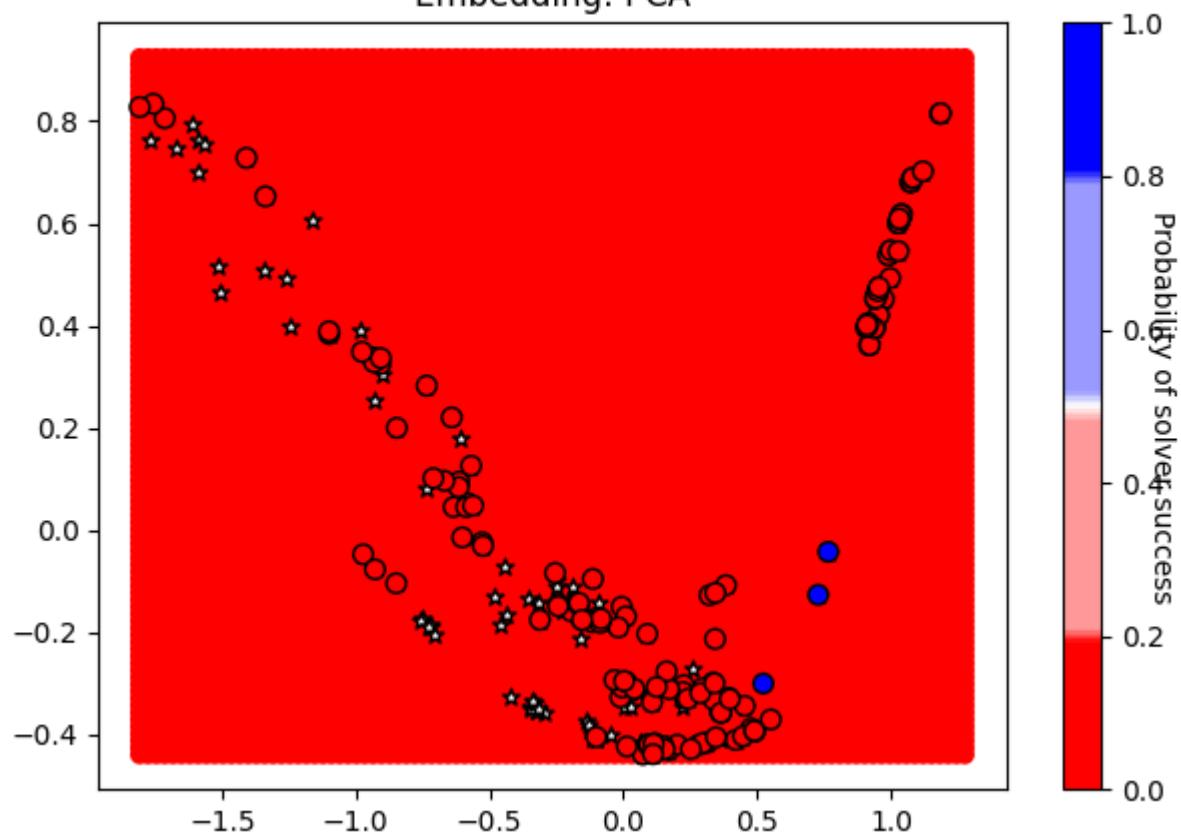
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/4b07...

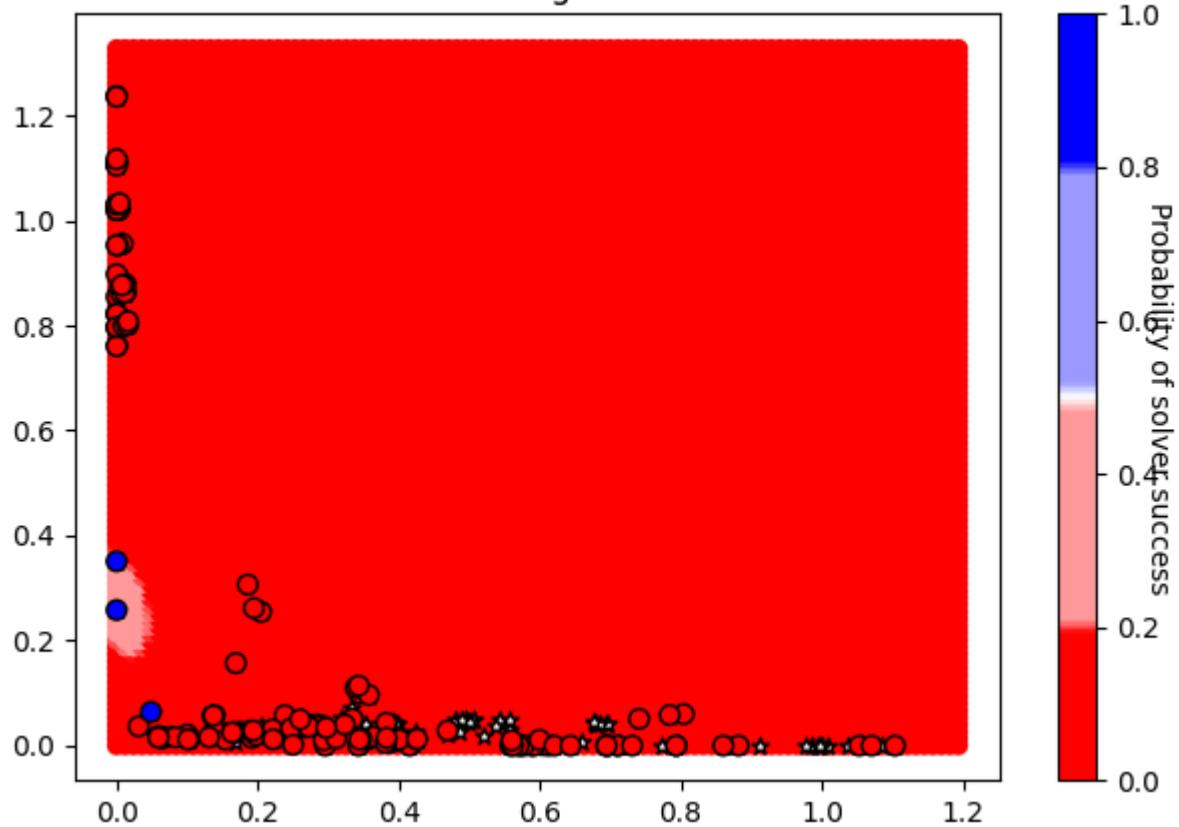
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



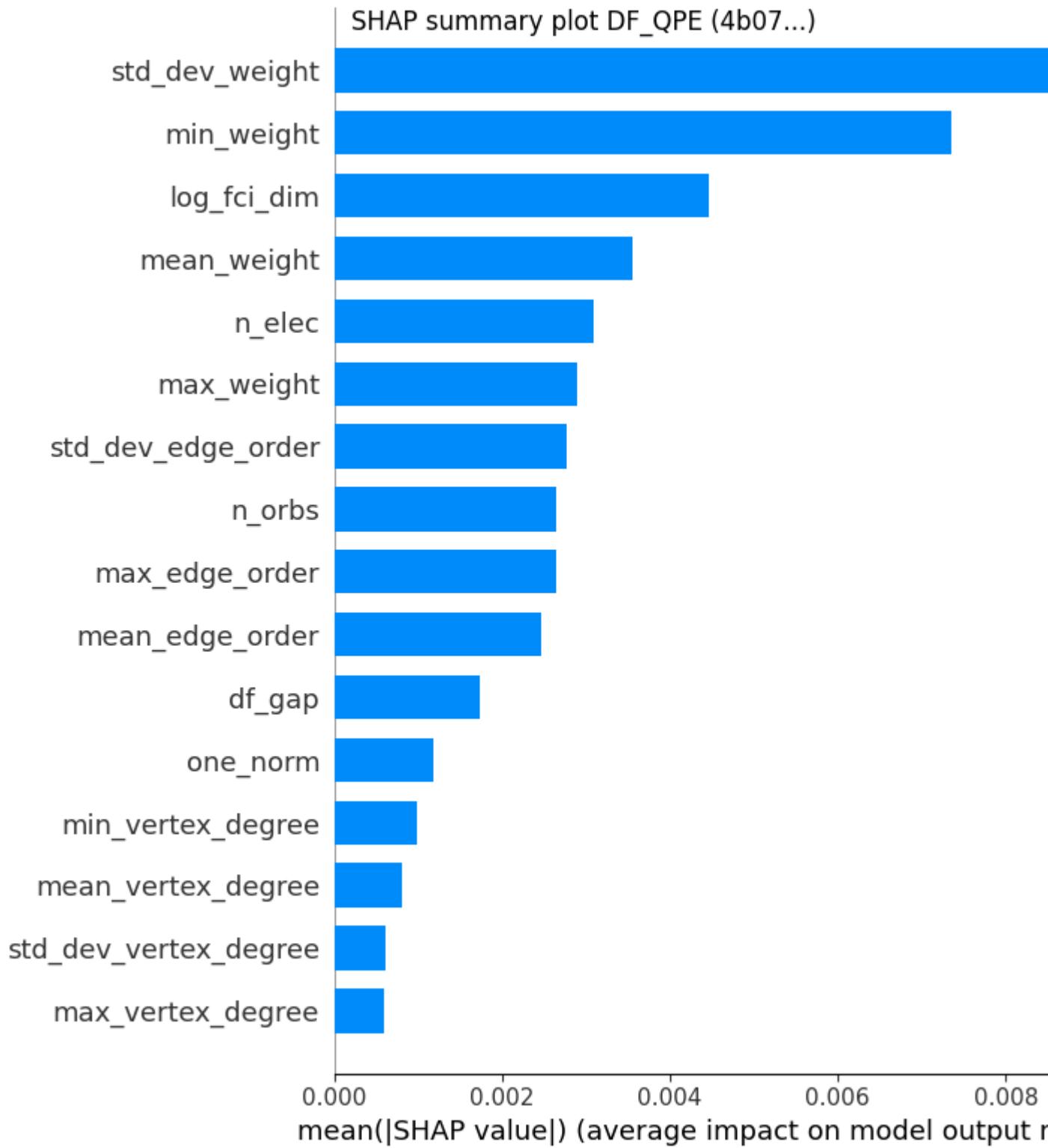
Solver DF_QPE (4b07...)
Embedding: PCA



Solver DF_QPE (4b07...)
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.

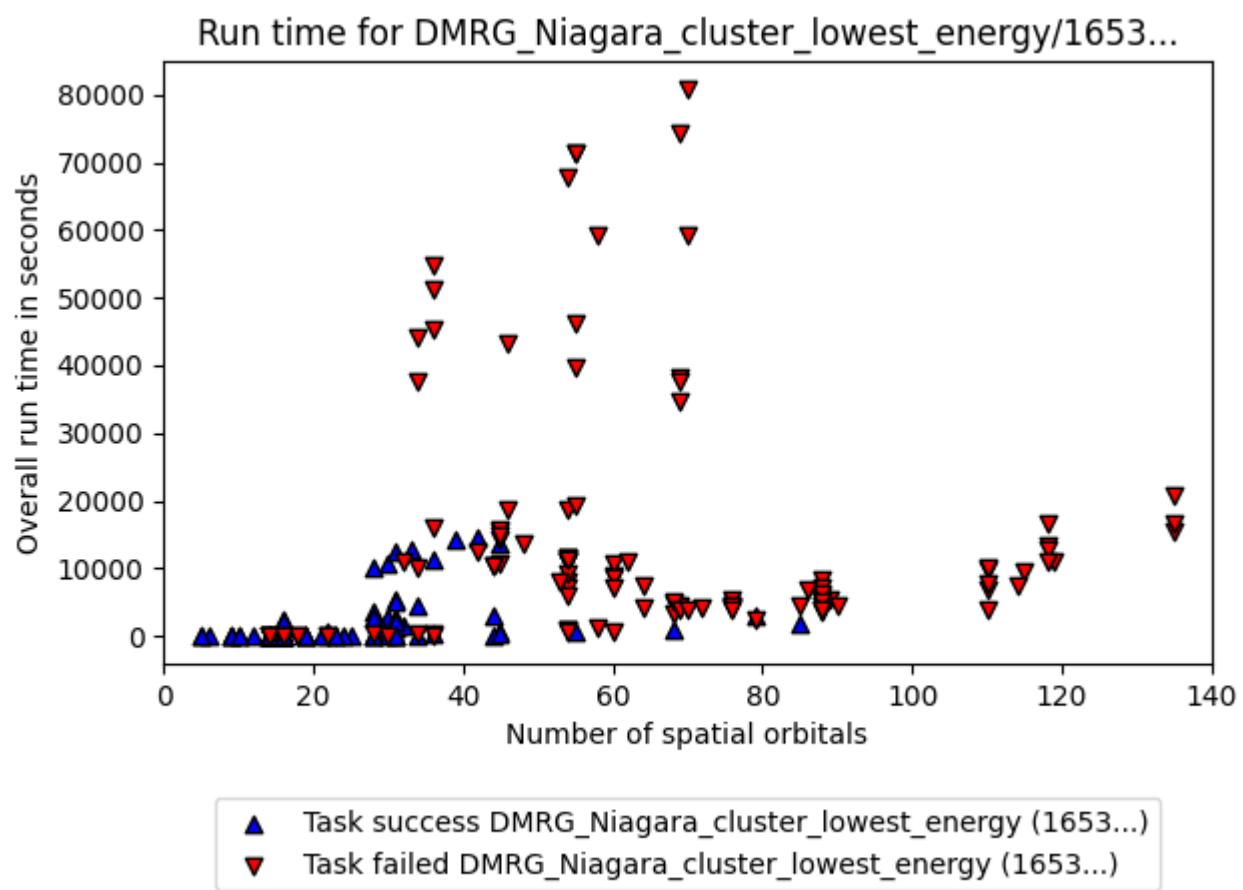


Solver DMRG_Niagara_cluster_lowest_energy, 16537433-9f4c-4eae-a65d-787dc3b35b59

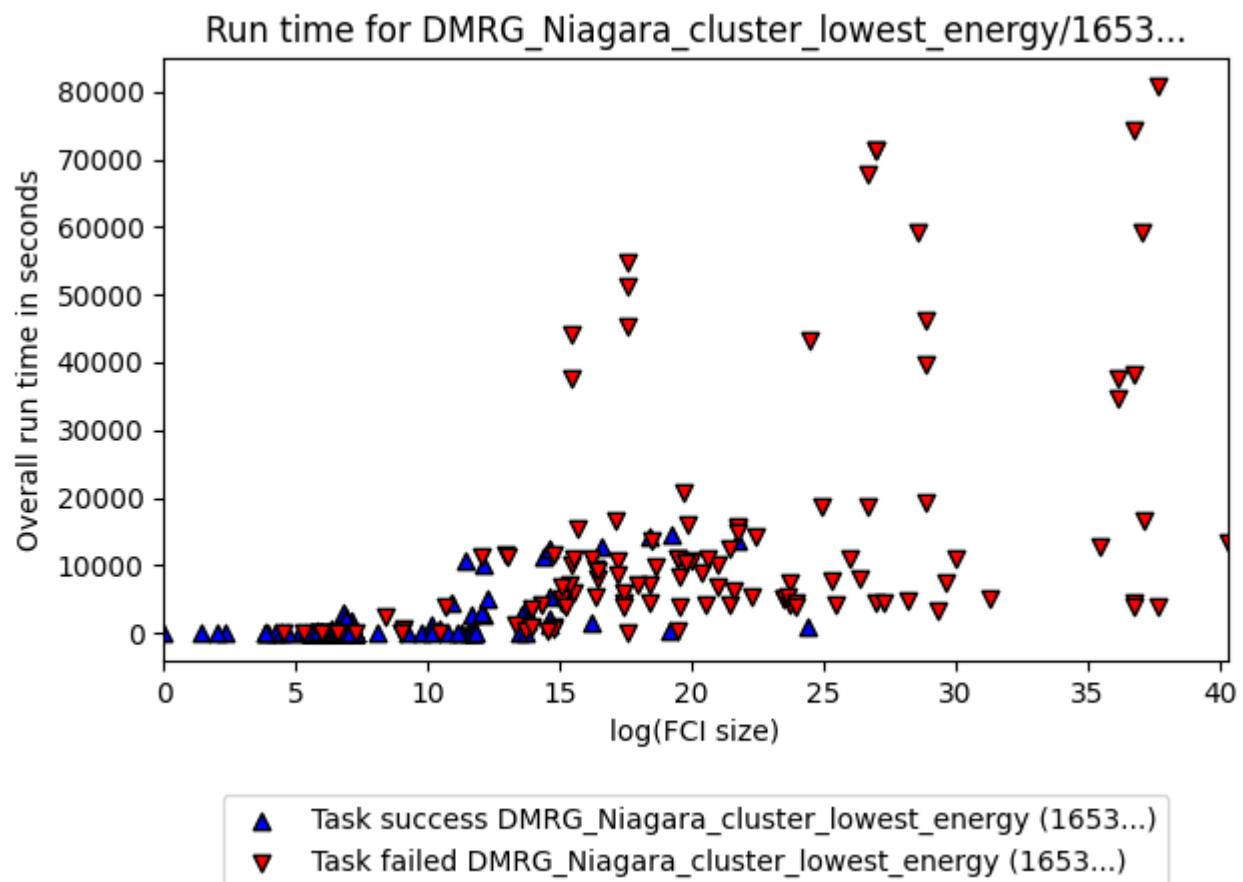
solver_uuid:16537433-9f4c-4eae-a65d-787dc3b35b59

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: 8220709d-362c-41a0-bf31-3126b7f6fa87
creation_timestamp: 2025-03-06T19:54:13.195807+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
comment: solvability ratio based on PCA embedding.
f1_score: [0.9130434782608695, 0.9626168224299065]
ml_metrics_calculator_version: 1



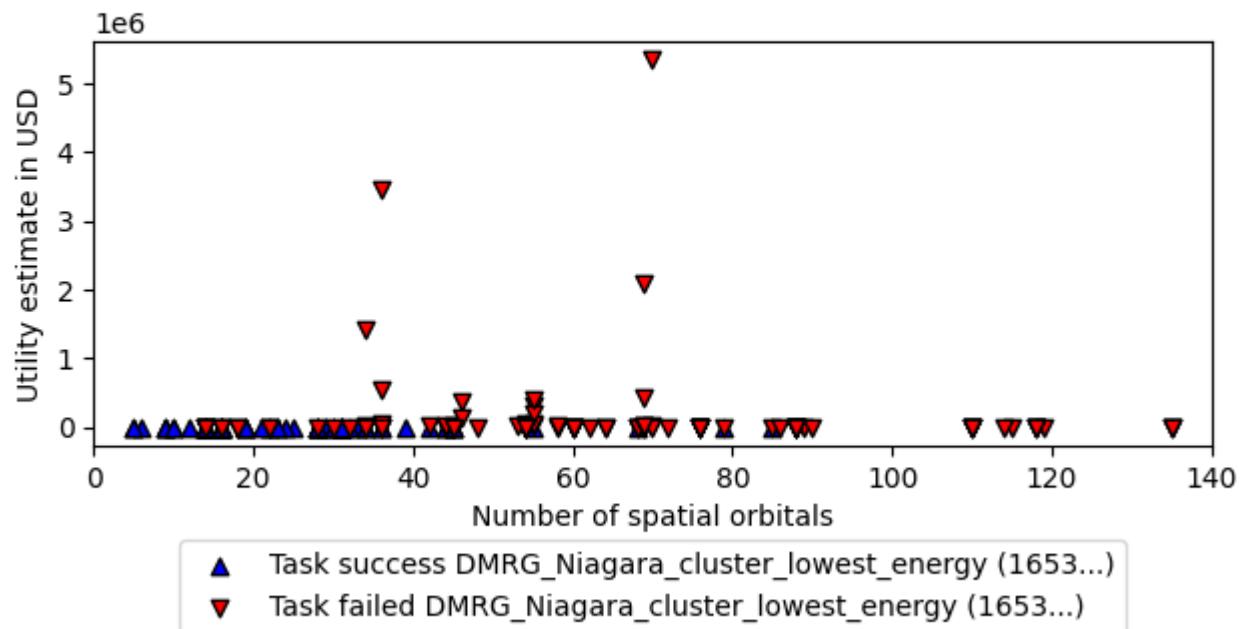
Note: plot only contains attempted tasks.



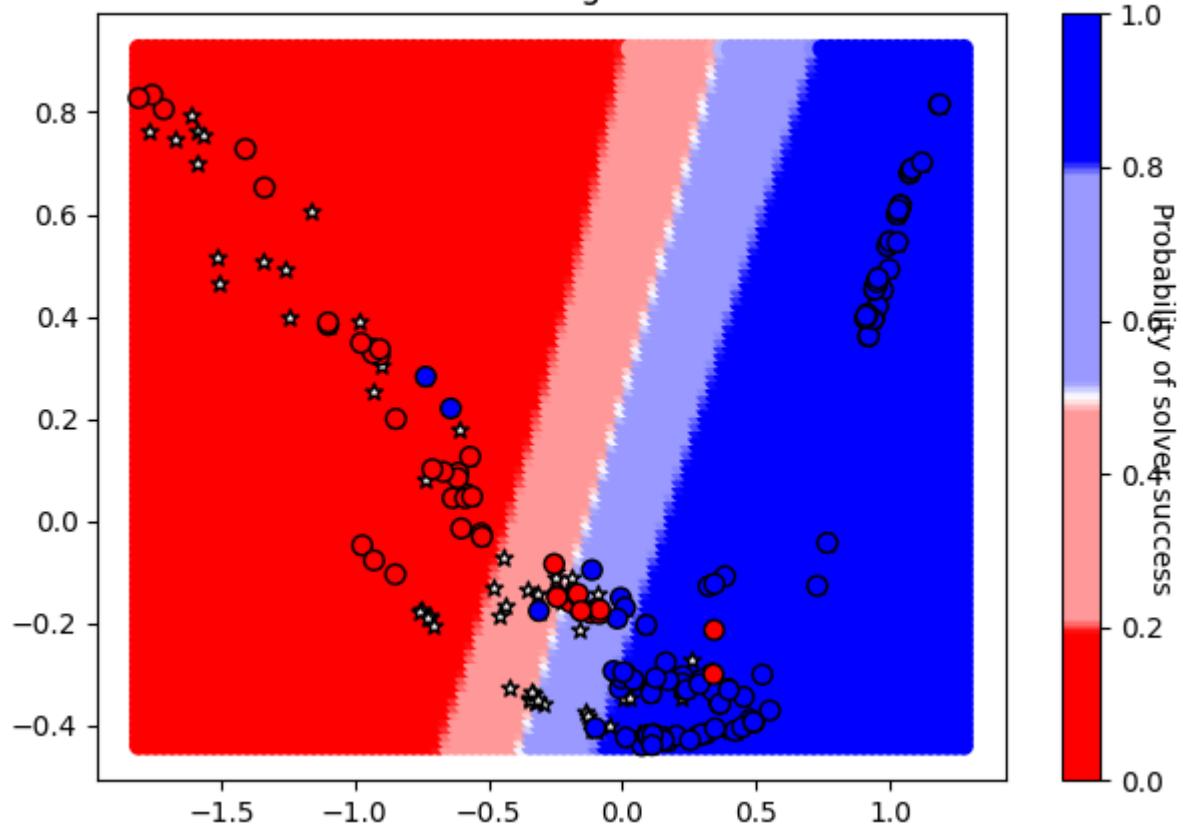
Note: plot only contains attempted tasks.

Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..

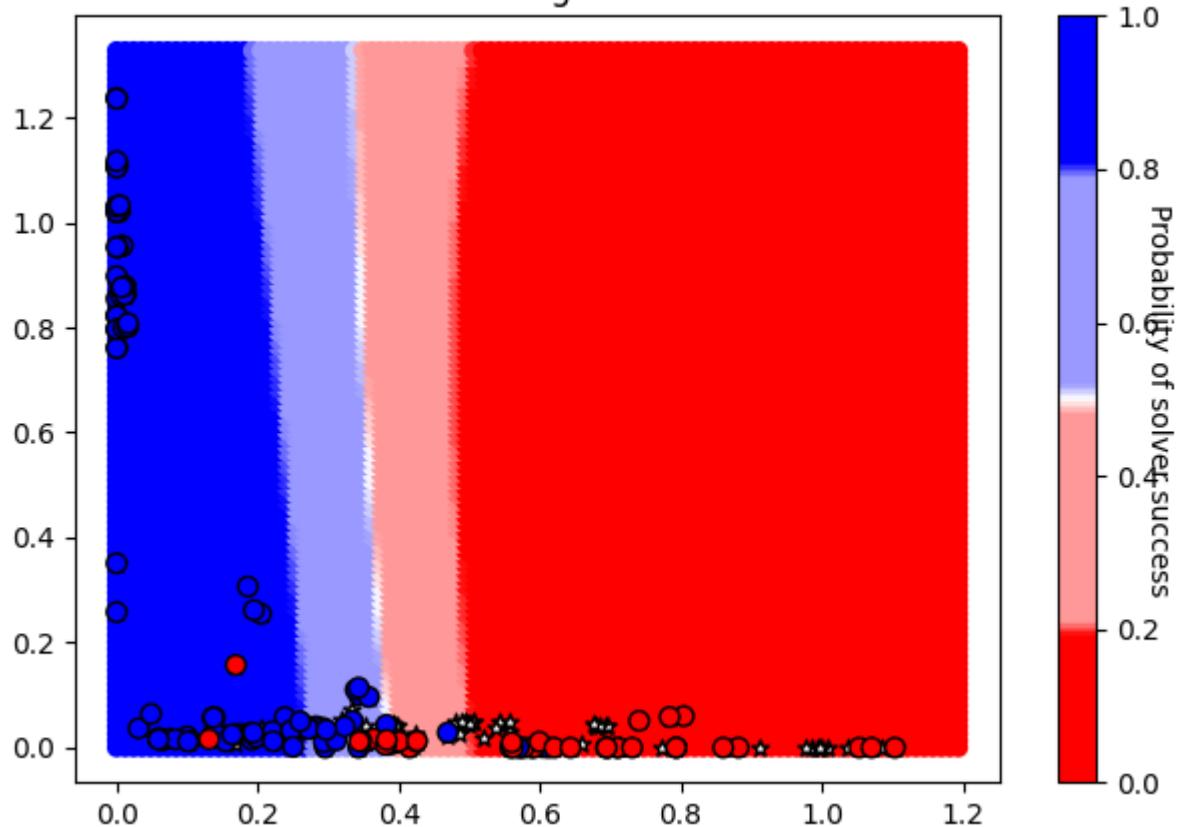
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: PCA

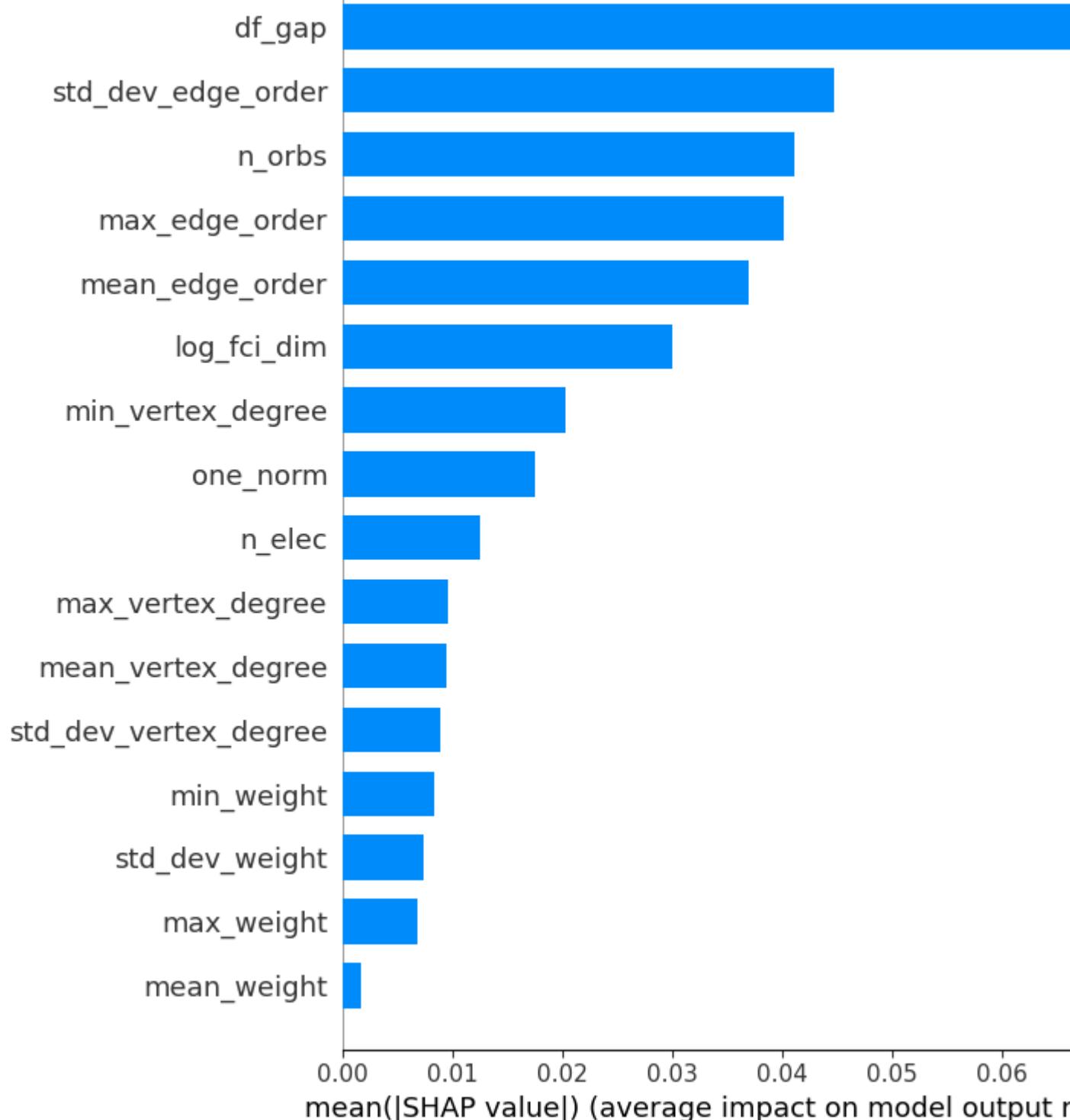


Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: NMF

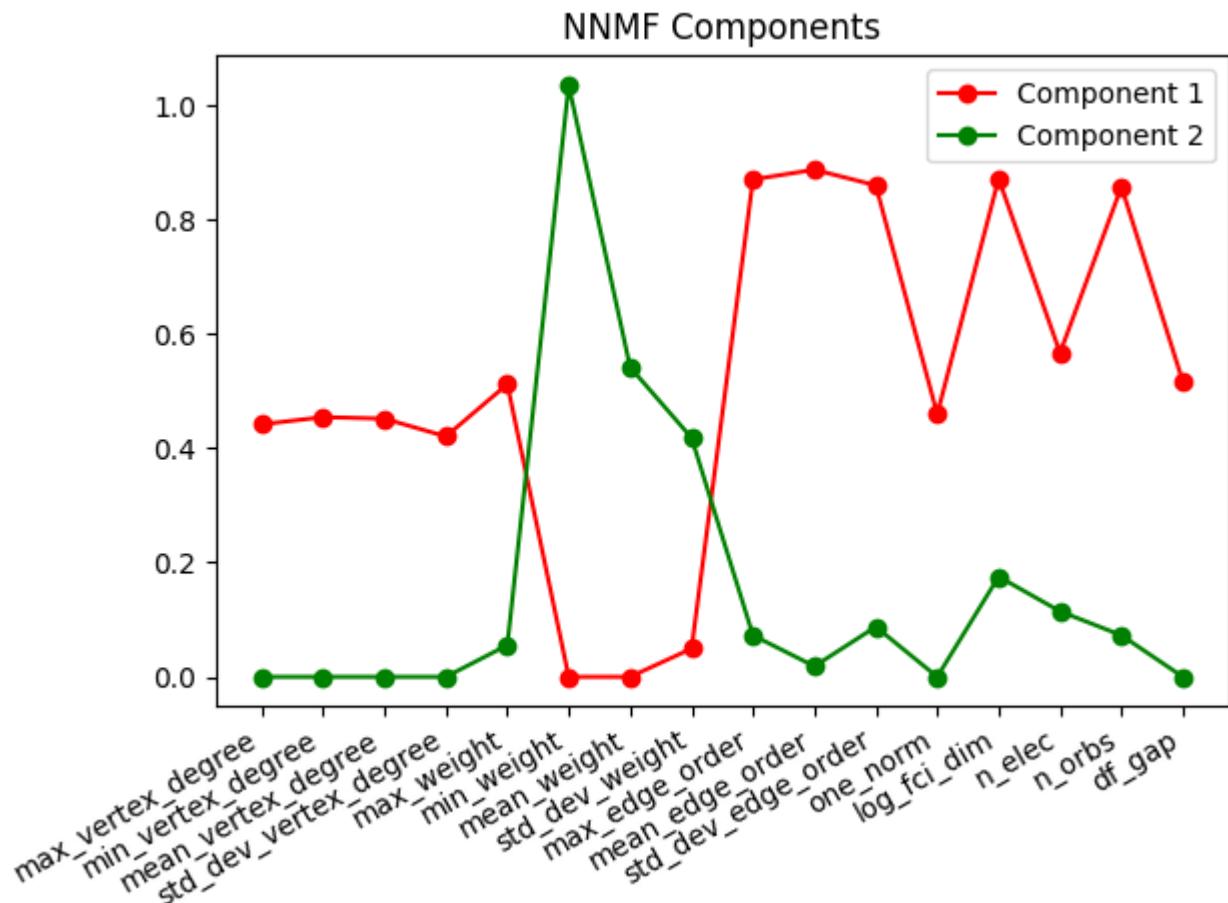


Note: attempted may be True or False. Tasks with a reference_energy can be labeled as solved or failed-to-solve. A task with a reference_energy that was NOT attempted is labeled as a failed-to-solve. White stars indicate Hamiltonians for which we do not have a reference_energy.

SHAP summary plot DMRG_Niagara_cluster_lowest_energy (1653...)



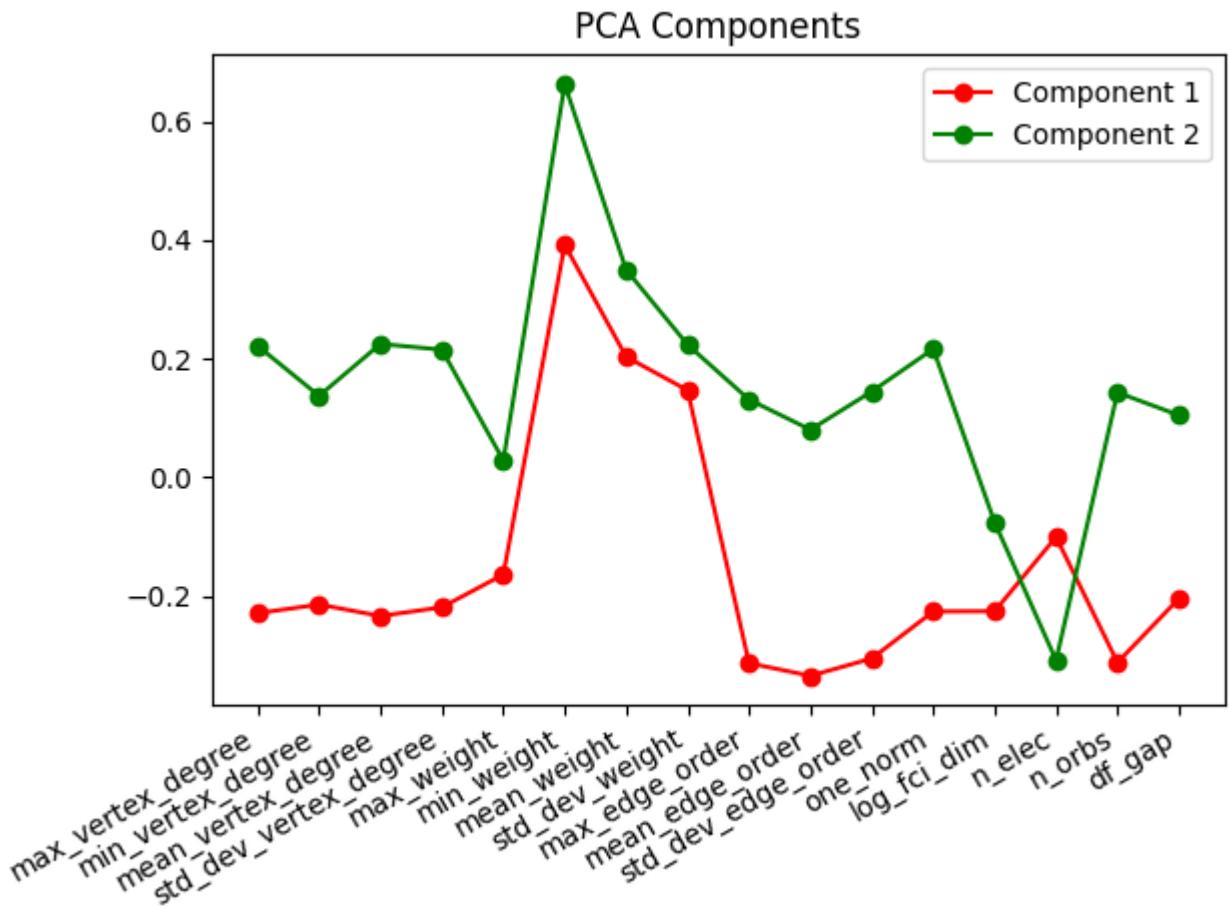
ML Feature Analysis



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.]

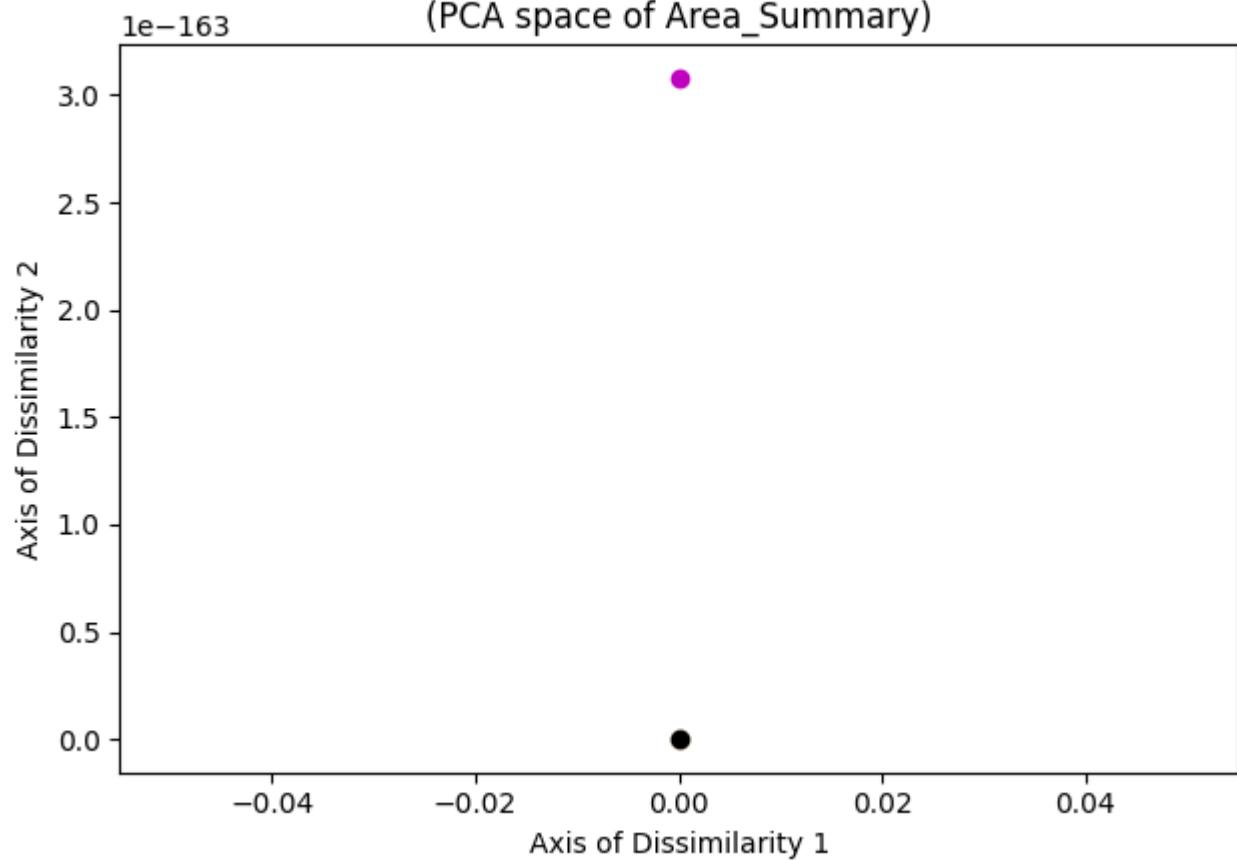


Features: ['max_vertex_degree', 'min_vertex_degree', 'mean_vertex_degree', 'std_dev_vertex_degree', 'max_weight', 'min_weight', 'mean_weight', 'std_dev_weight', 'max_edge_order', 'mean_edge_order', 'std_dev_edge_order', 'one_norm', 'log_fci_dim', 'n_elec', 'n_orbs', 'df_gap']

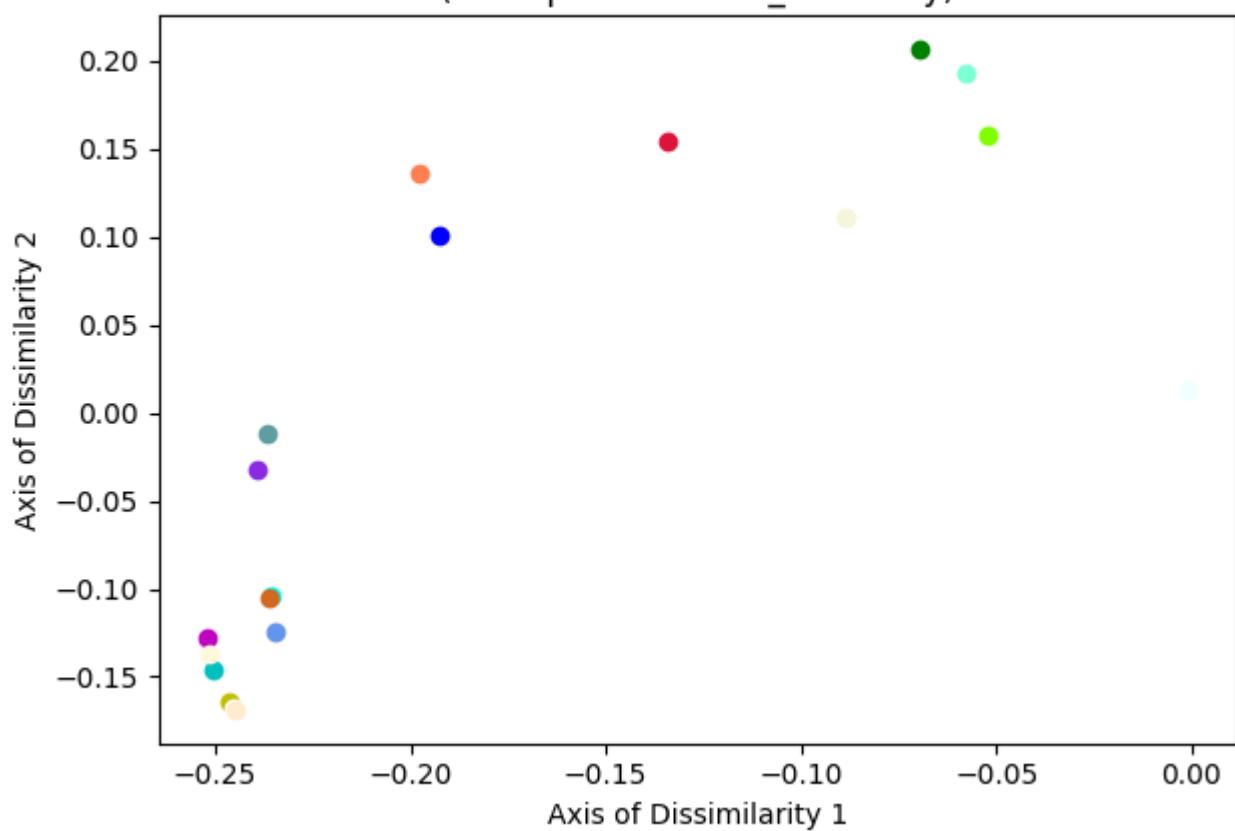
PCA Component 1: [-0.22922229 -0.21461603 -0.23398401 -0.21923522
 -0.16402432 0.39183587 0.20302013 0.14659357 -0.3134204 -0.33485059
 -0.30553226 -0.22630863 -0.2258685 -0.10070305 -0.31226268
 -0.20457232]

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]

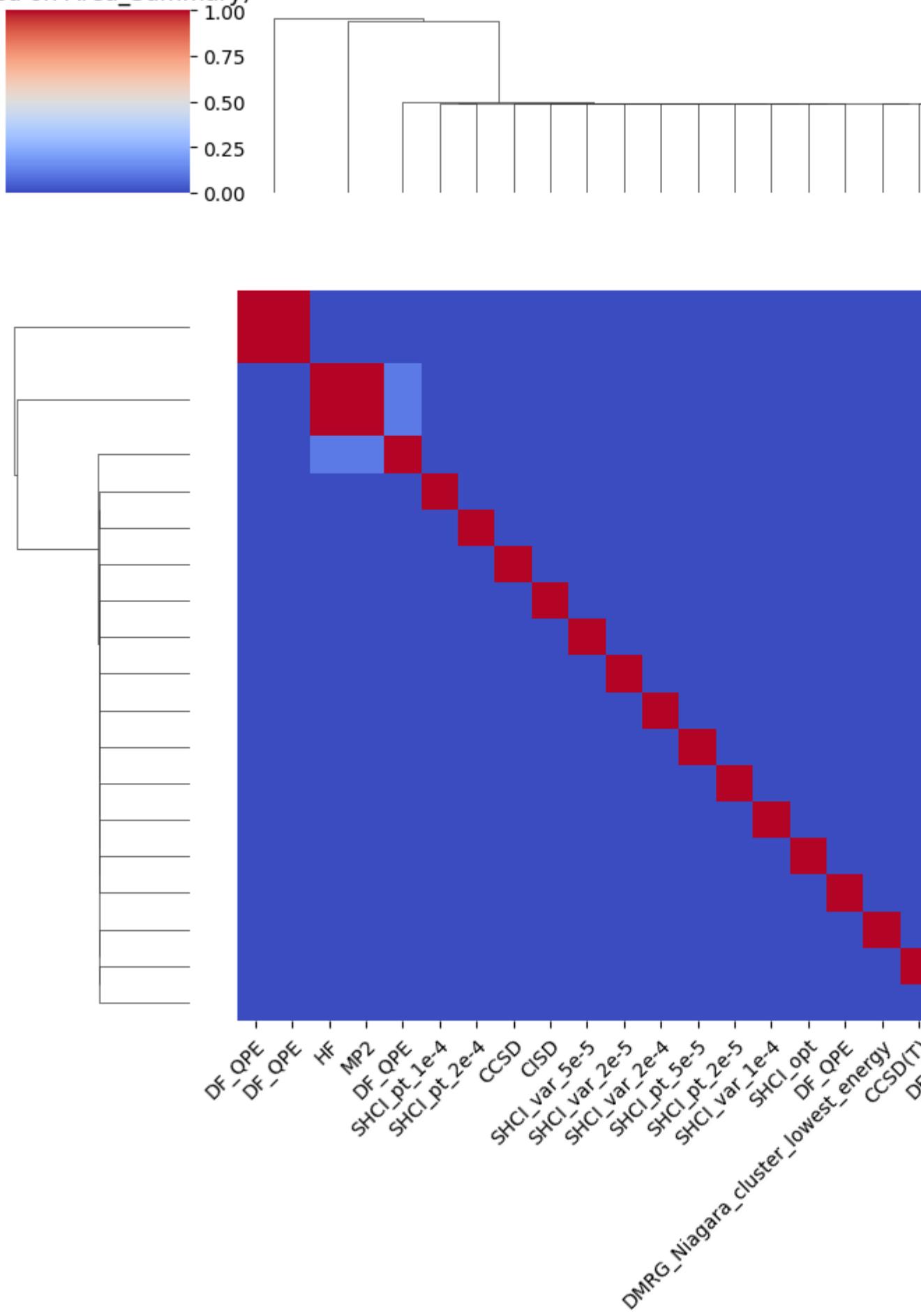
Solver points in PCA space
(PCA space of Area_Summary)



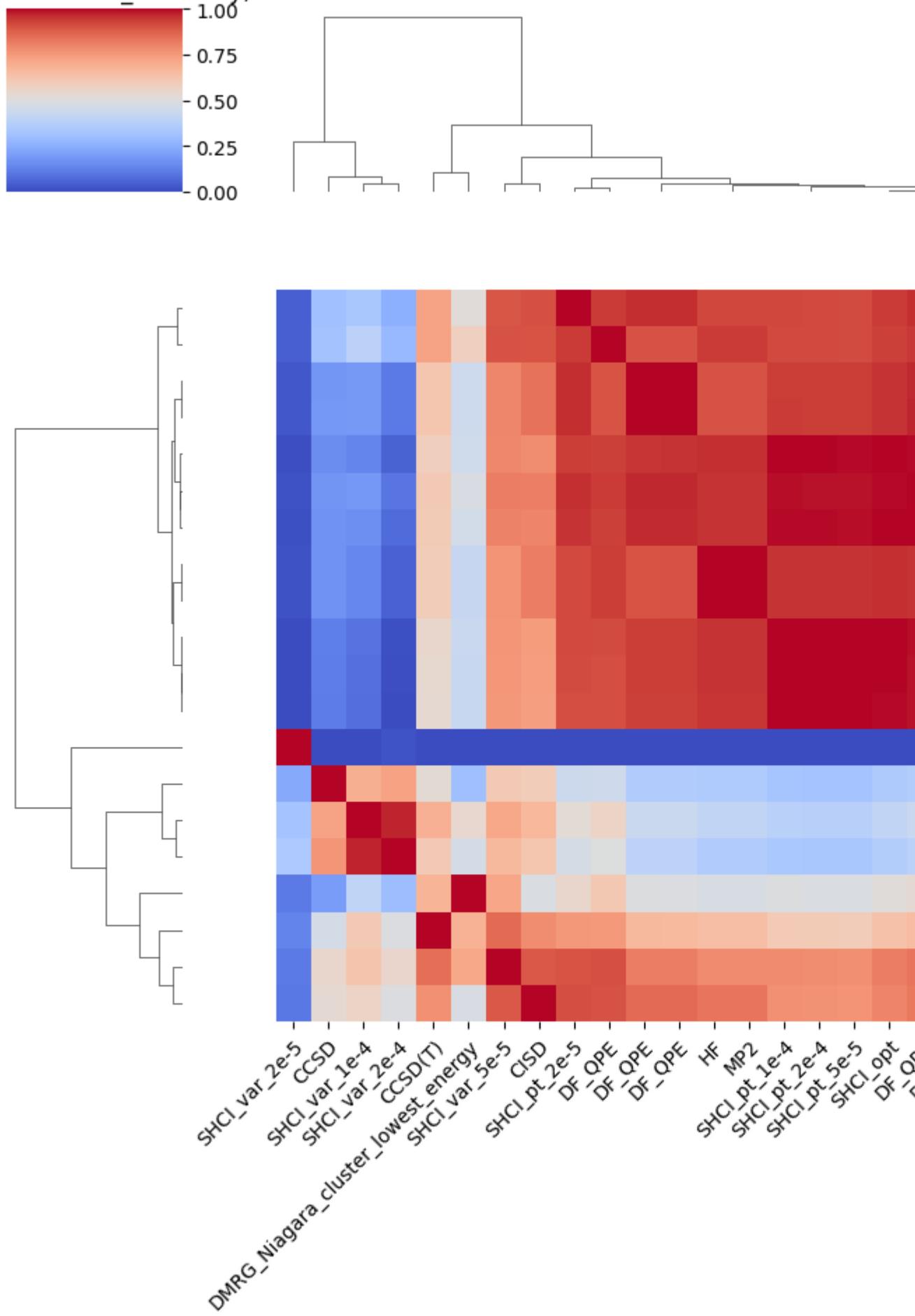
Solver points in PCA space
(PCA space of SHAP_summary)

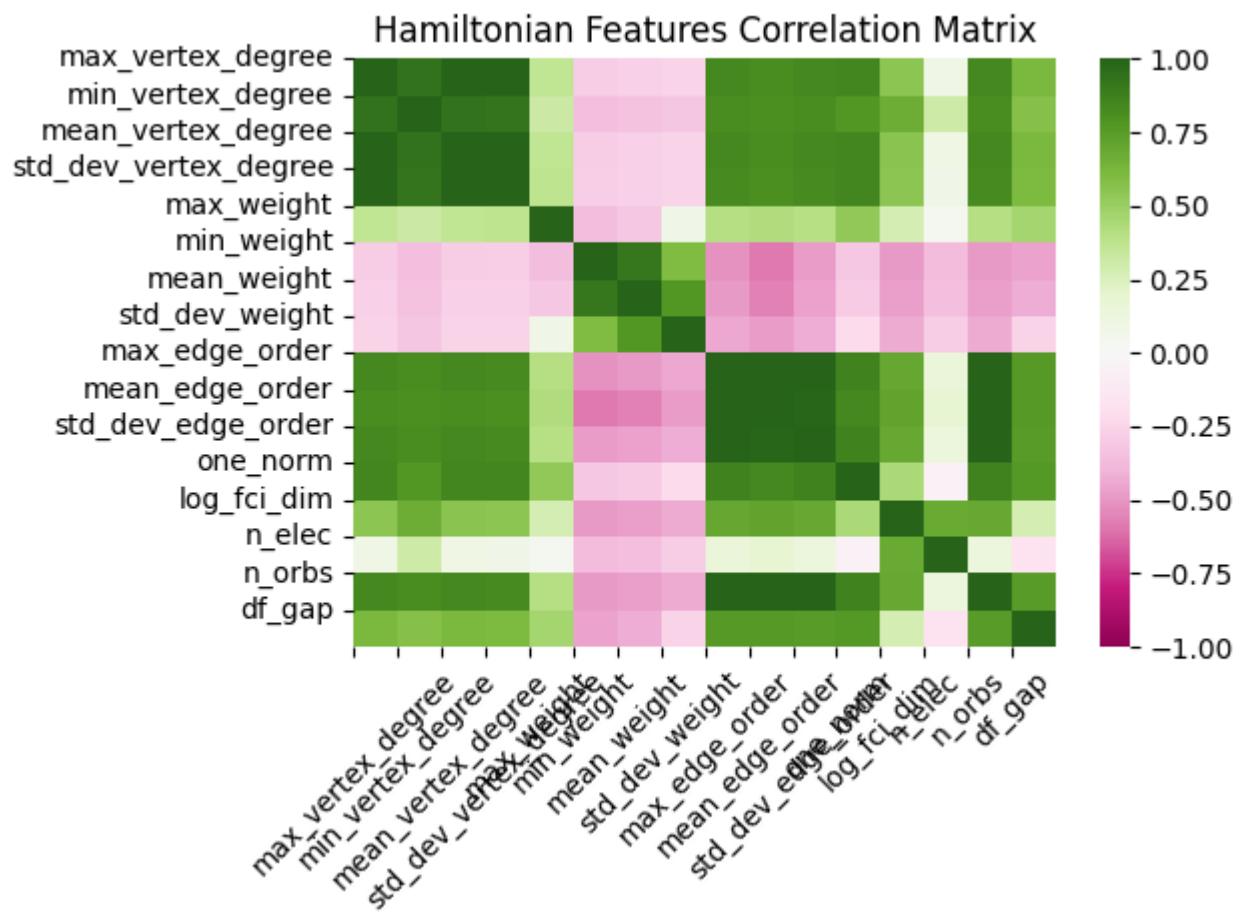


Solver similarity matrix
(based on Area_Summary)

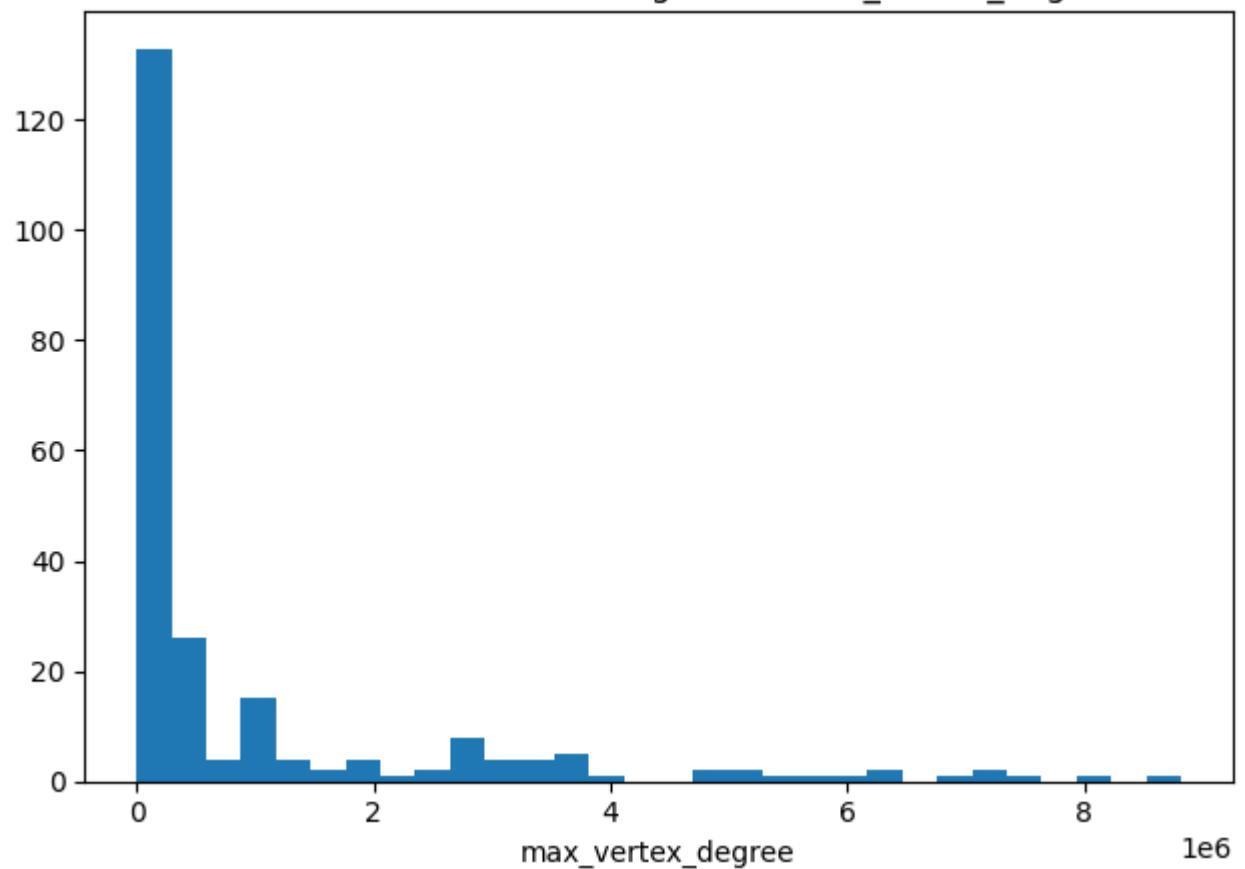


Solver similarity matrix
(based on SHAP_summary)

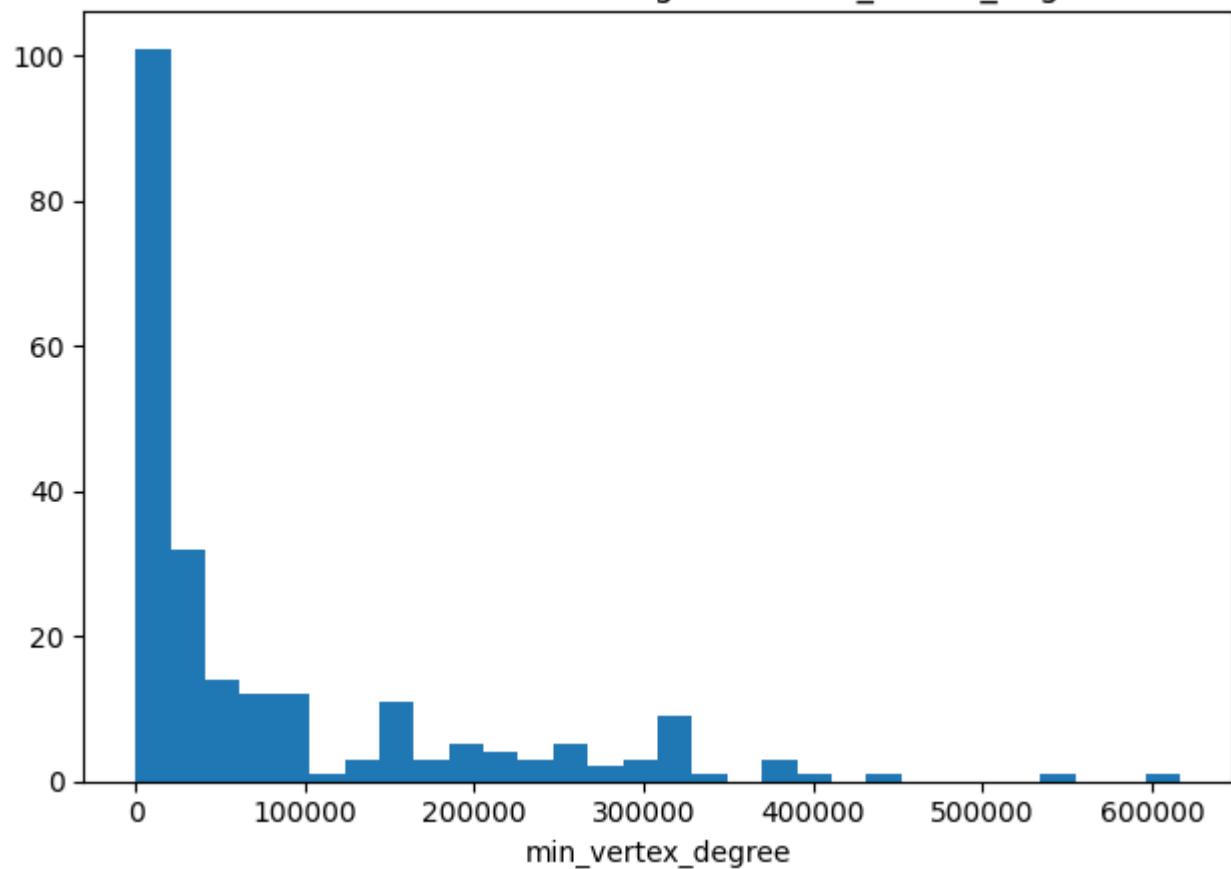




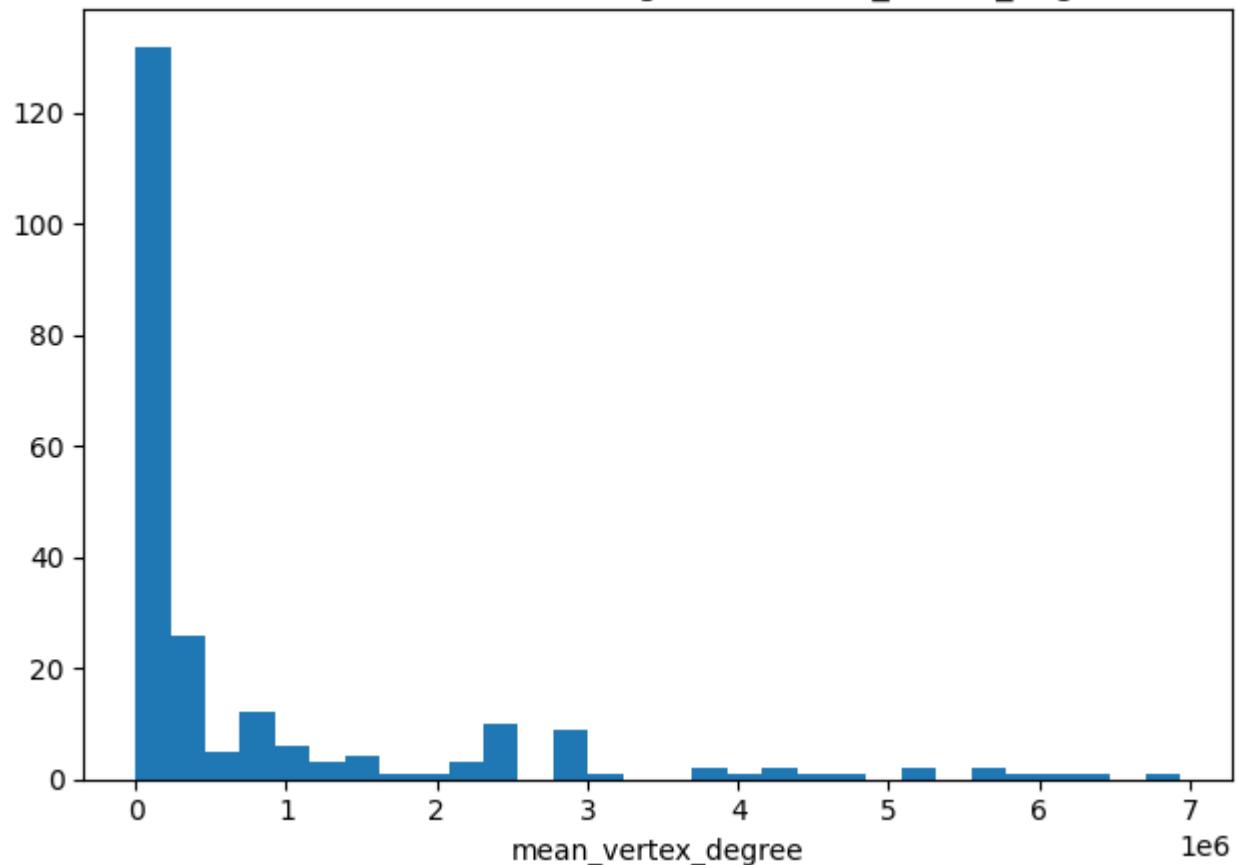
Hamiltonian features: histogram of max_vertex_degree



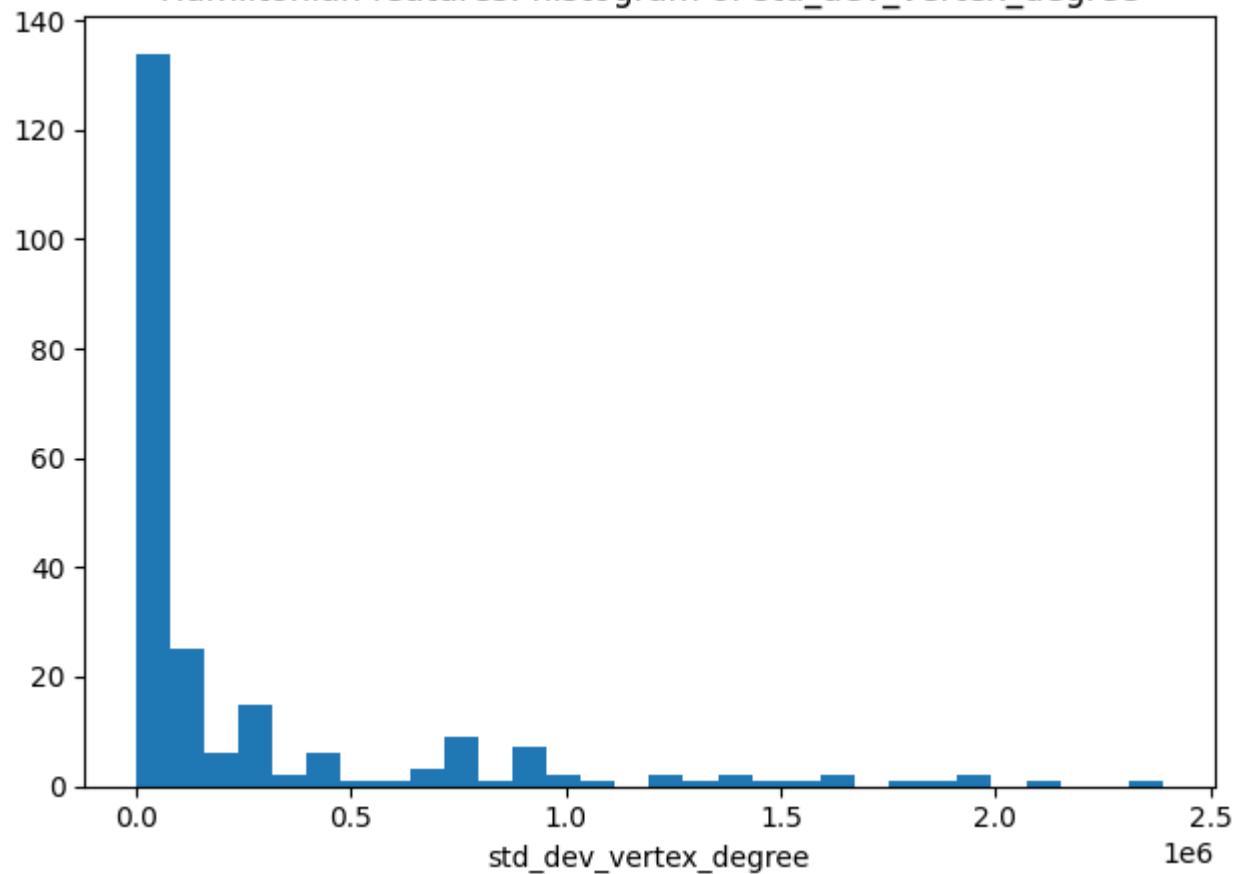
Hamiltonian features: histogram of min_vertex_degree



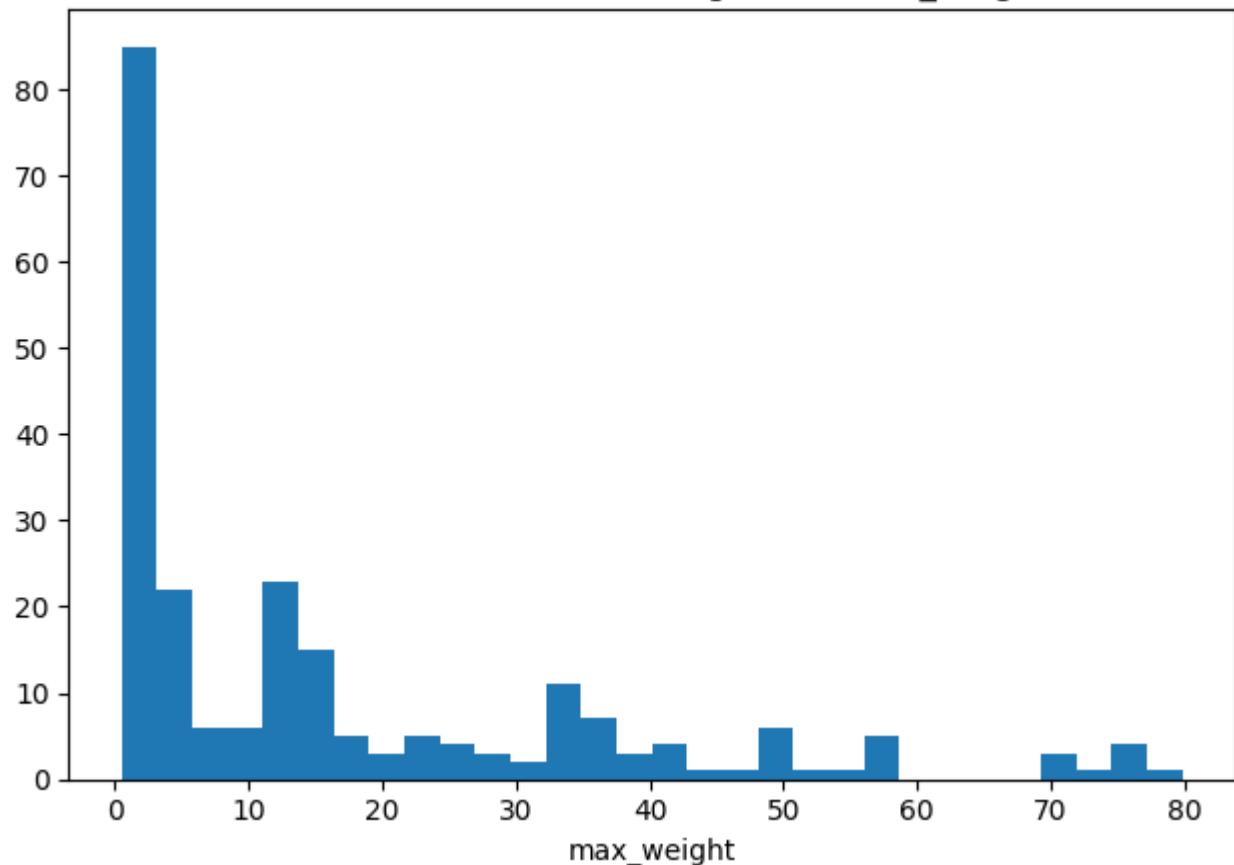
Hamiltonian features: histogram of mean_vertex_degree



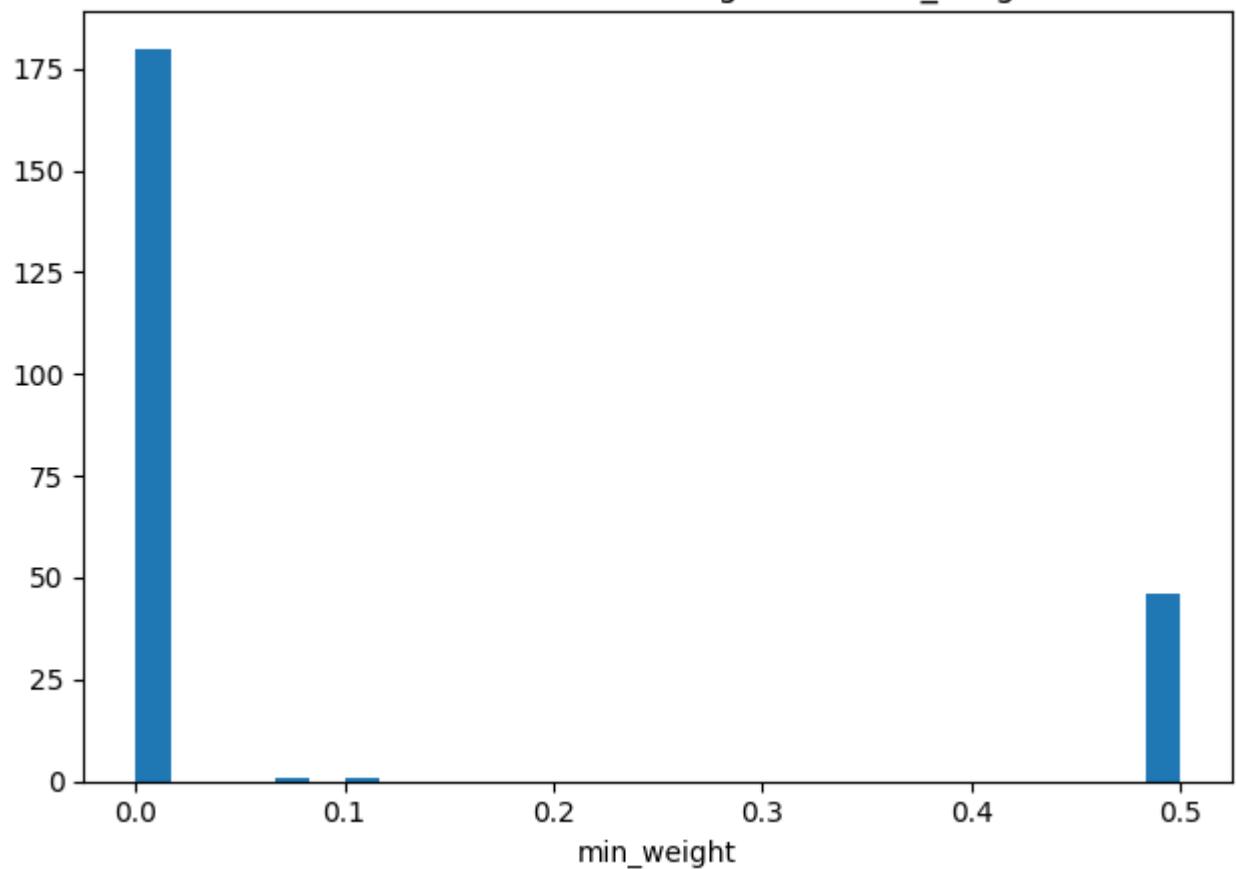
Hamiltonian features: histogram of std_dev_vertex_degree



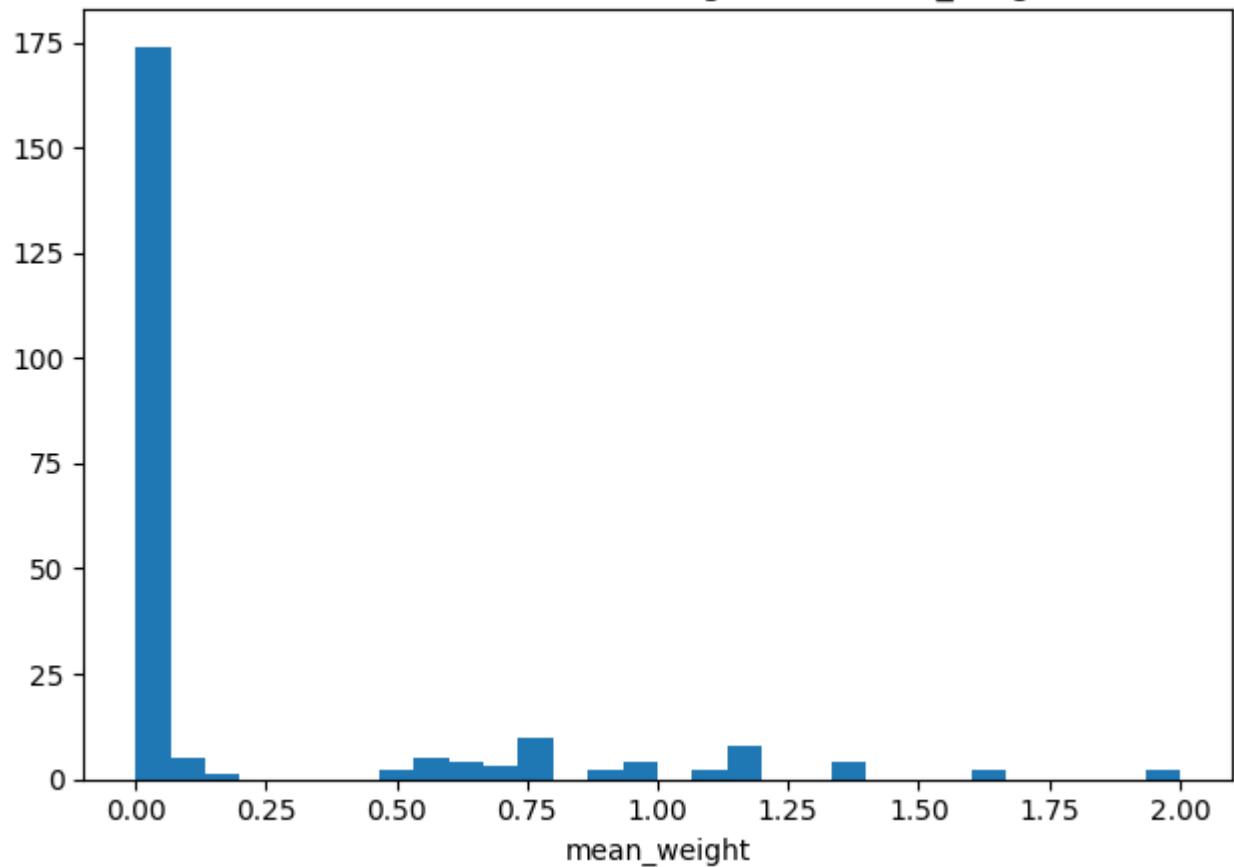
Hamiltonian features: histogram of max_weight



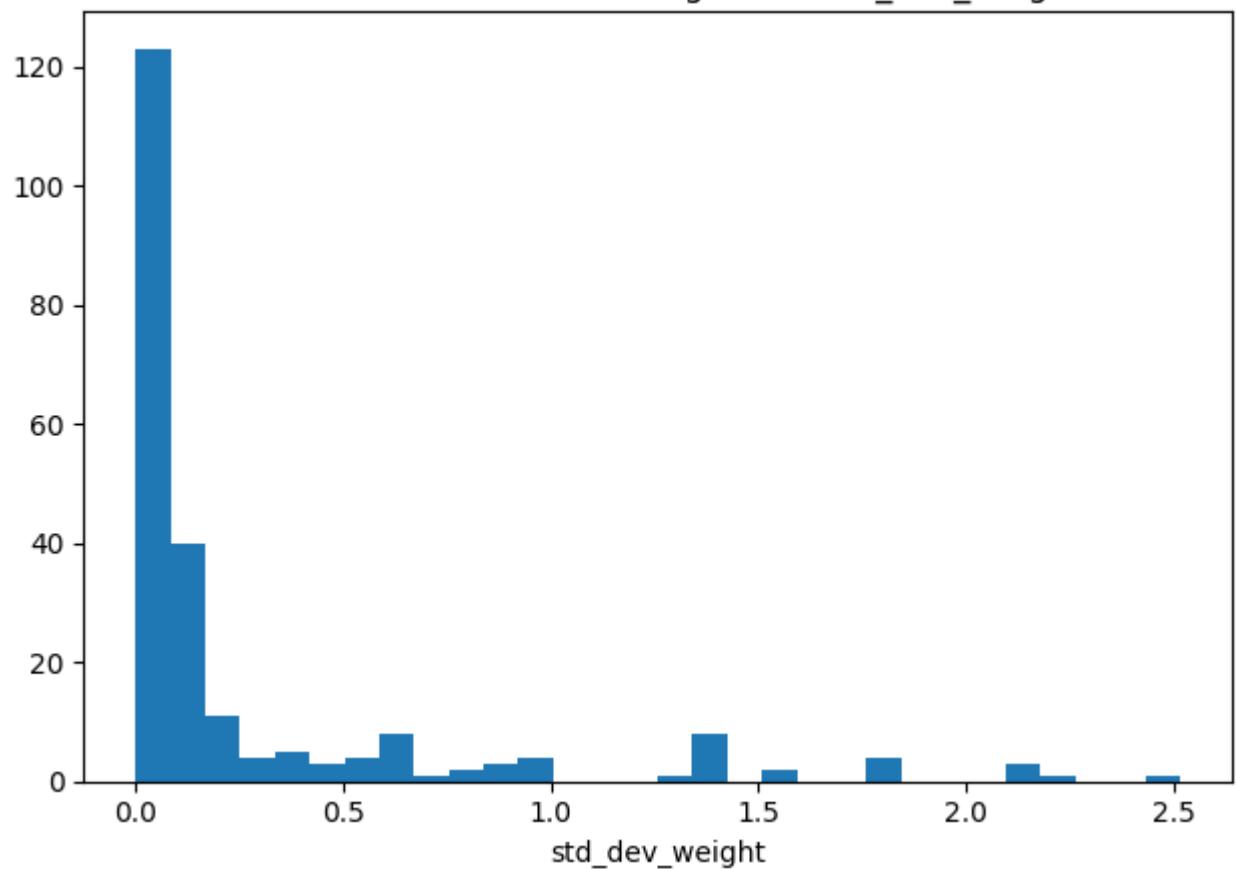
Hamiltonian features: histogram of min_weight



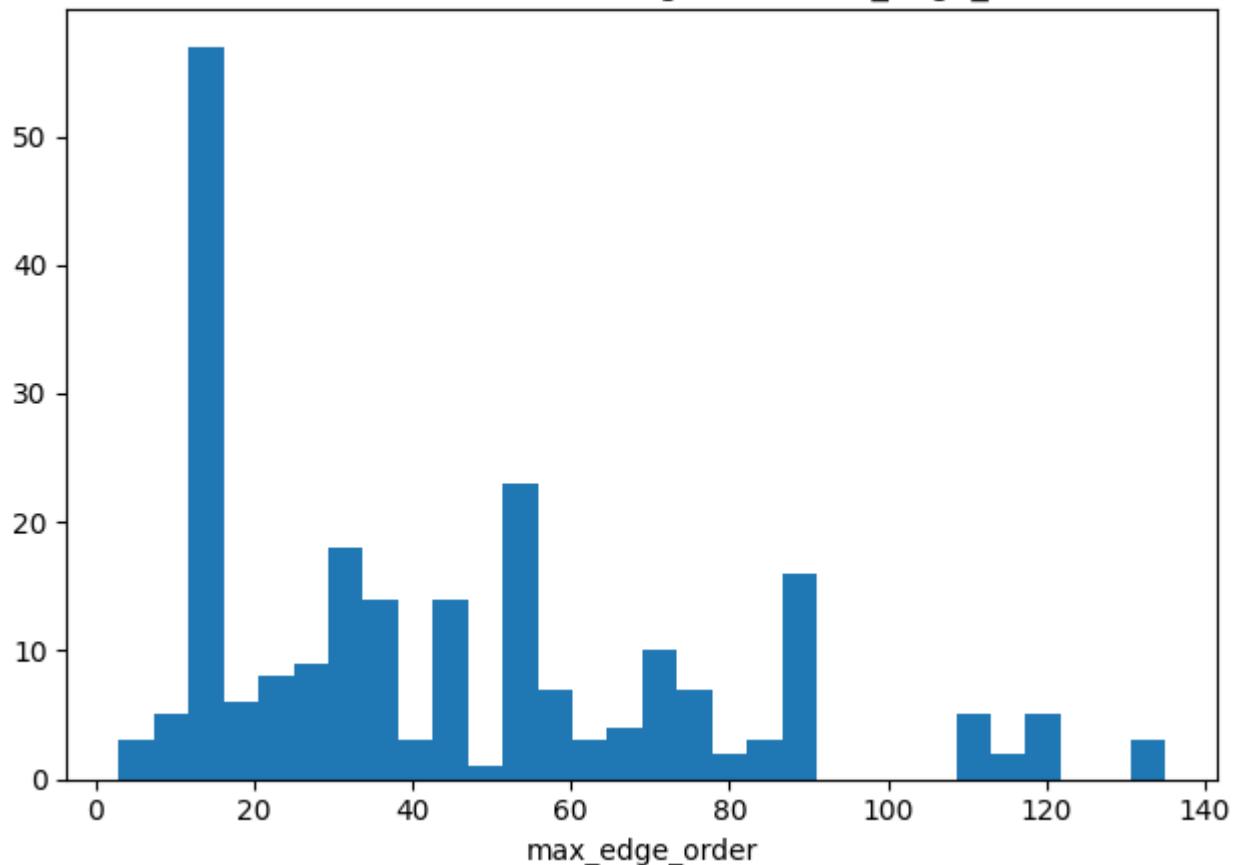
Hamiltonian features: histogram of mean_weight



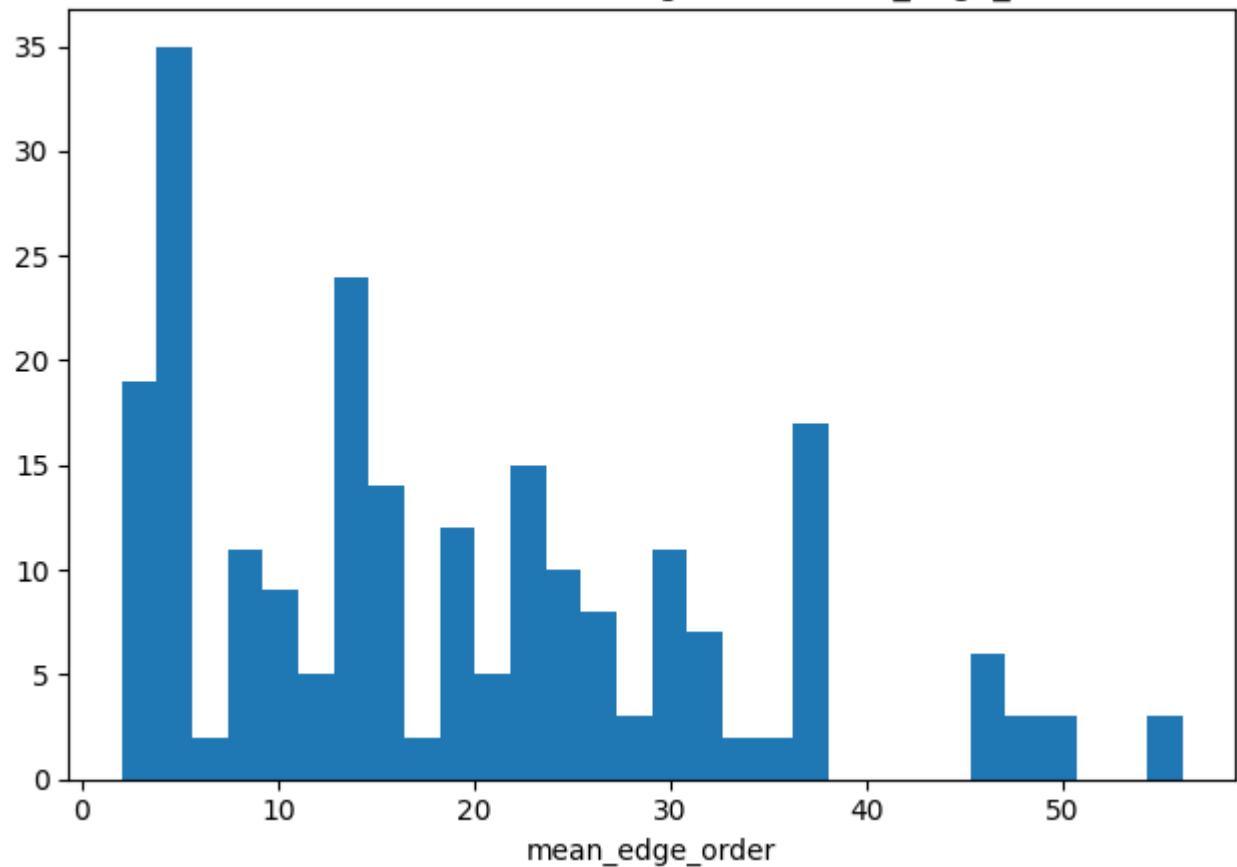
Hamiltonian features: histogram of std_dev_weight



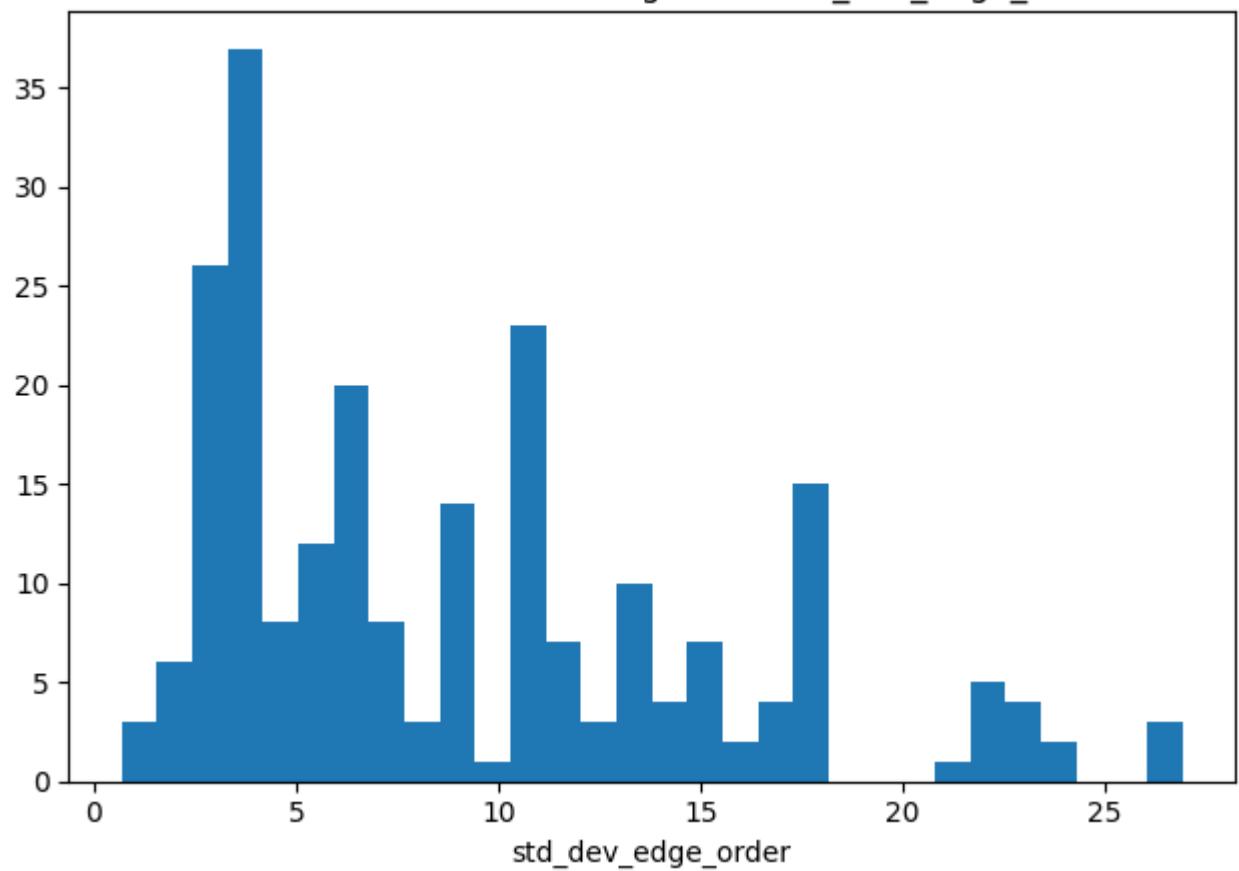
Hamiltonian features: histogram of max_edge_order



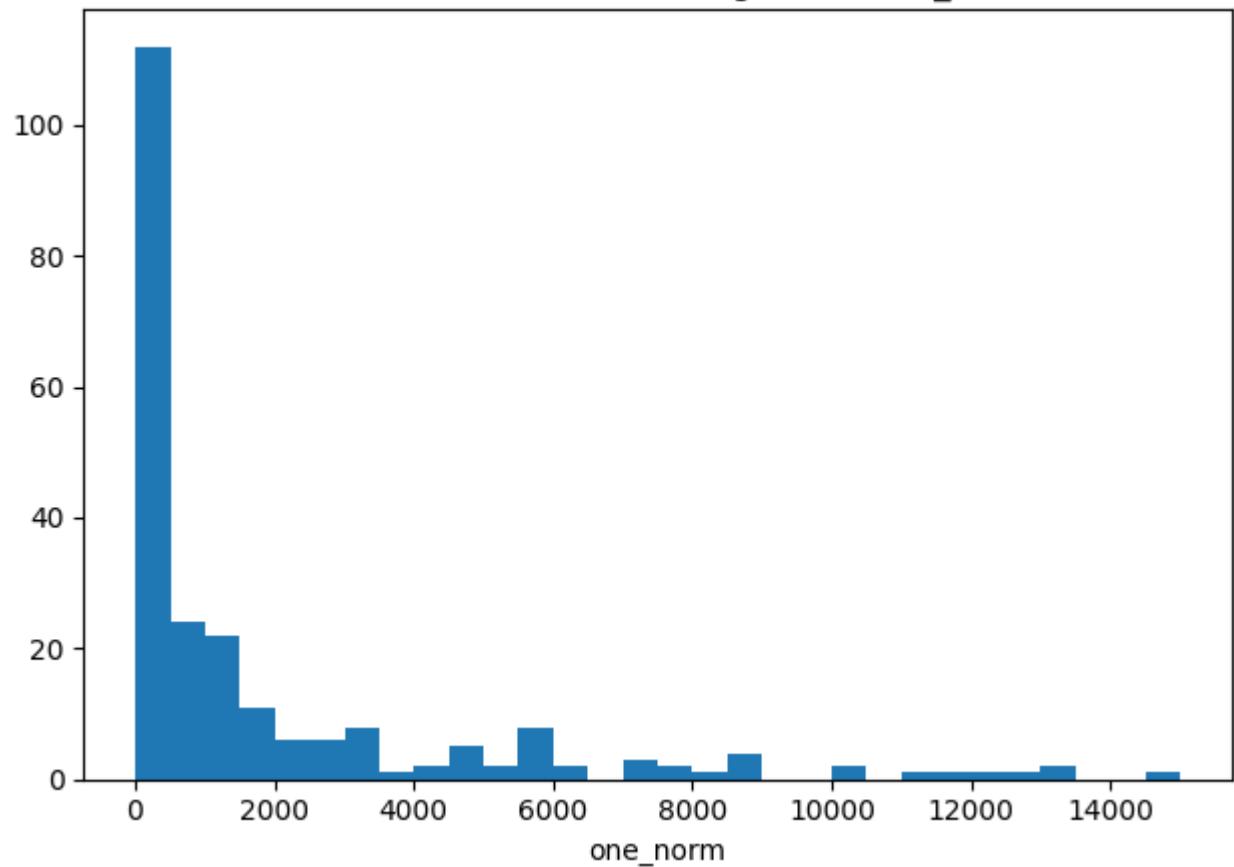
Hamiltonian features: histogram of mean_edge_order



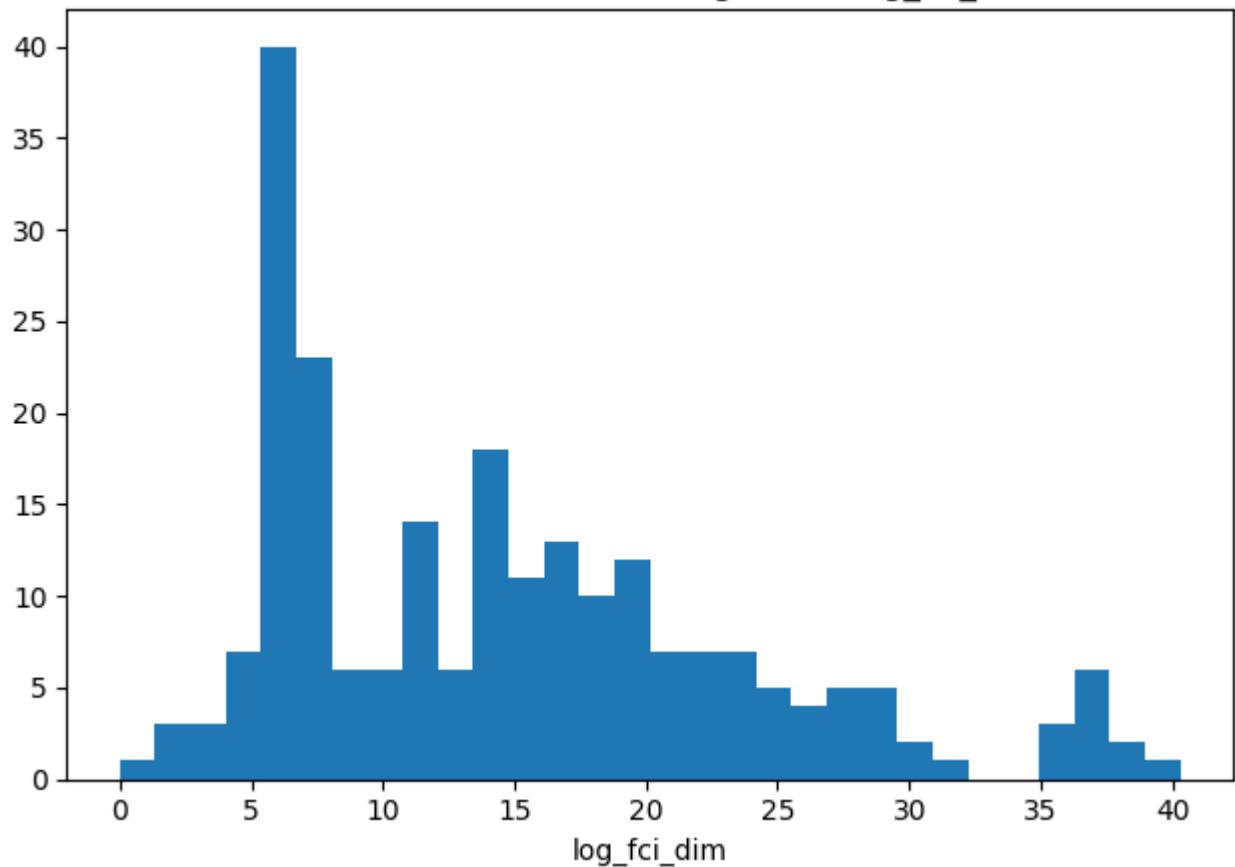
Hamiltonian features: histogram of std_dev_edge_order



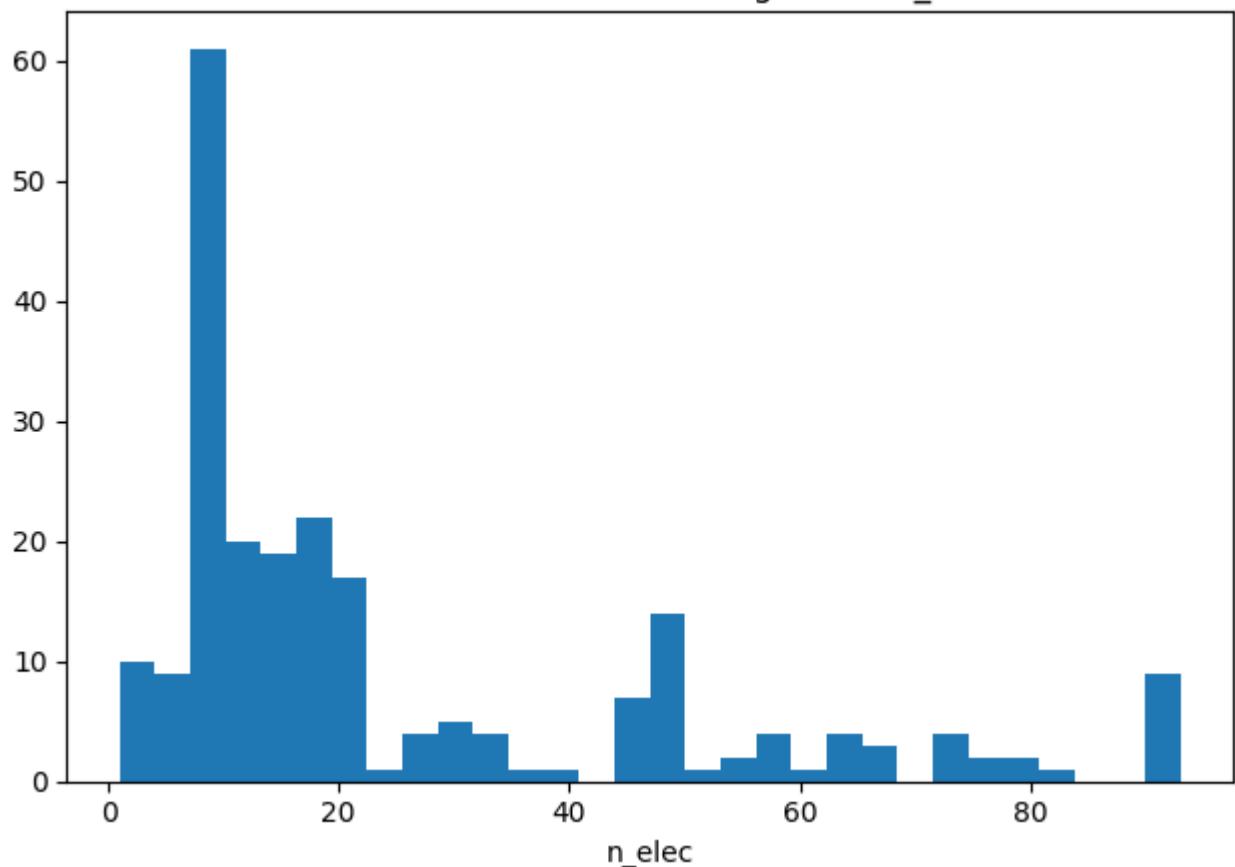
Hamiltonian features: histogram of one_norm



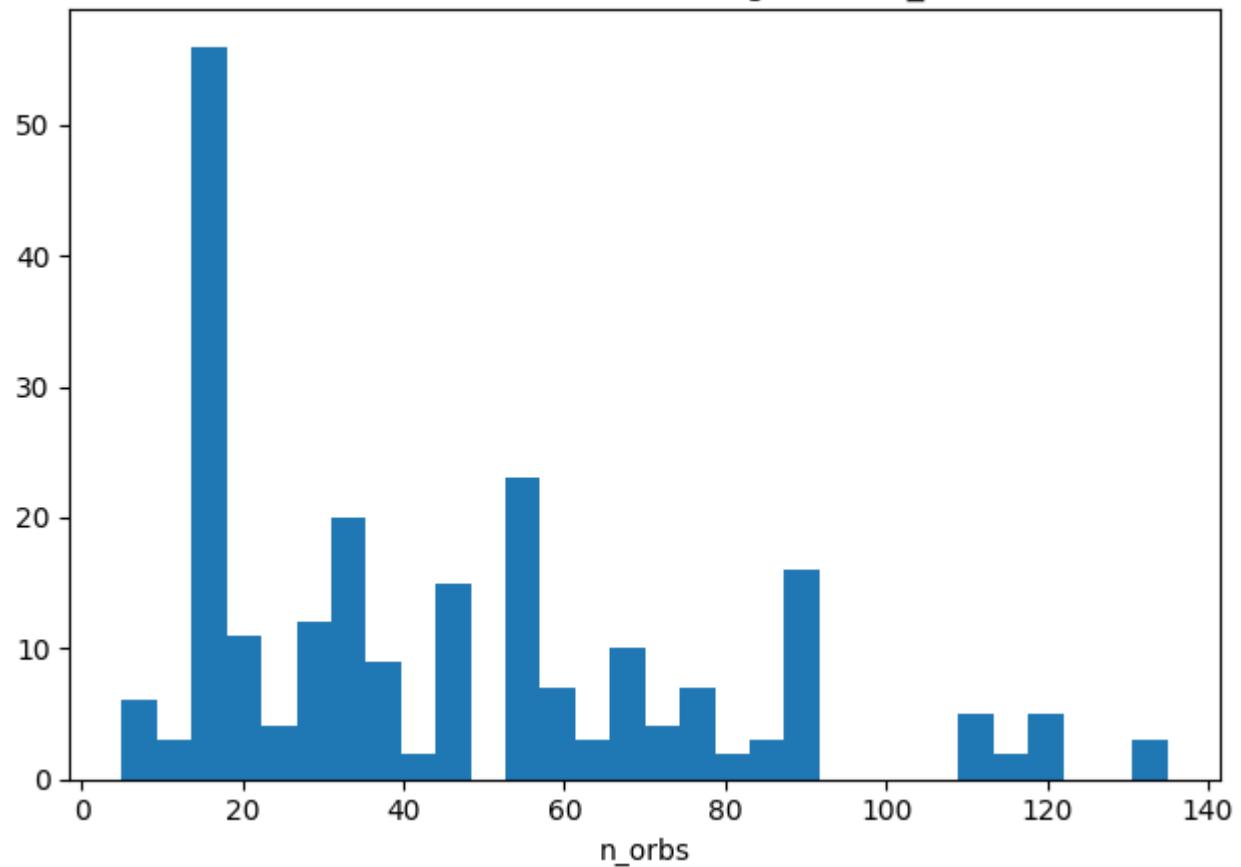
Hamiltonian features: histogram of log_fci_dim



Hamiltonian features: histogram of n_elec



Hamiltonian features: histogram of n_orbs



Hamiltonian features: histogram of df_gap

