

GSEE Benchmark Standard Report

Report based on data from 2025-02-24T20:41:03.349036+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Mon Feb 24 12:56:15 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 Feb 24 12:56:15 2025

Latest creation time for a `solution.json` file: Mon Feb 24 14:43:26 2025

Problem Instance Summary Statistics

number of `problem_instances`: 68.

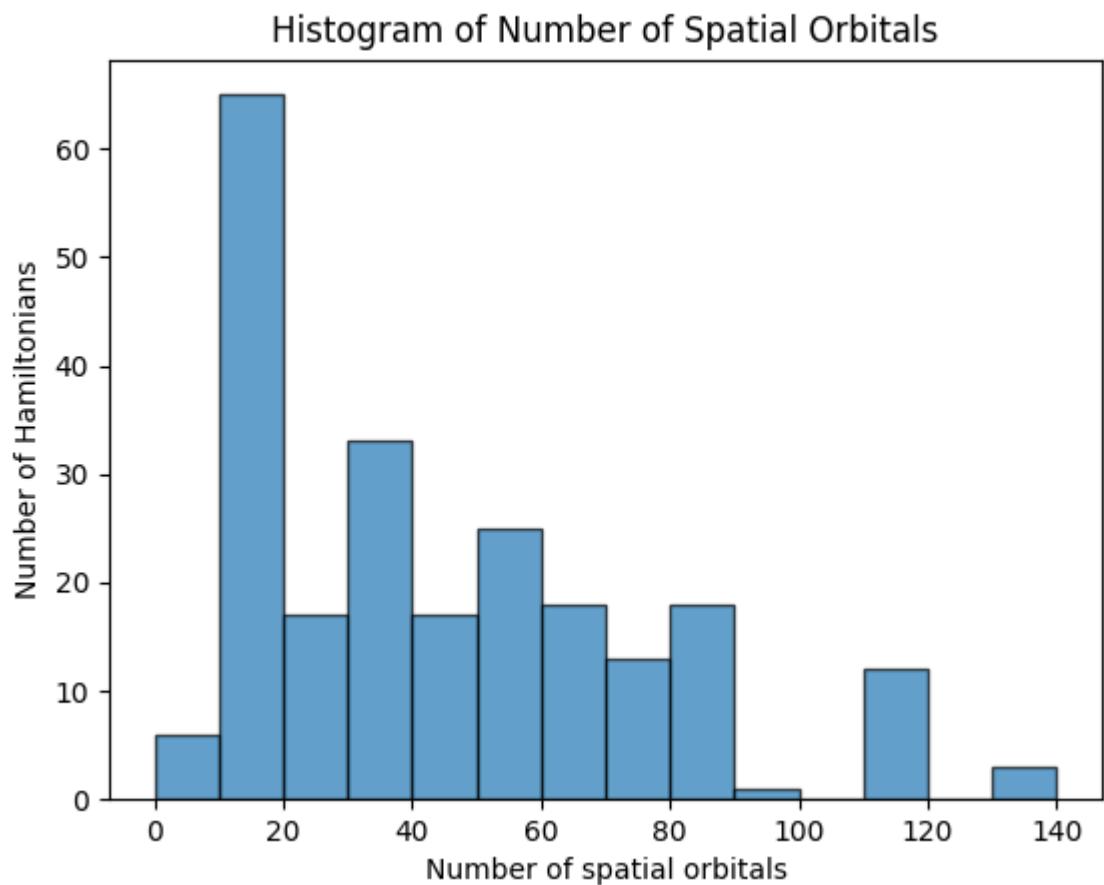
`problem_instance.json` with the most tasks: 30 (`hubbard_square/614c4444-a31a-4348-b24d-01040208651c`)

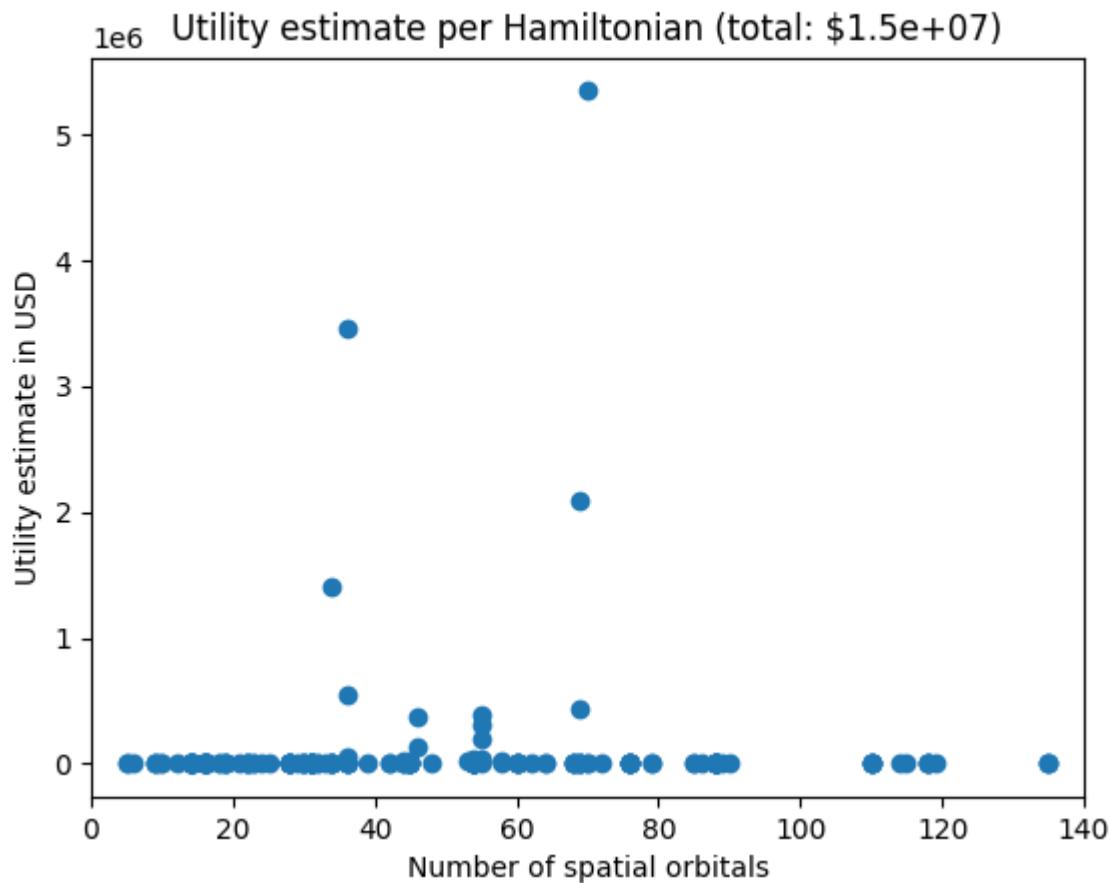
number of Hamiltonians (i.e., tasks) we have features calculated for: 228

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/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]

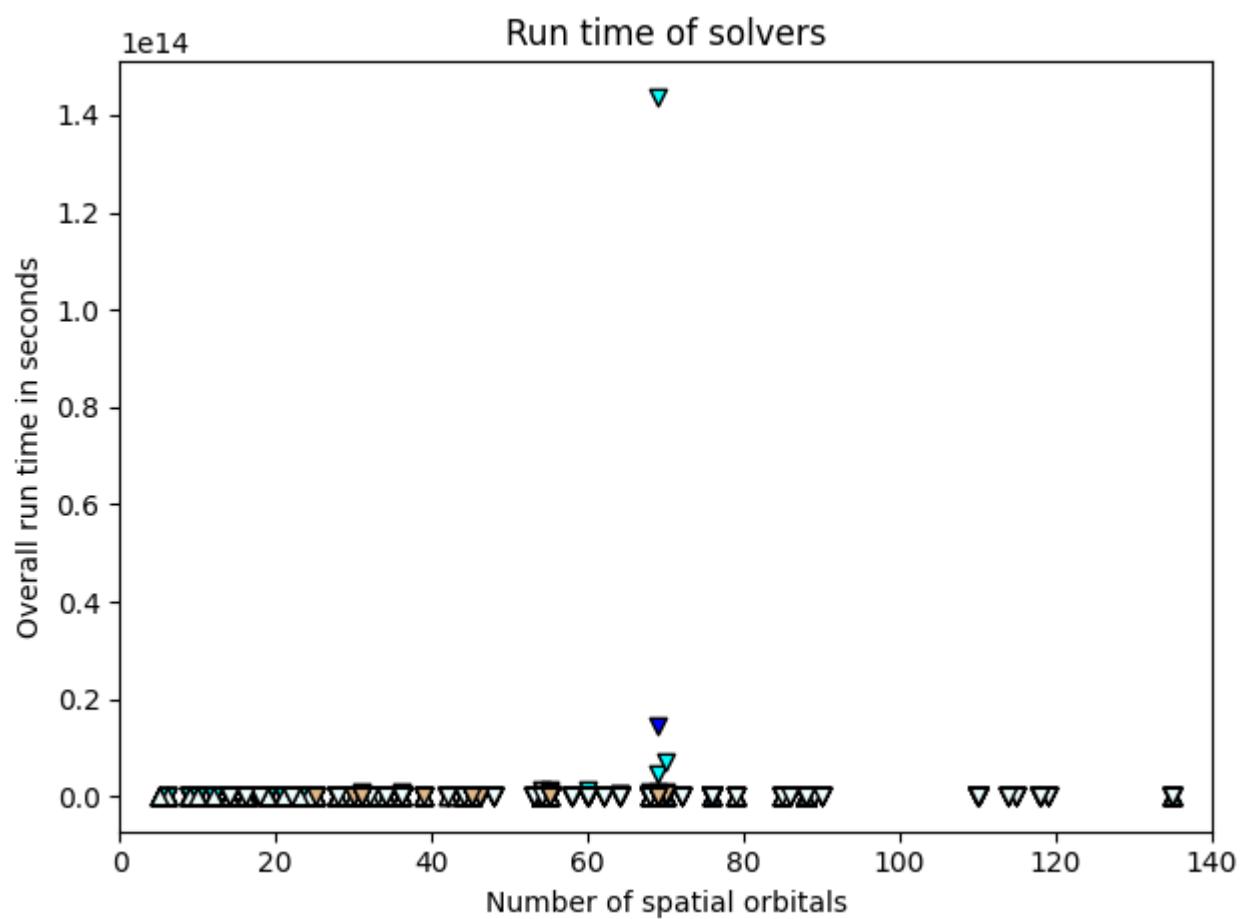
Solver: DF_QPE/5d768520-b3d0-4292-bbb4-9776fa128107, ML Solvability
Ratio: {'PCA': 0.0394, 'NNMF': 0.0199}, F1 Score: [1. 1.]

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

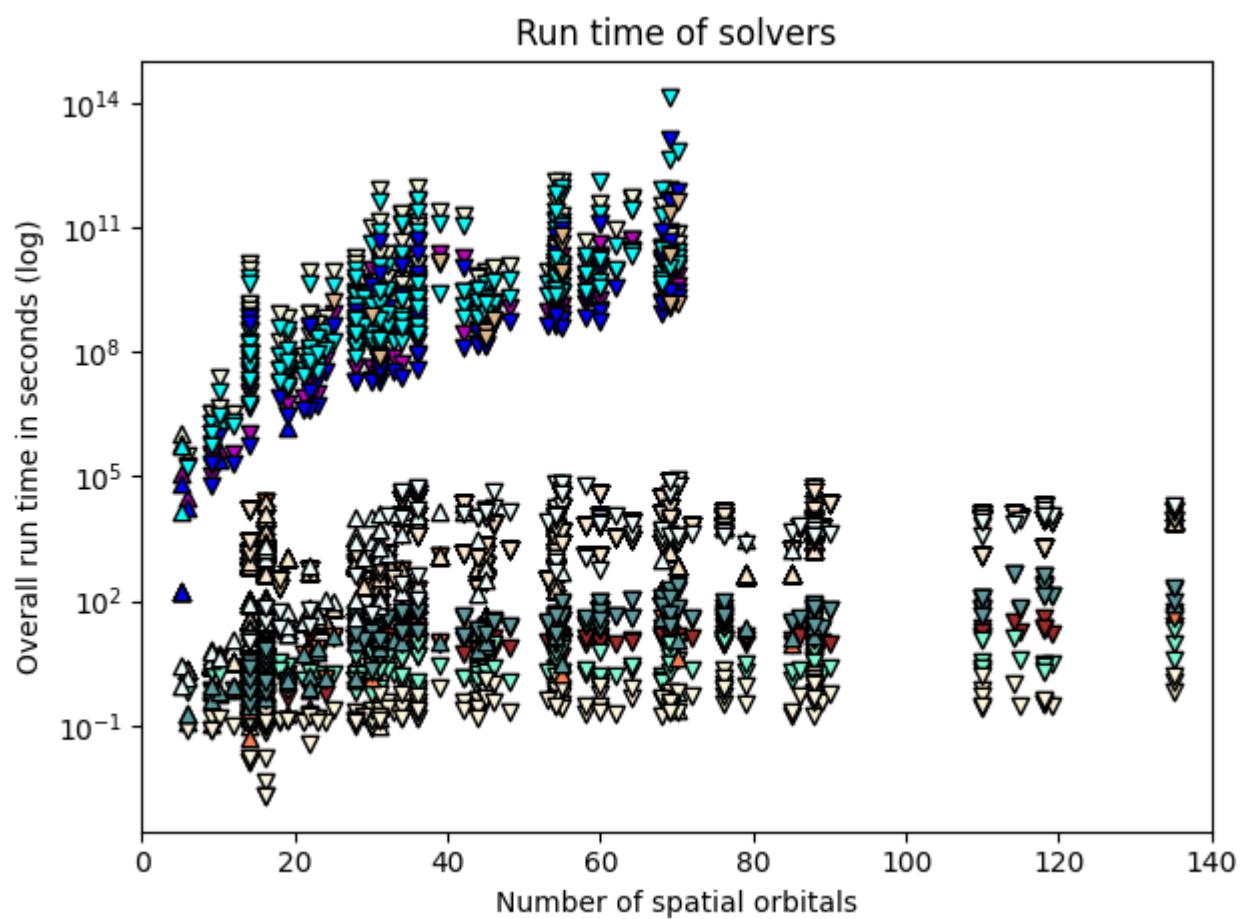
Solver: DF_QPE/4b07b89f-c66f-4e72-8c24-df3e4222cb41, ML Solvability
Ratio: {'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [1. 1.]

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]

Solver: DF_QPE/6f385080-934b-4cbb-b813-39c2cb61349e, Model could not
be calculated.

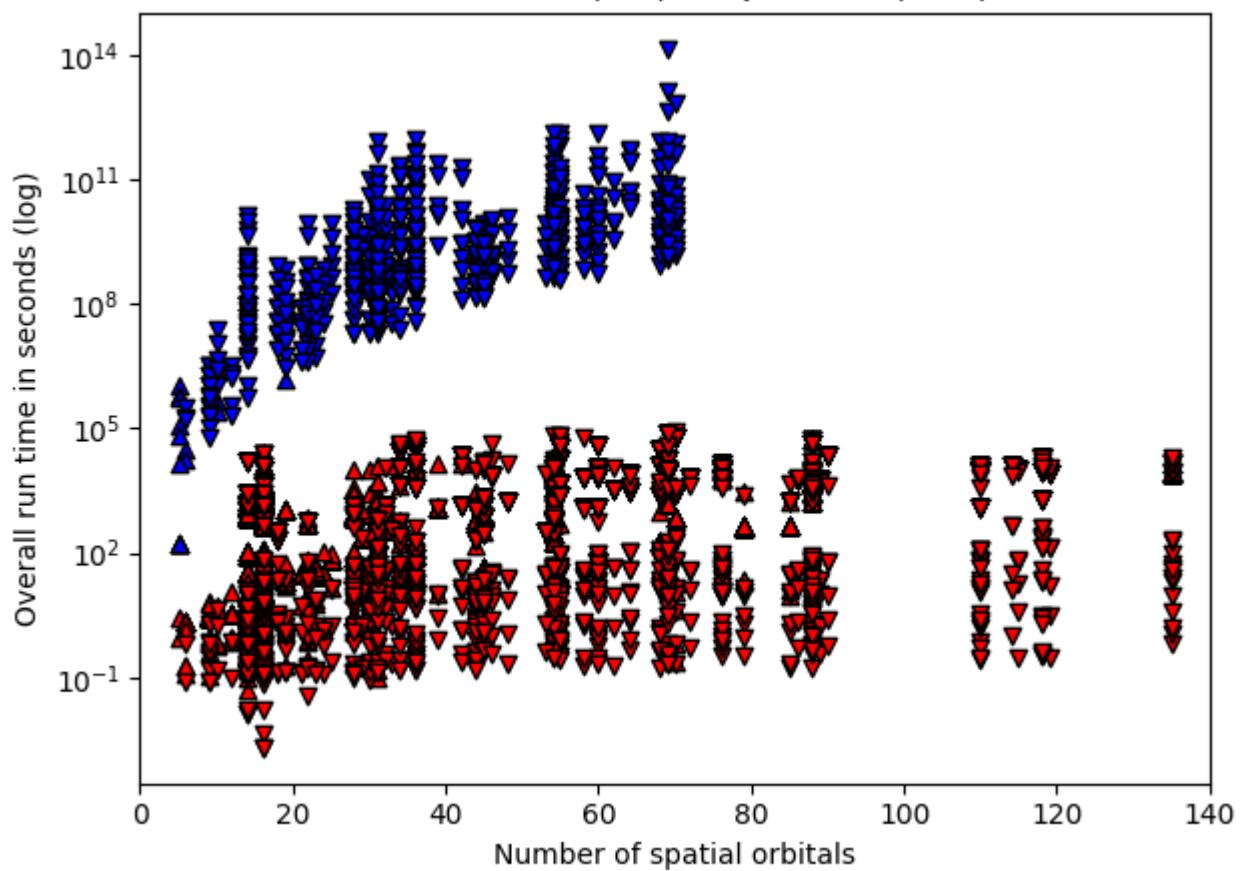


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

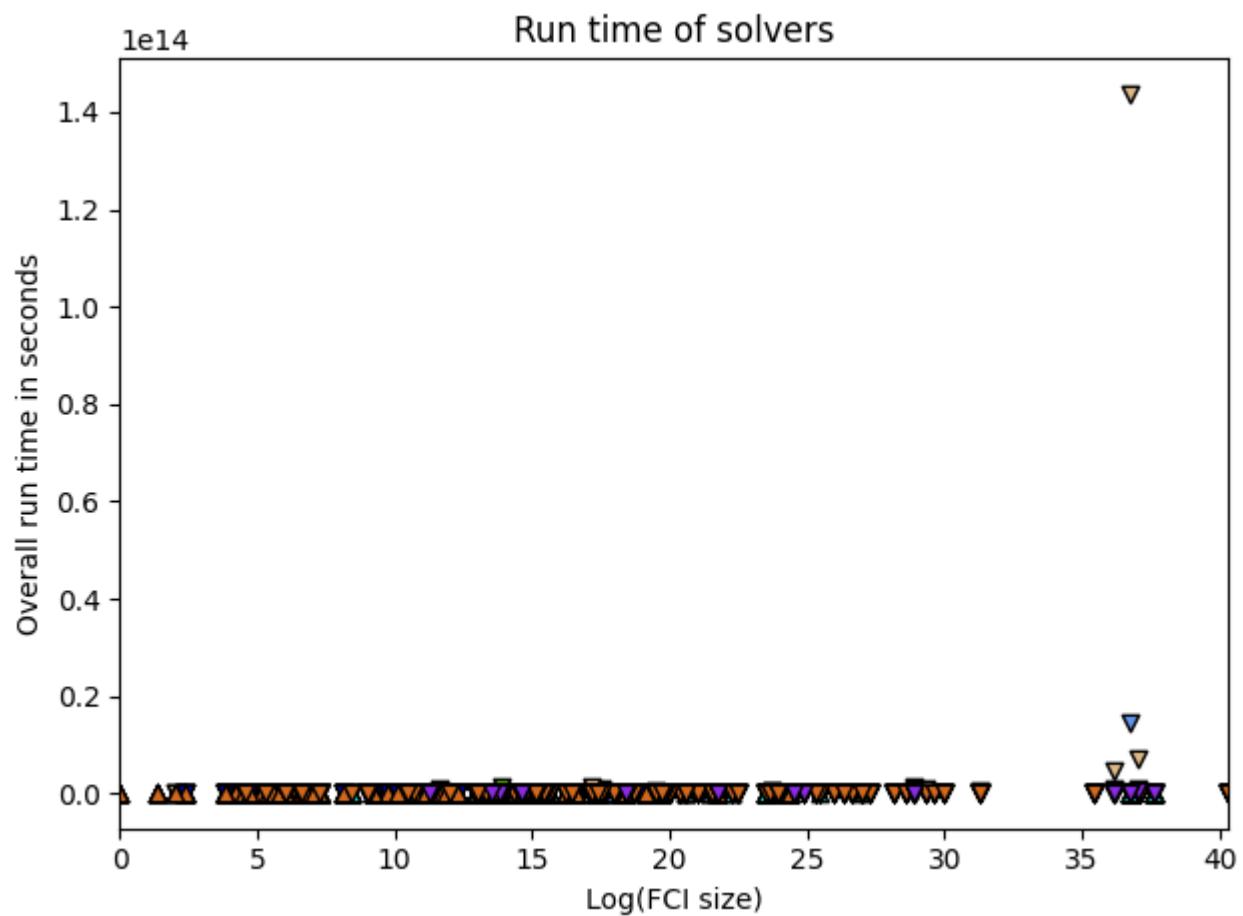


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

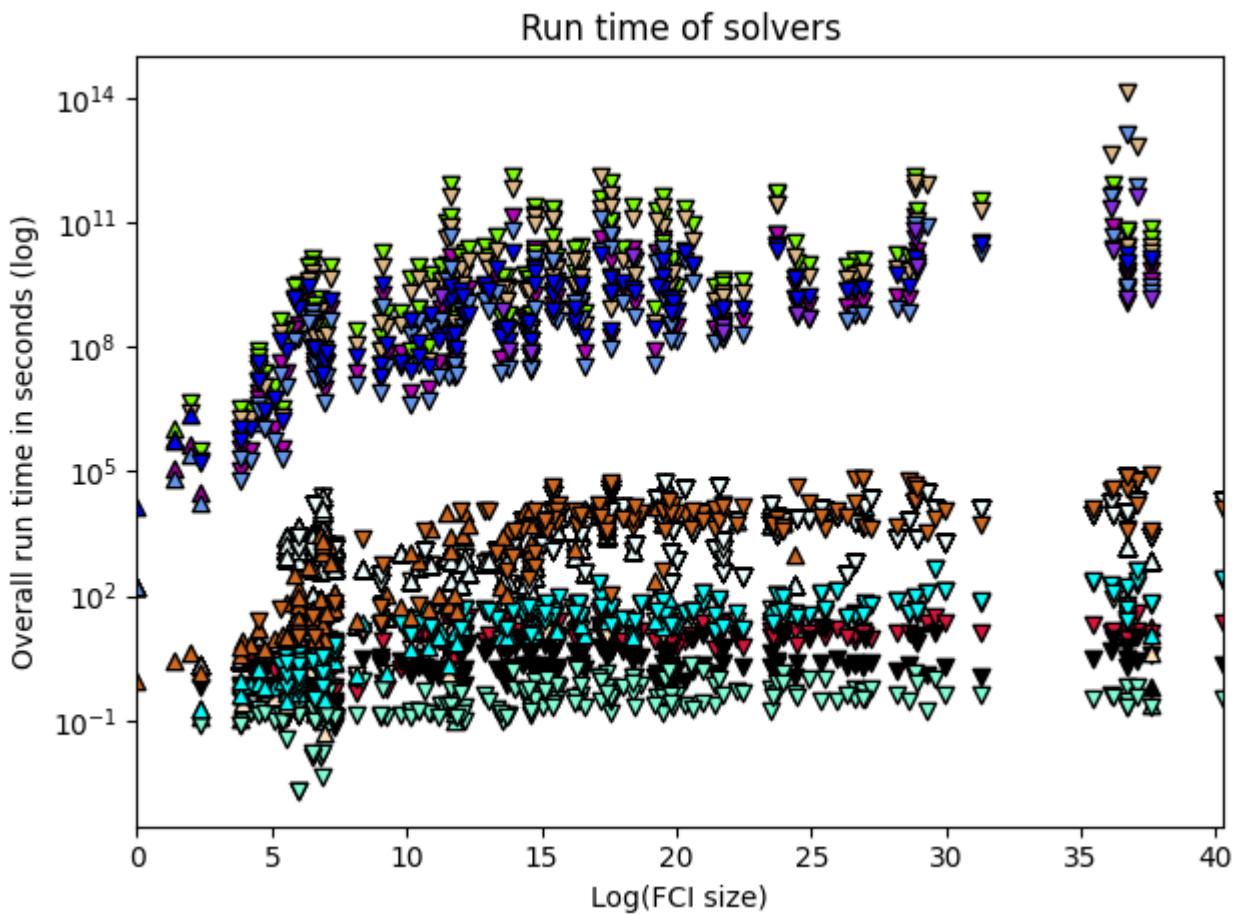
Run time of Classical (red) vs Quantum (blue) solvers



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

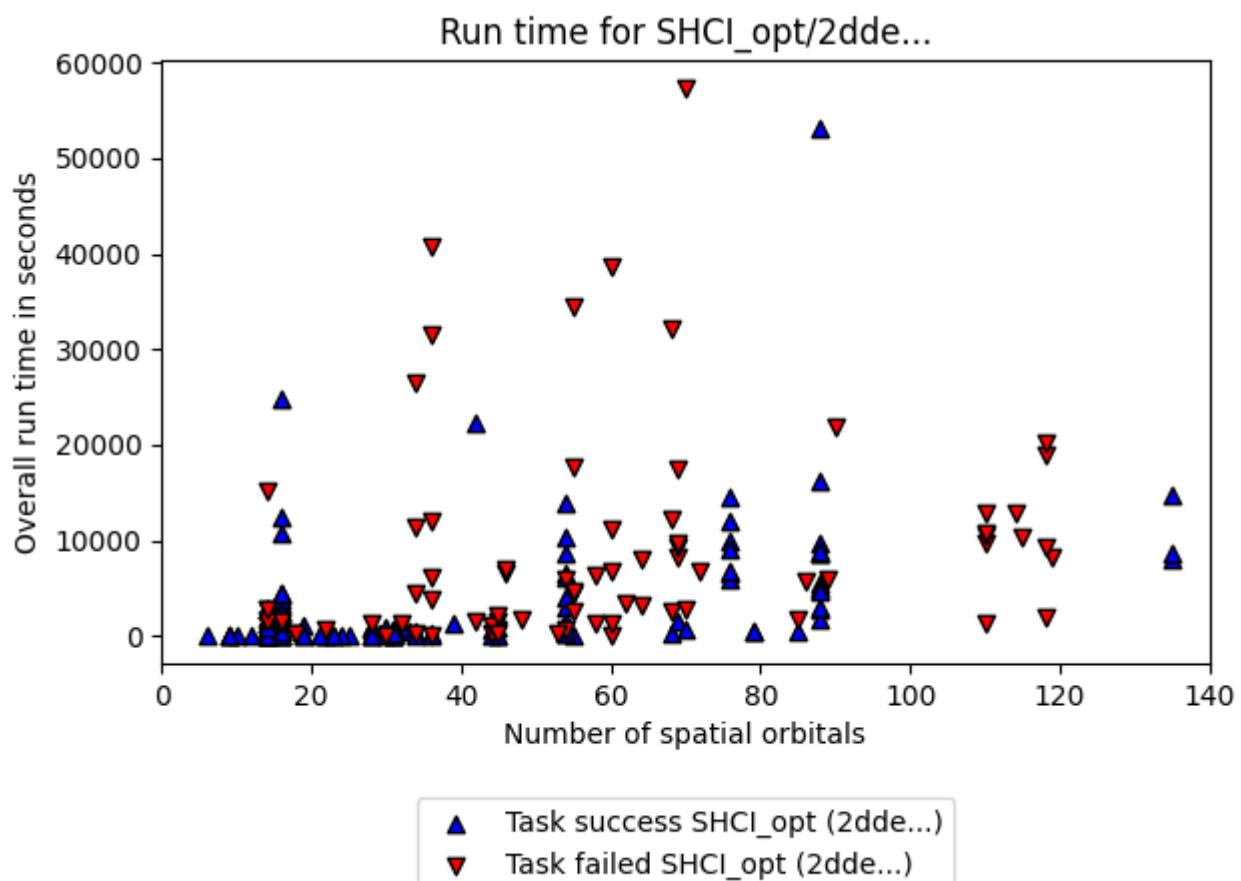
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance_metrics_uuid: 999f842a-3dd5-40cc-92a4-714ef3b1e5b8

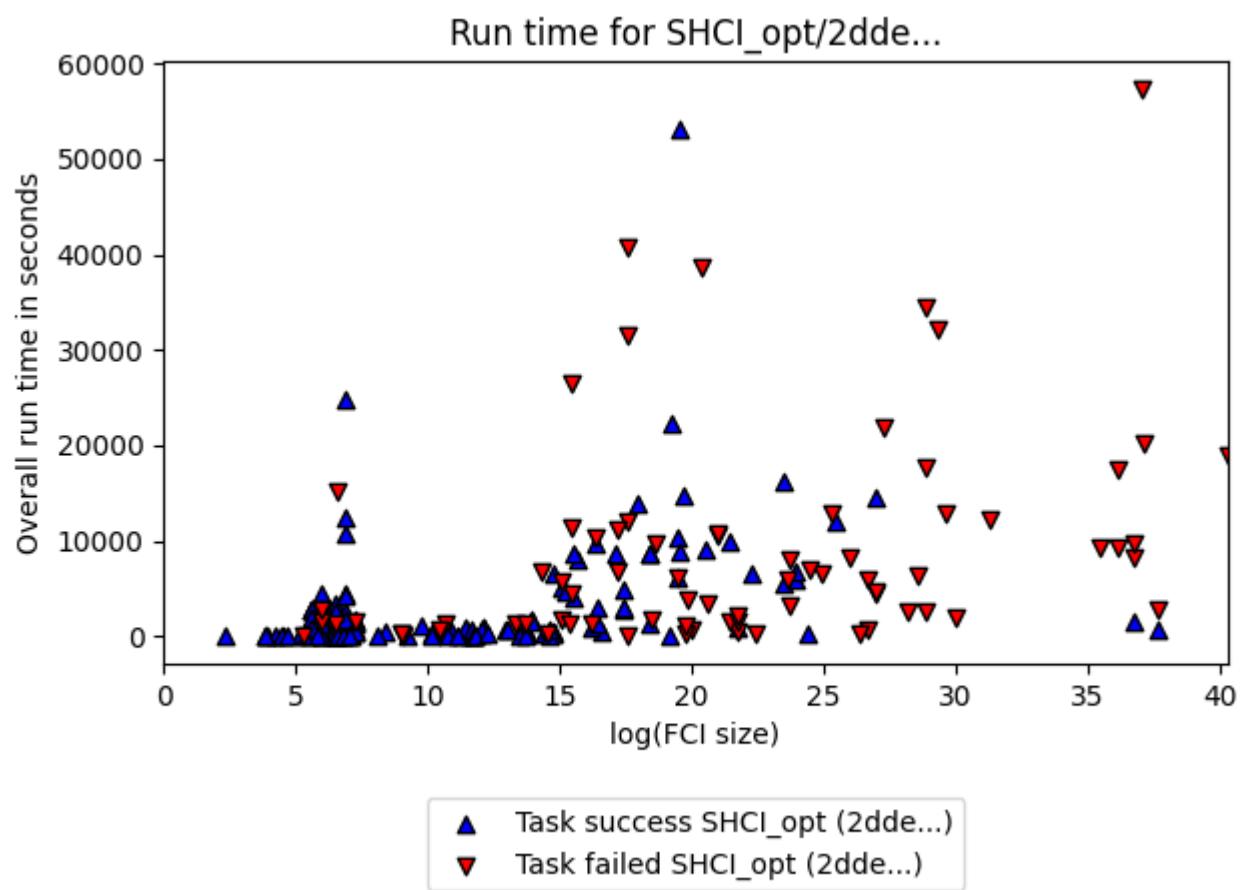
creation_timestamp: 2025-02-24T20:41:03.349036+00:00

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



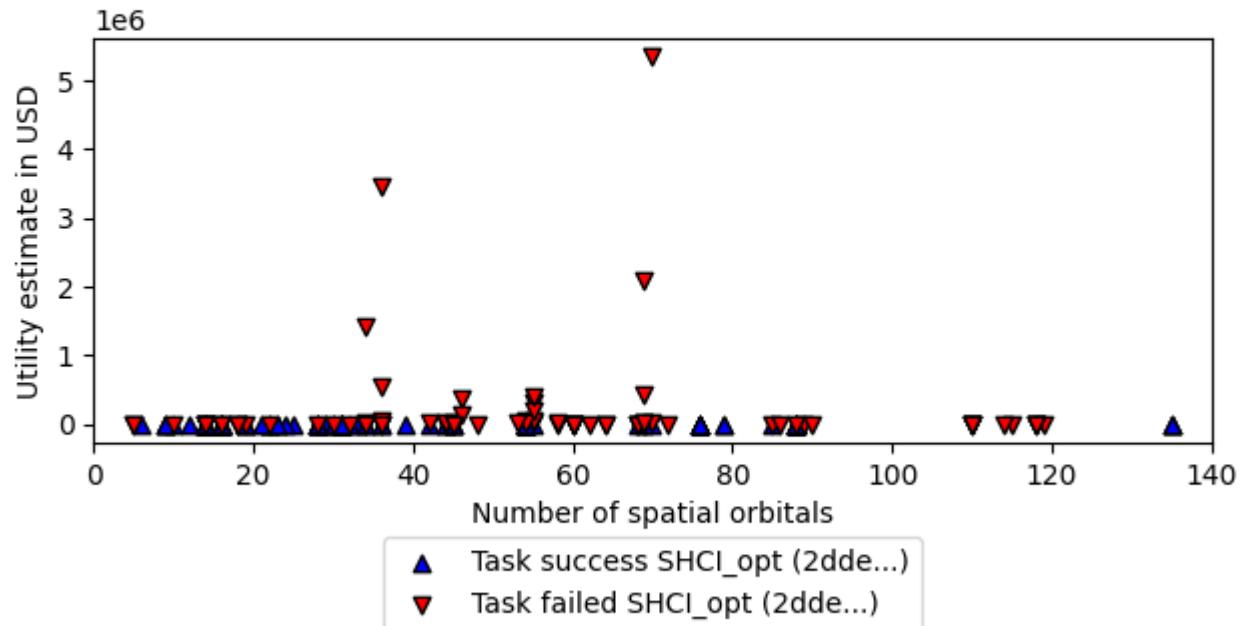
Note: plot only contains attempted tasks.



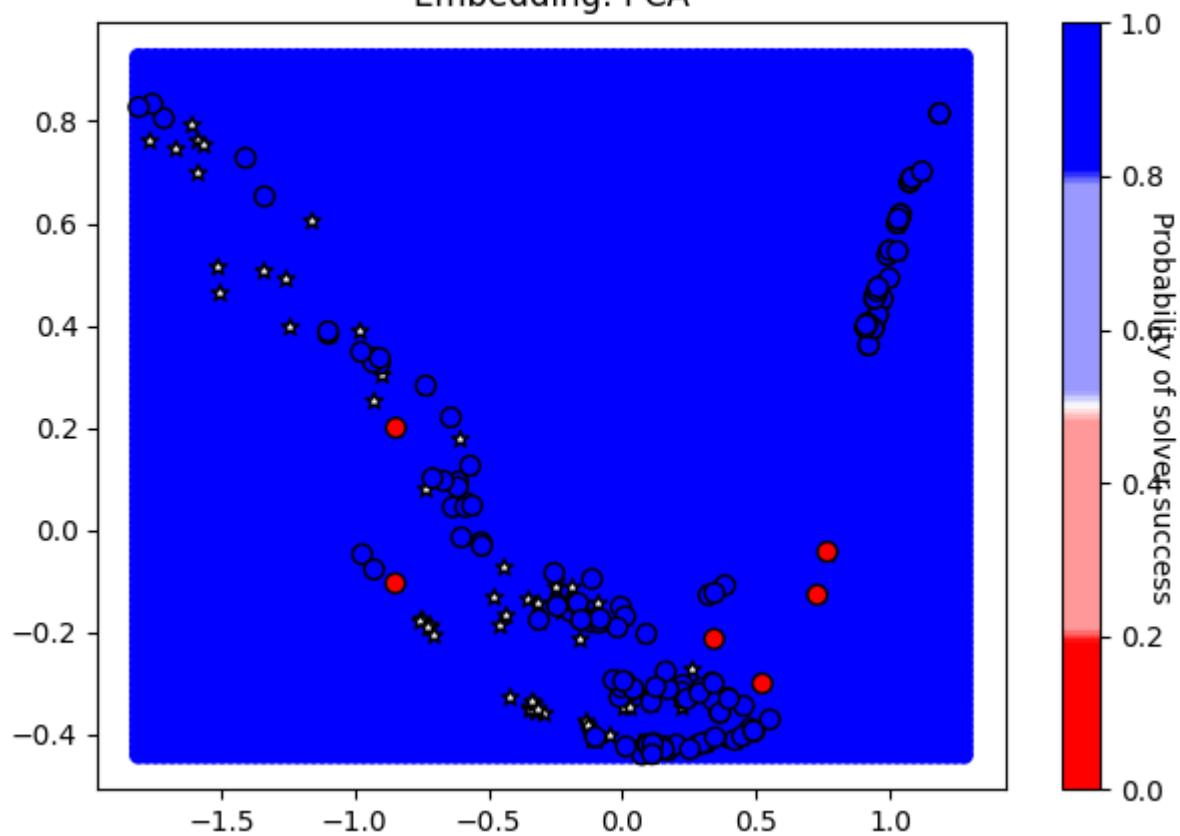
Note: plot only contains attempted tasks.

Utility capture from SHCI_opt/2dde...

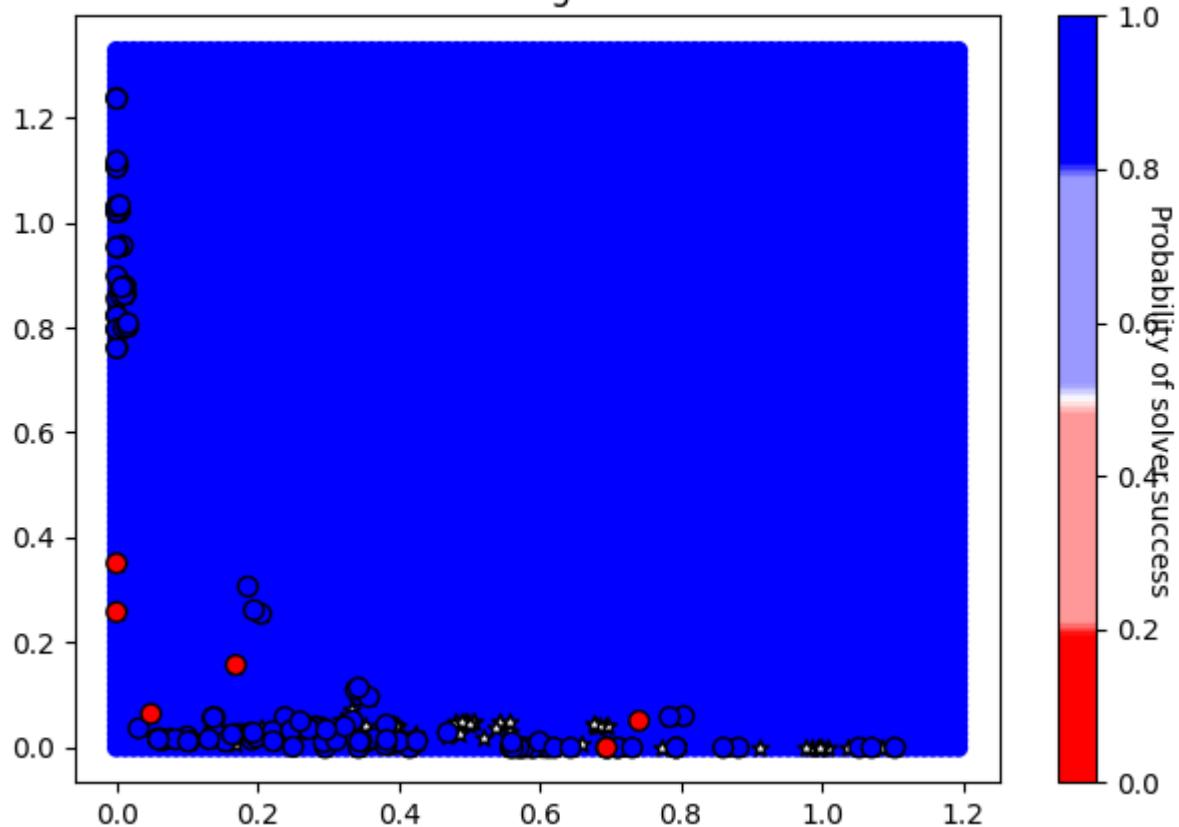
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



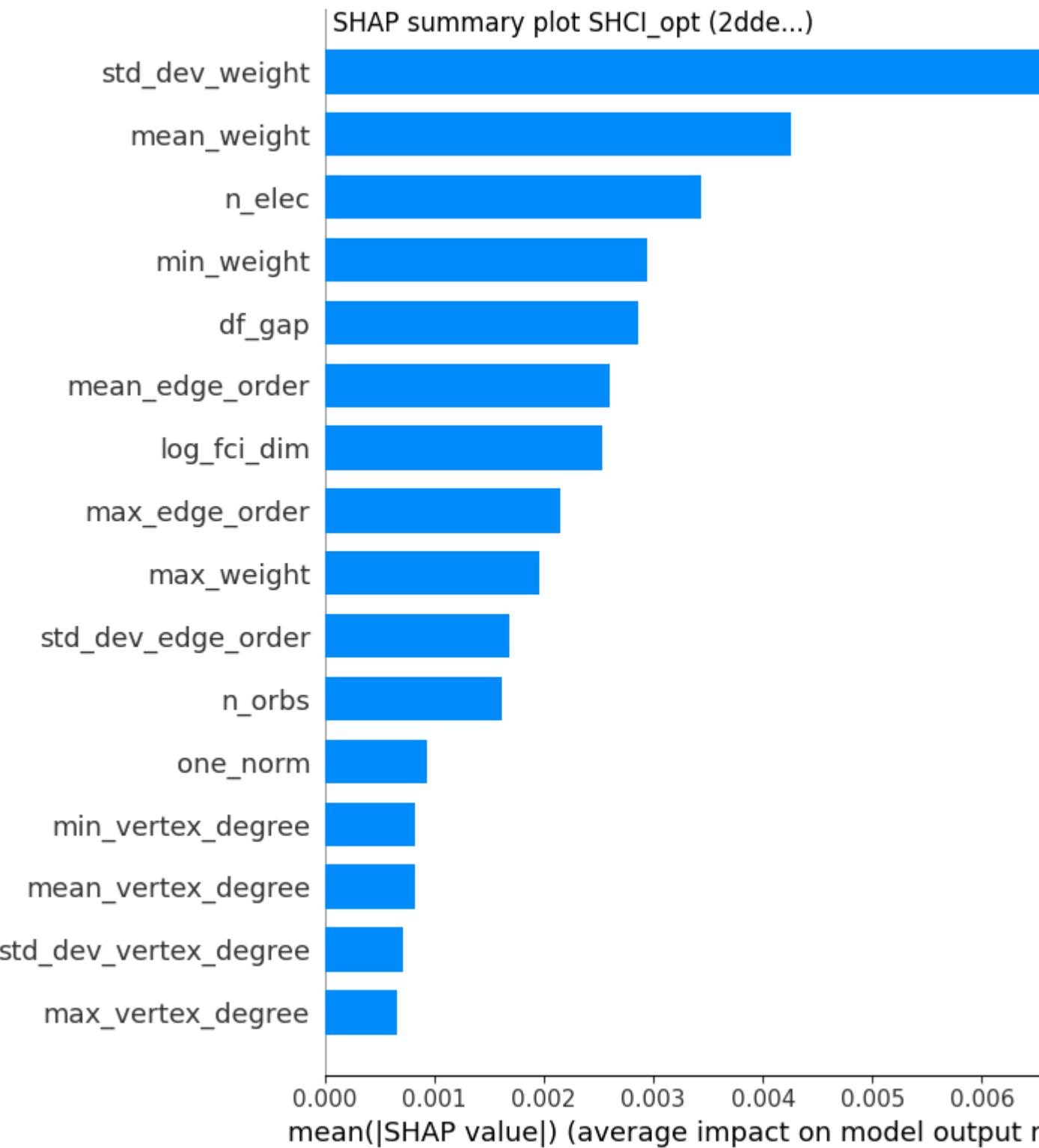
Solver SHCI_opt (2dde...)
Embedding: PCA



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: f482dfe8-2212-4c36-970c-025b4dc34b22

creation_timestamp: 2025-02-24T20:41:03.349036+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

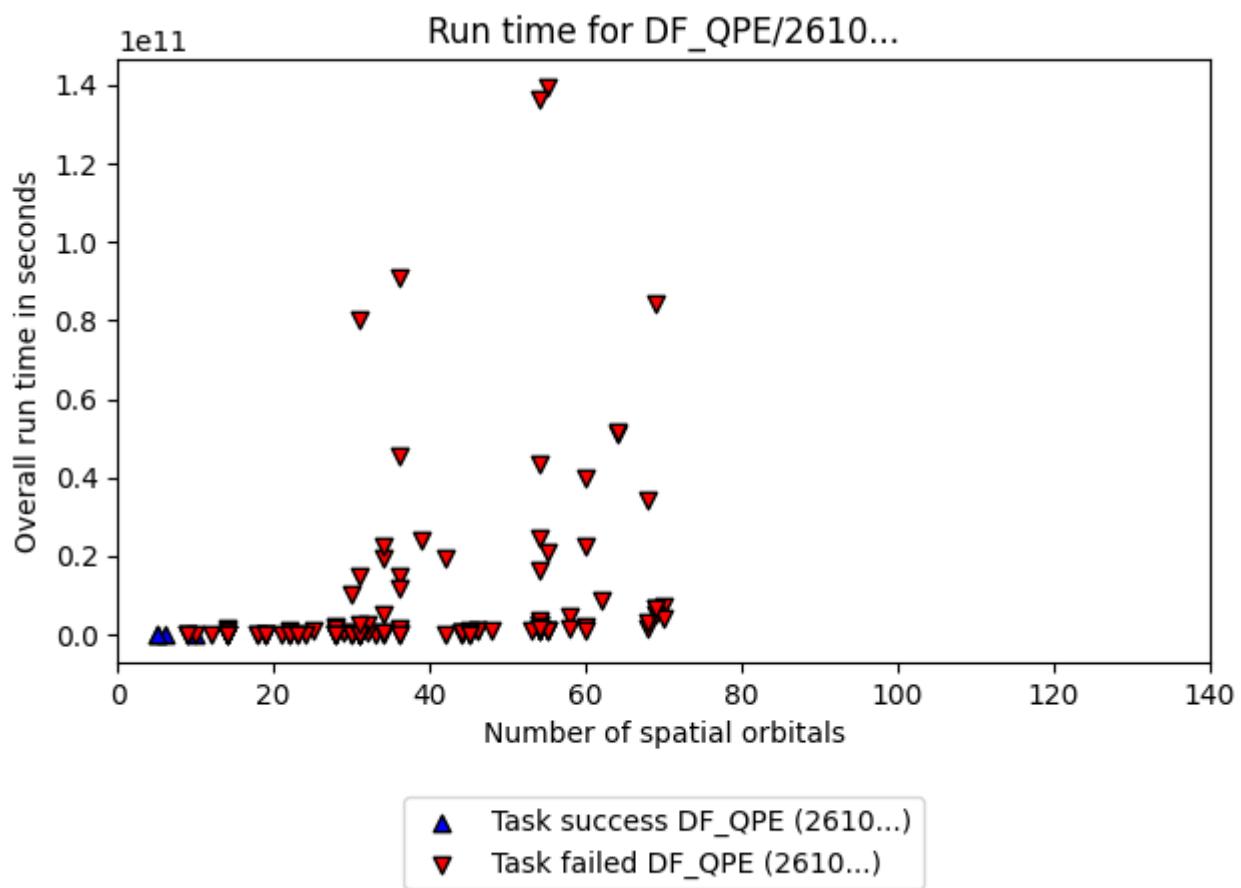
sum_of_run_time_of_attempted_tasks: 1131474650773.224

solvability_ratio: 0.0716

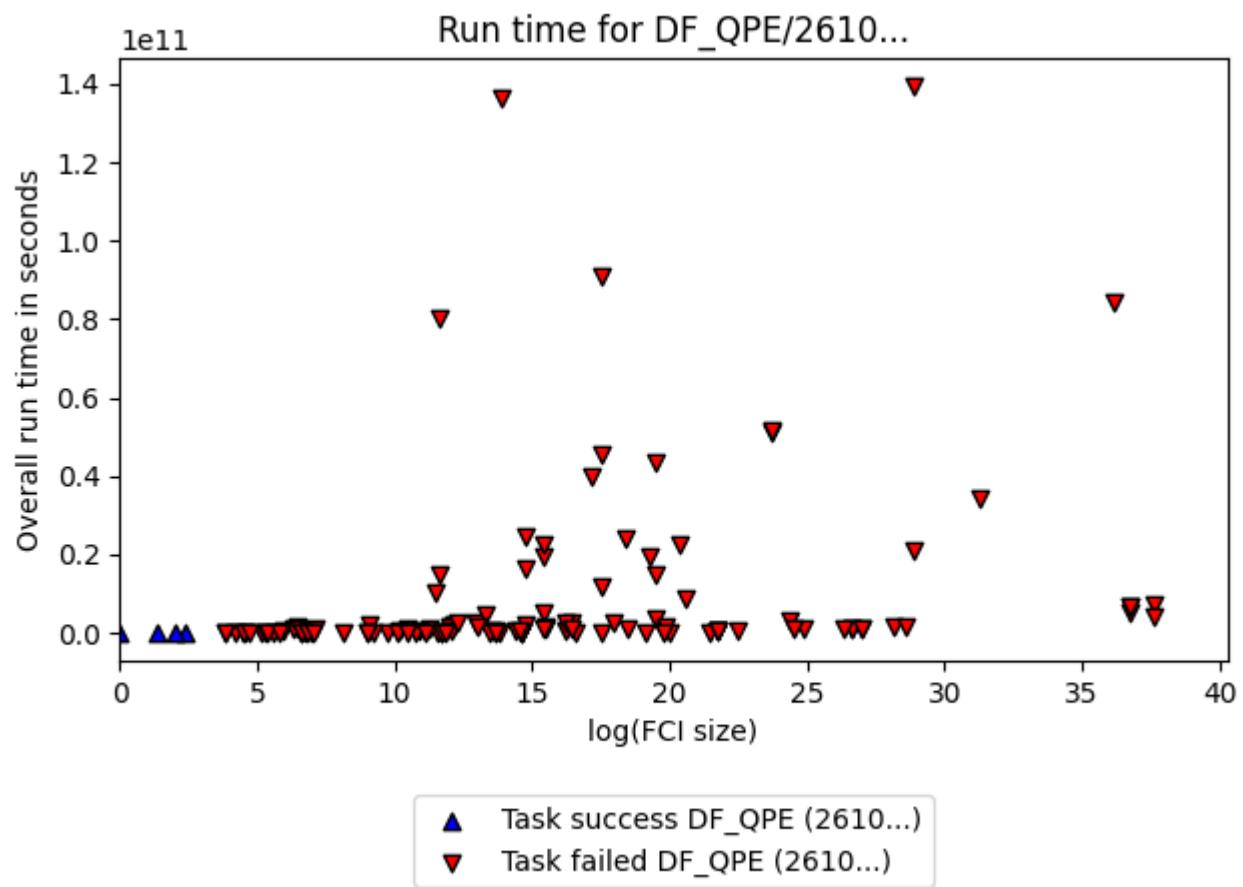
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



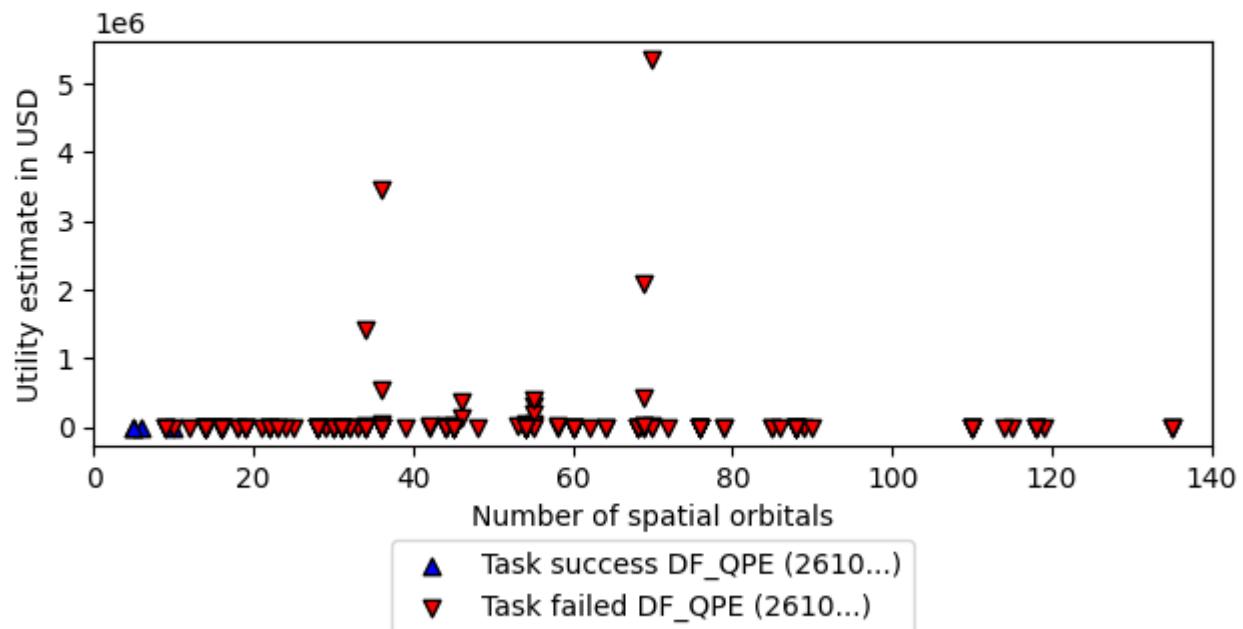
Note: plot only contains attempted tasks.



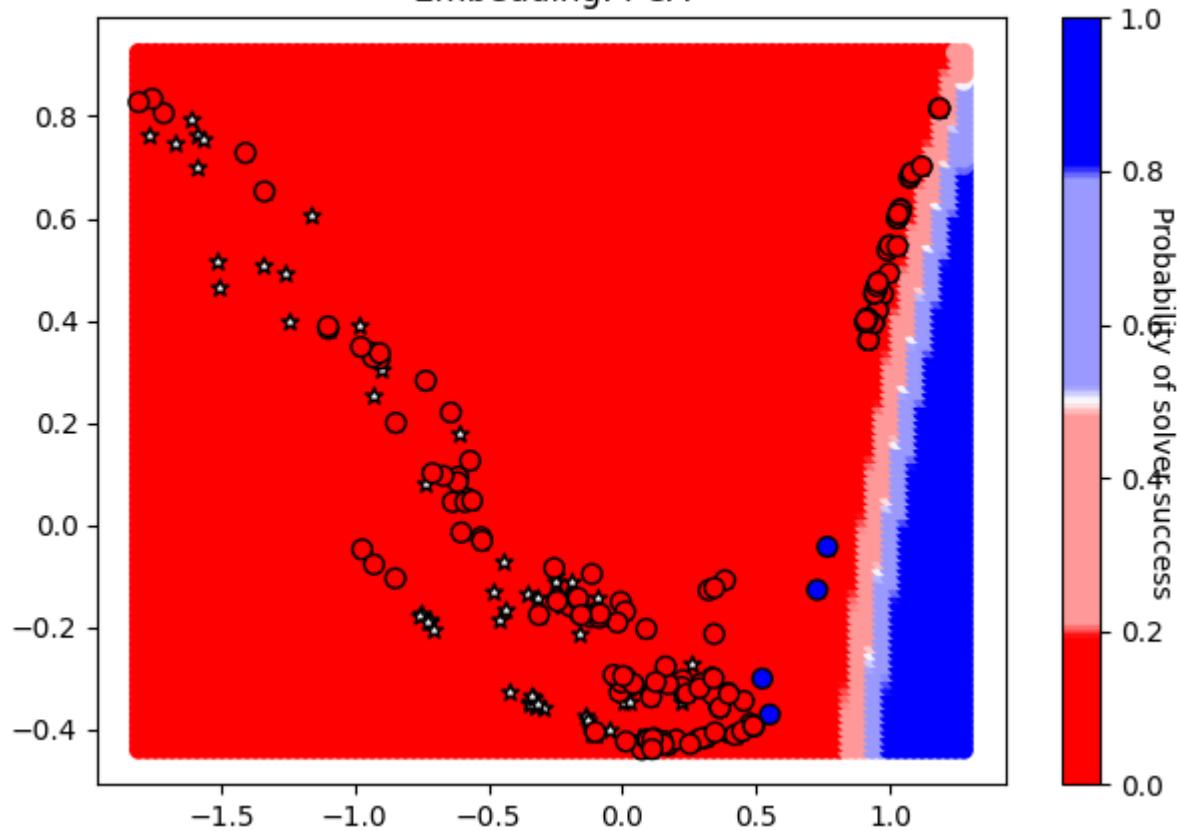
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/2610...

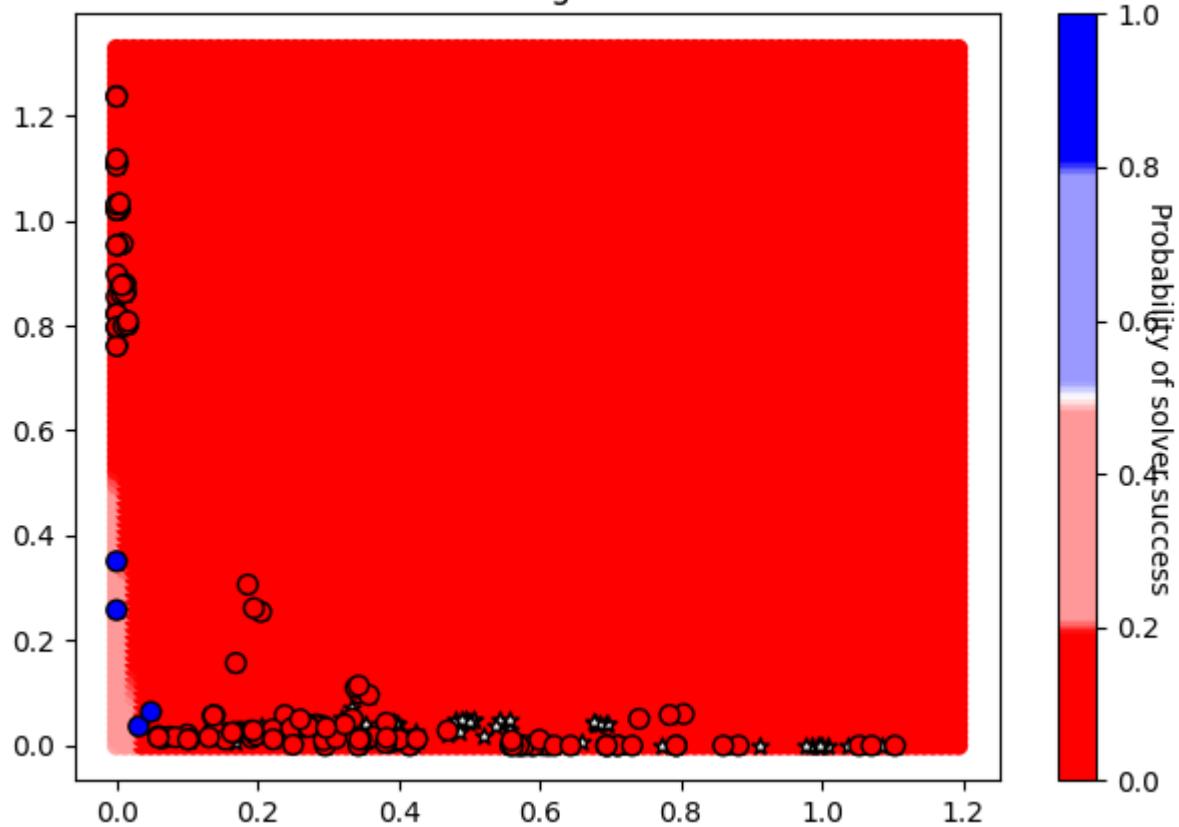
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



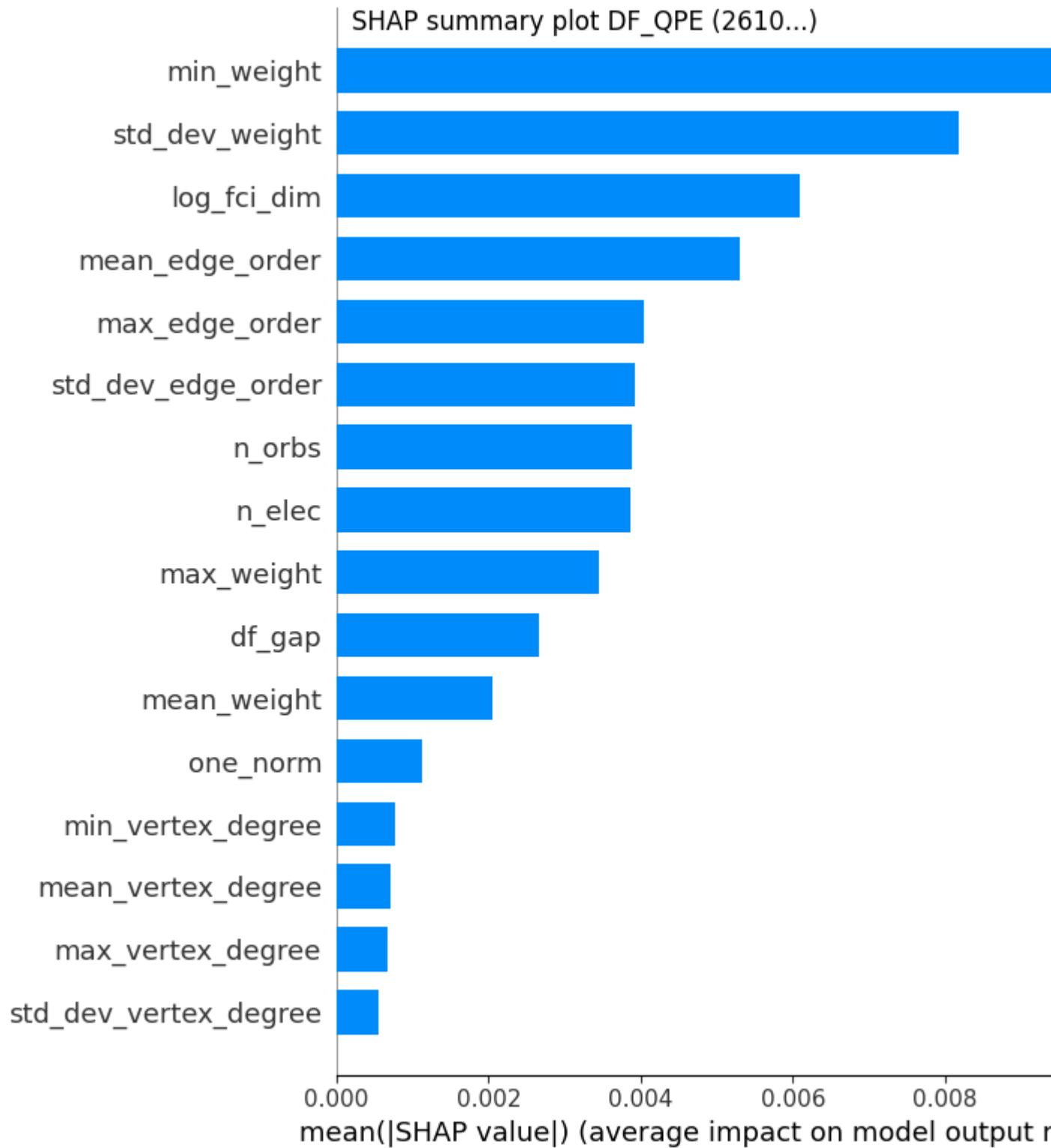
Solver DF_QPE (2610...)
Embedding: PCA



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.

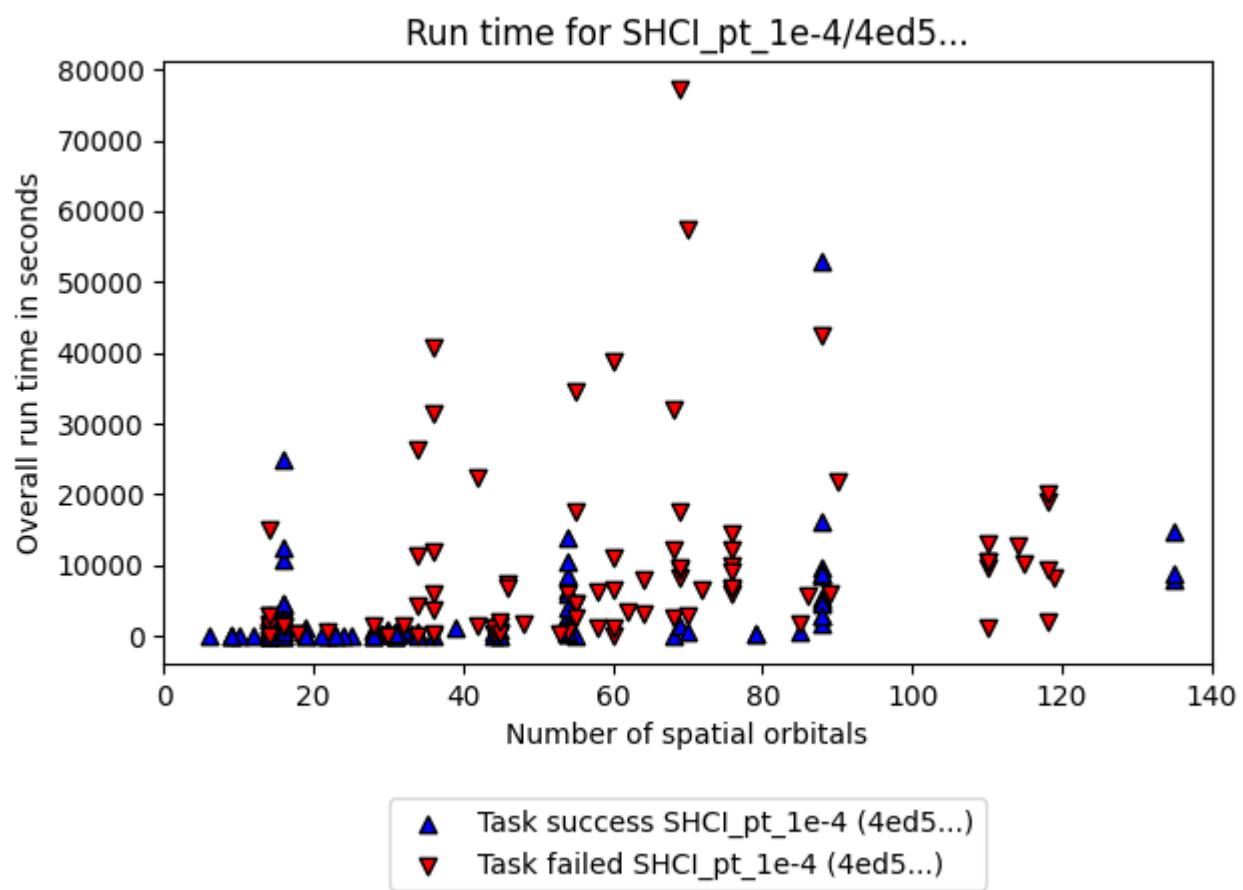


Solver SHCI_pt_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4

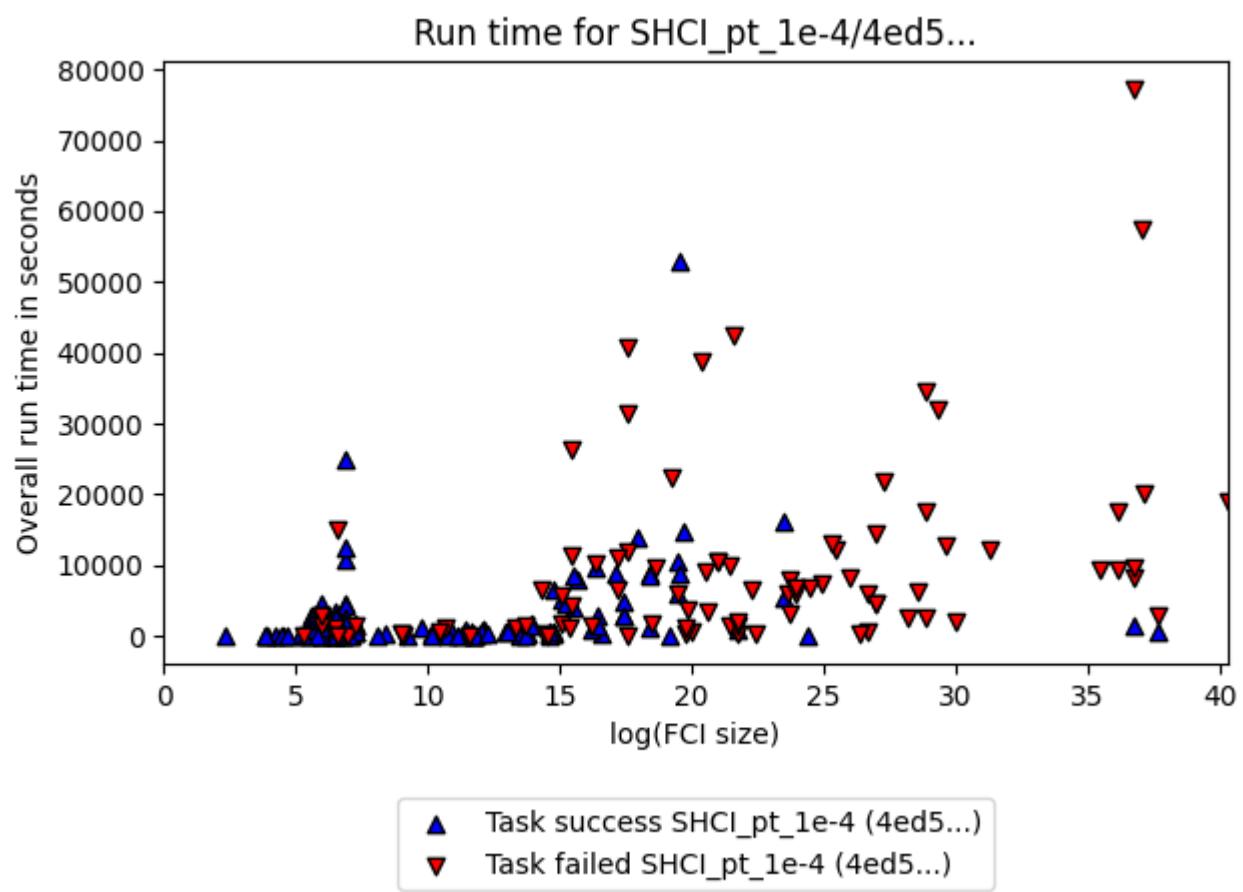
solver_uuid:4ed500f1-0650-41e3-af00-e4d0359394b4

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: 336e206c-5eae-4c62-98fb-de83e6b61f58
creation.timestamp: 2025-02-24T20:41:03.349036+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



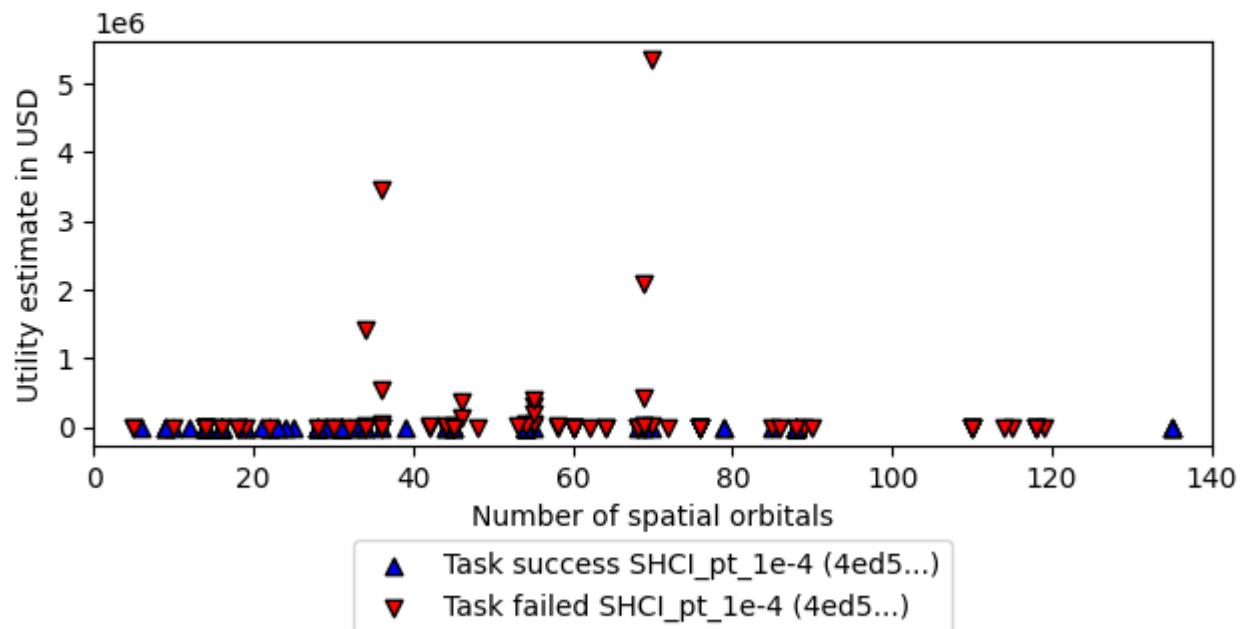
Note: plot only contains attempted tasks.



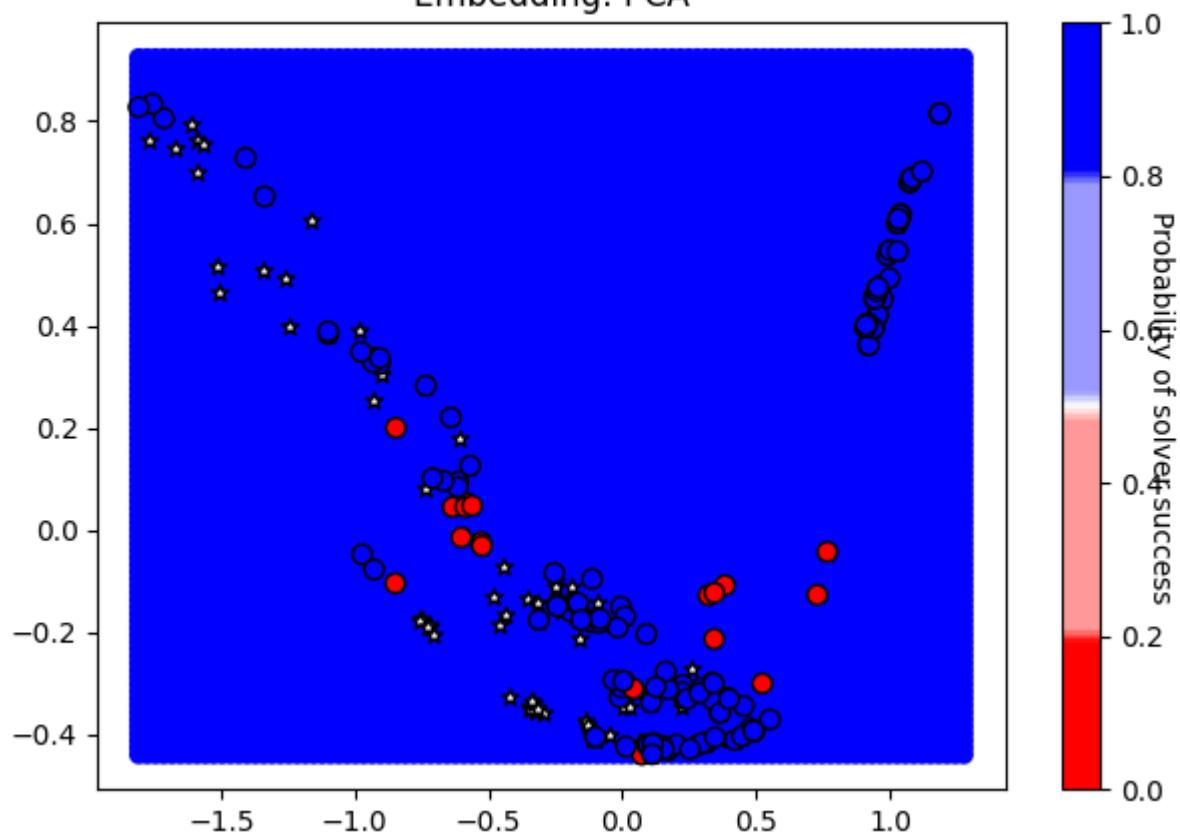
Note: plot only contains attempted tasks.

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

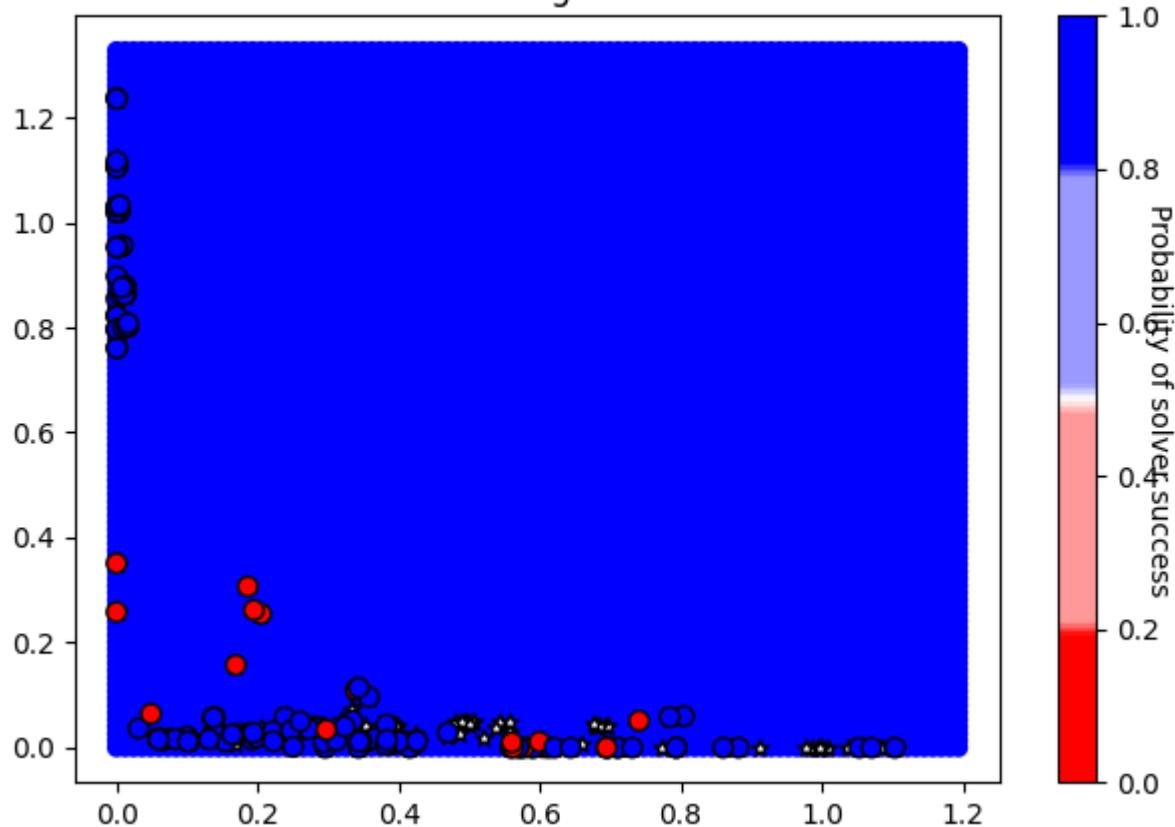
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



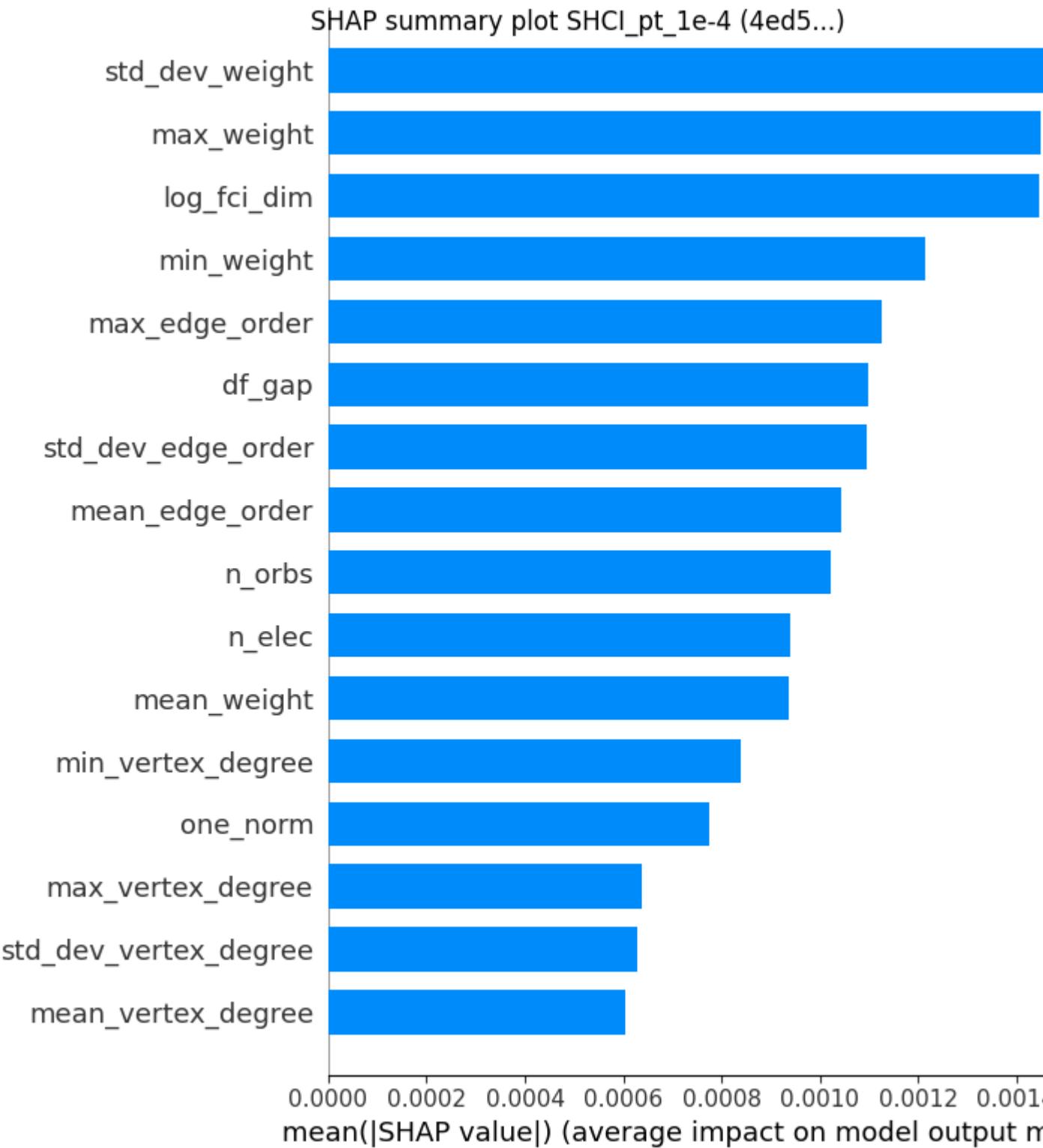
Solver SHCI_pt_1e-4 (4ed5...)
Embedding: PCA



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.

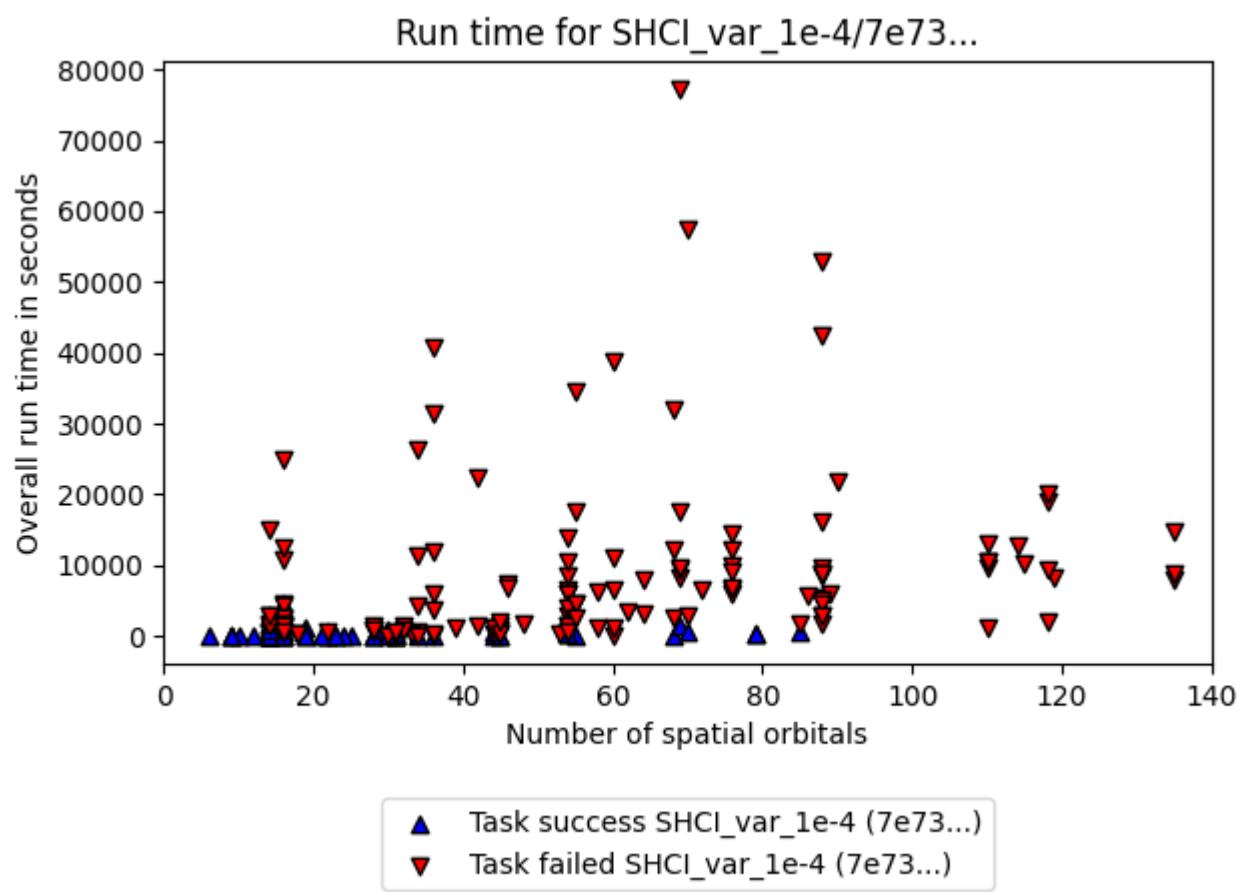


Solver SHCI_var_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54

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

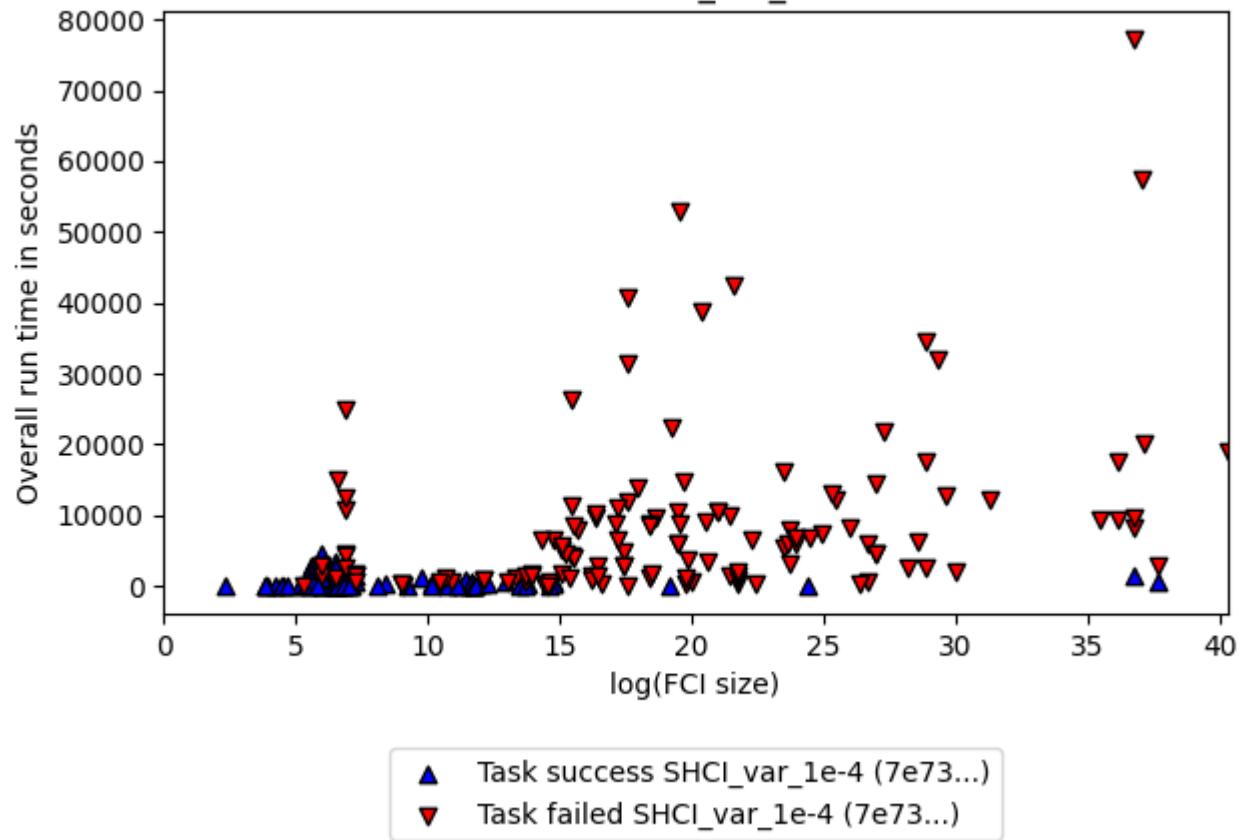
solver_short_name:SHCI_var_1e-4

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: 8f799fe4-3f49-482a-9b07-0c3a32139531
creation_timestamp: 2025-02-24T20:41:03.349036+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.

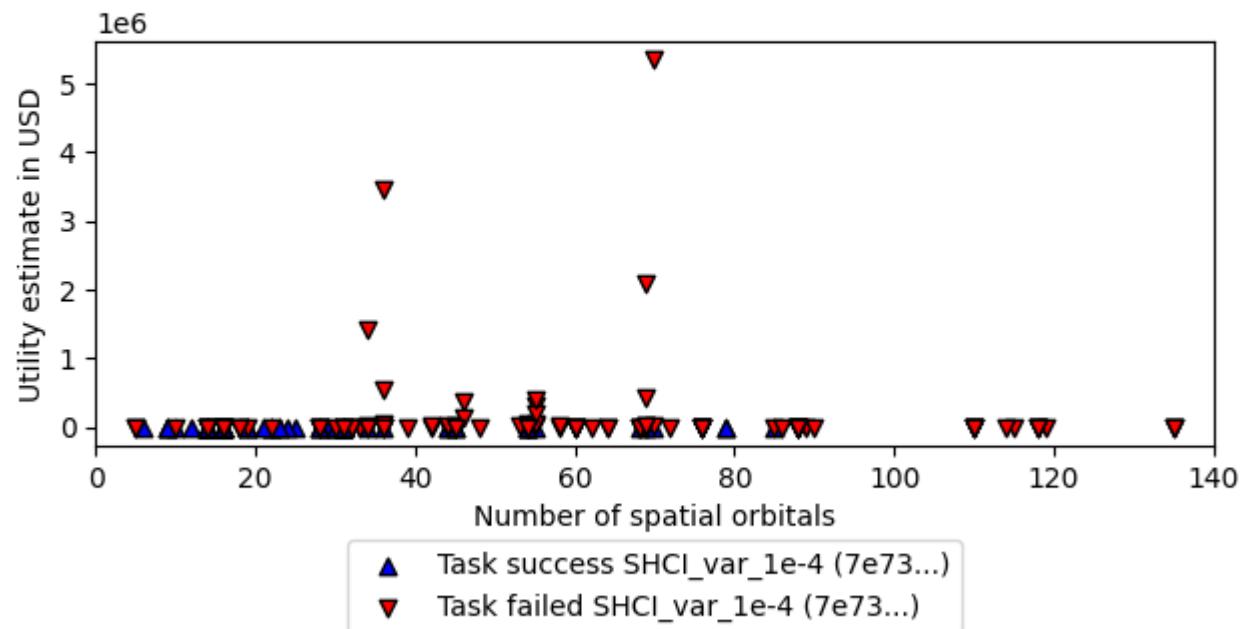
Run time for SHCI_var_1e-4/7e73...



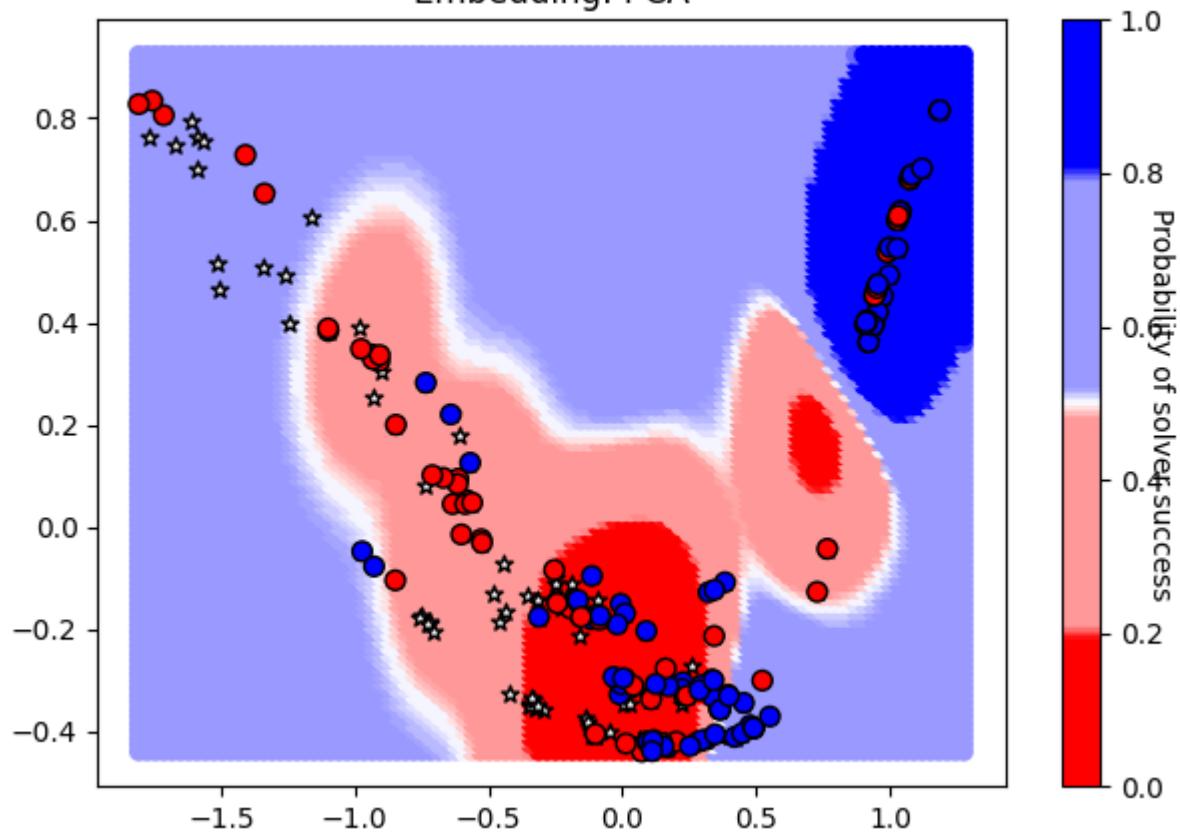
Note: plot only contains attempted tasks.

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

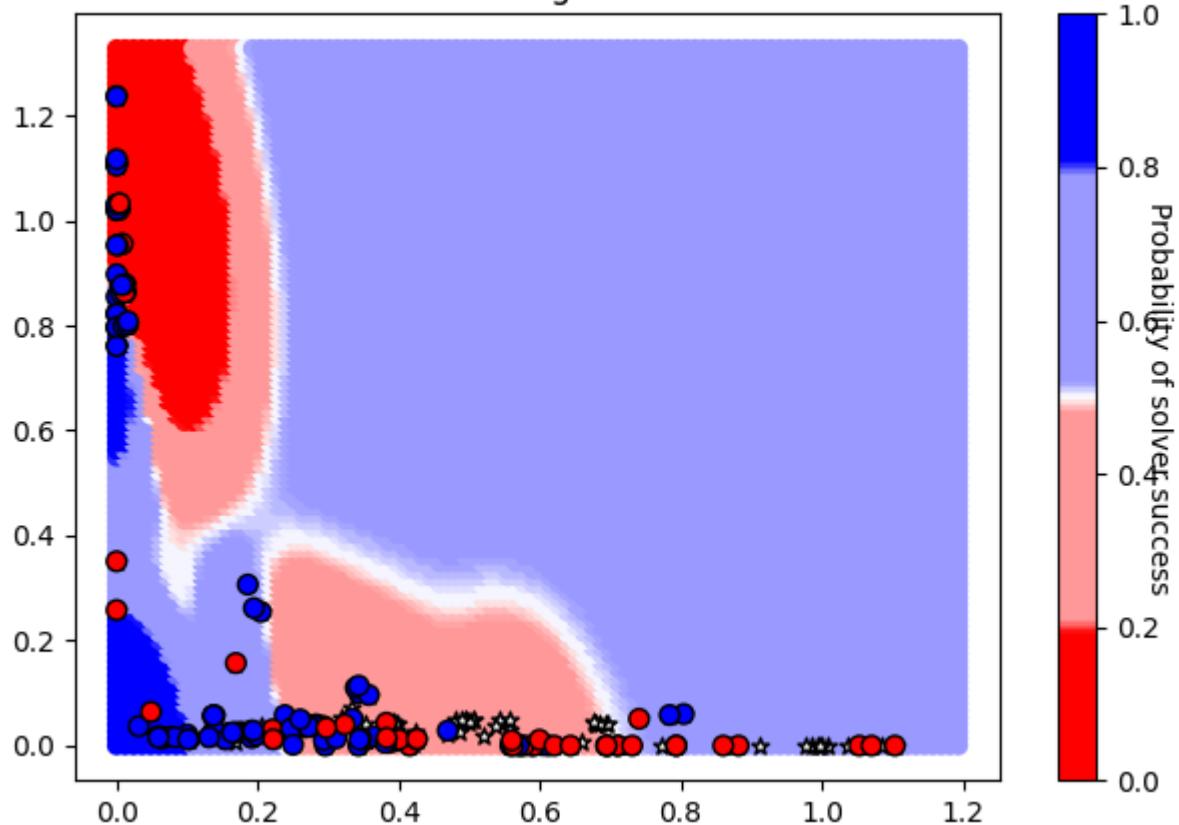
(captured: $\$1.0\text{e}+02/1.5\text{e}+07$, approximately $6.8\text{e}-04\%$)



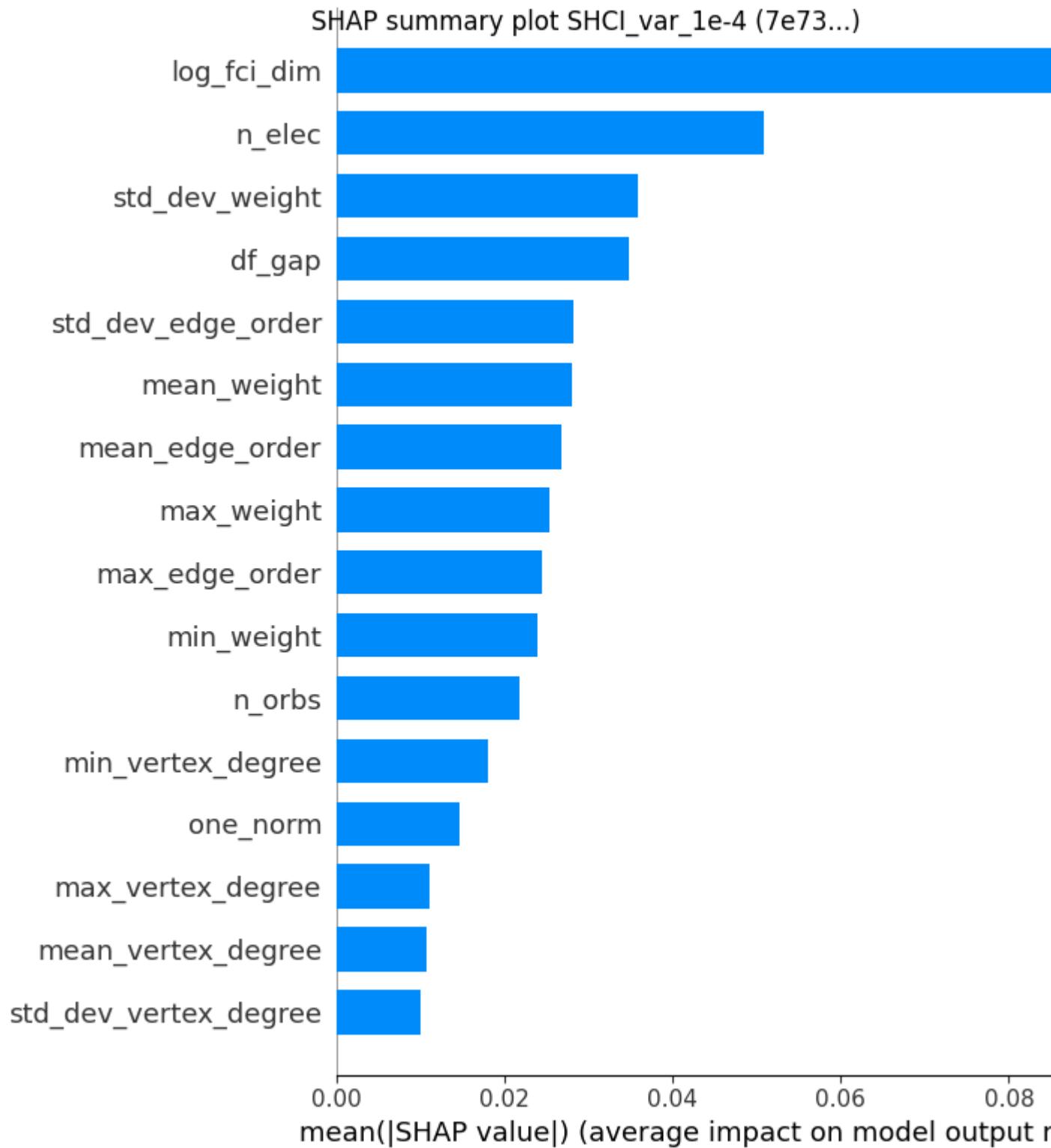
Solver SHCI_var_1e-4 (7e73...)
Embedding: PCA



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.



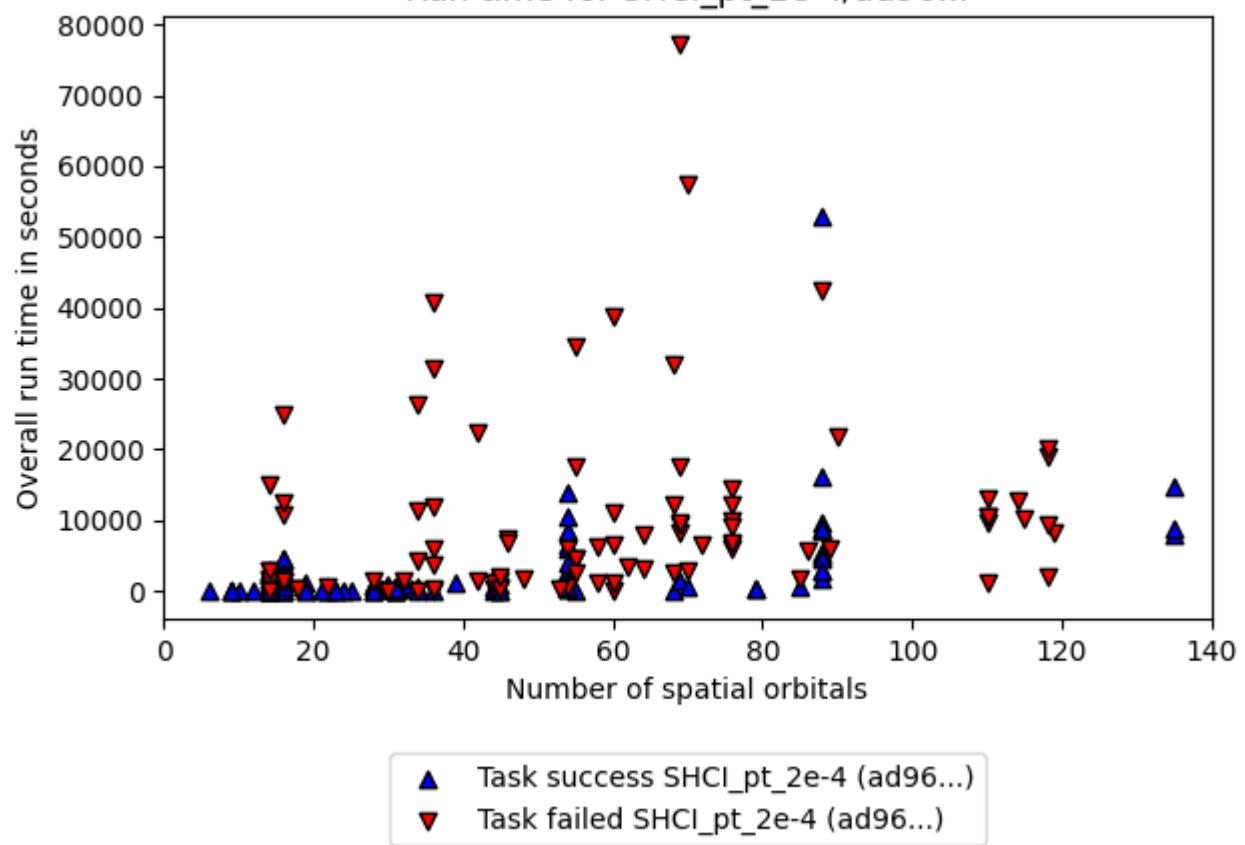
Solver SHCI_pt_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb

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

solver_short_name:SHCI_pt_2e-4

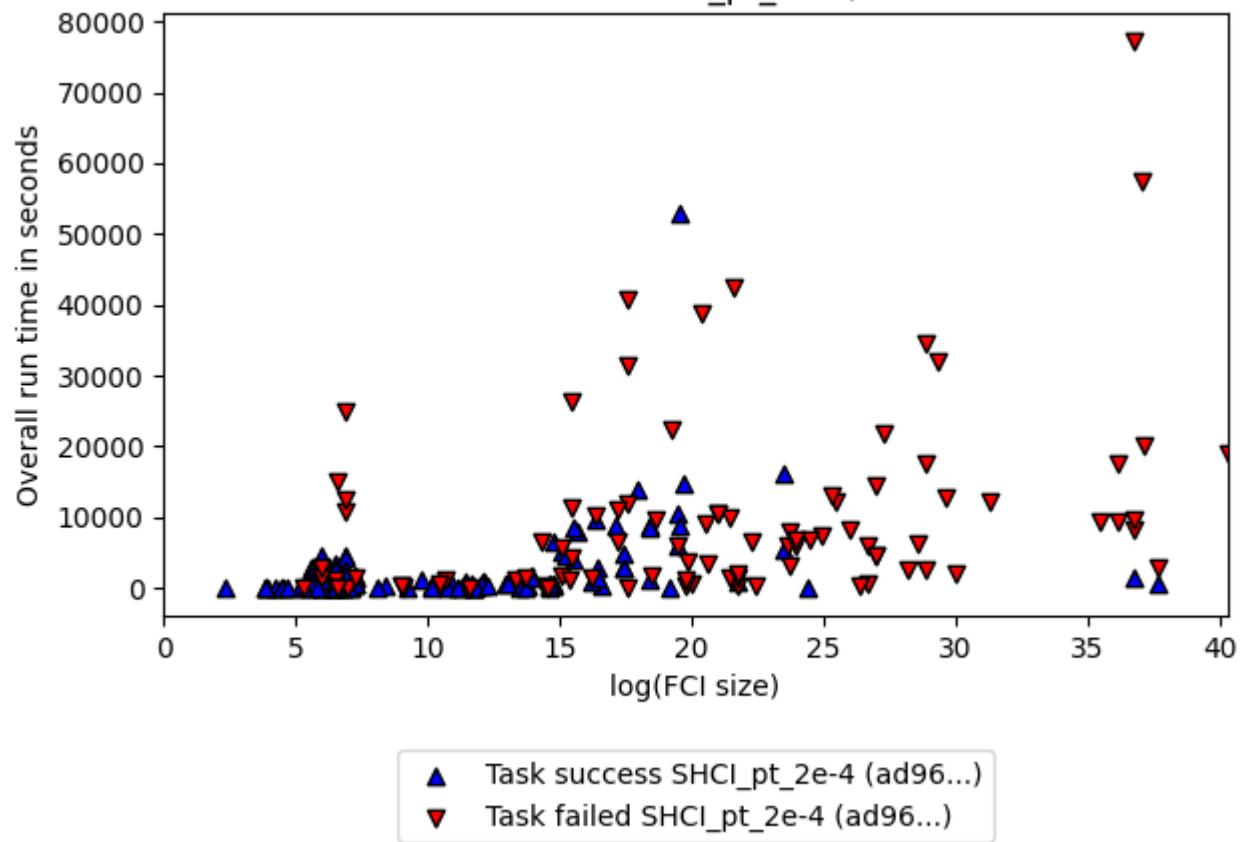
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-4 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: 6c97e0b0-8103-4dc6-8331-b131efaf320c
creation.timestamp: 2025-02-24T20:41:03.349036+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.

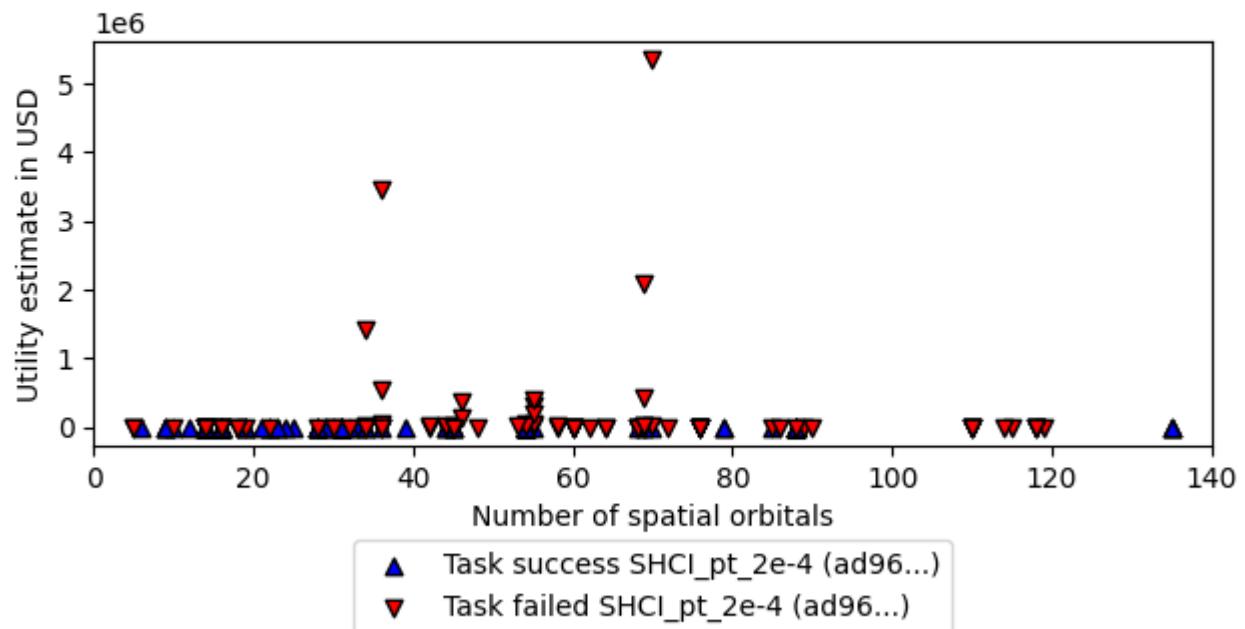
Run time for SHCI_pt_2e-4/ad96...



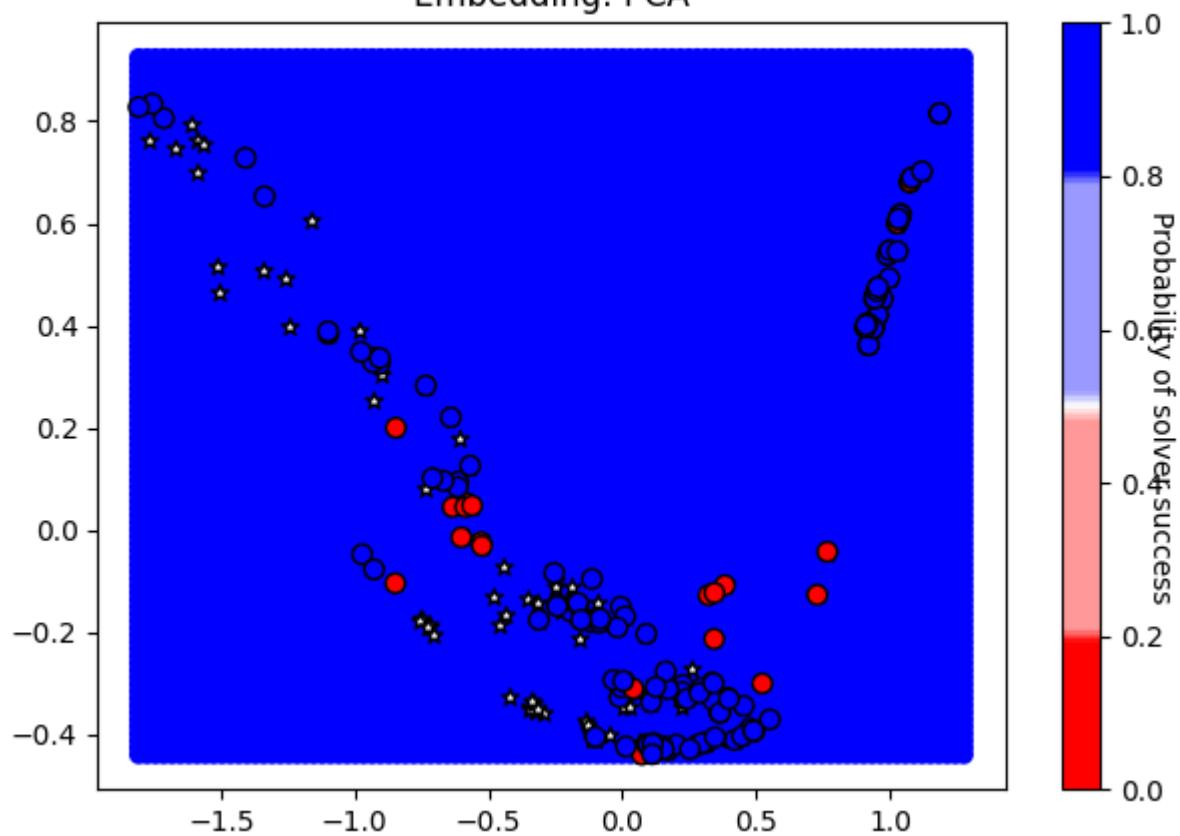
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-4/ad96...

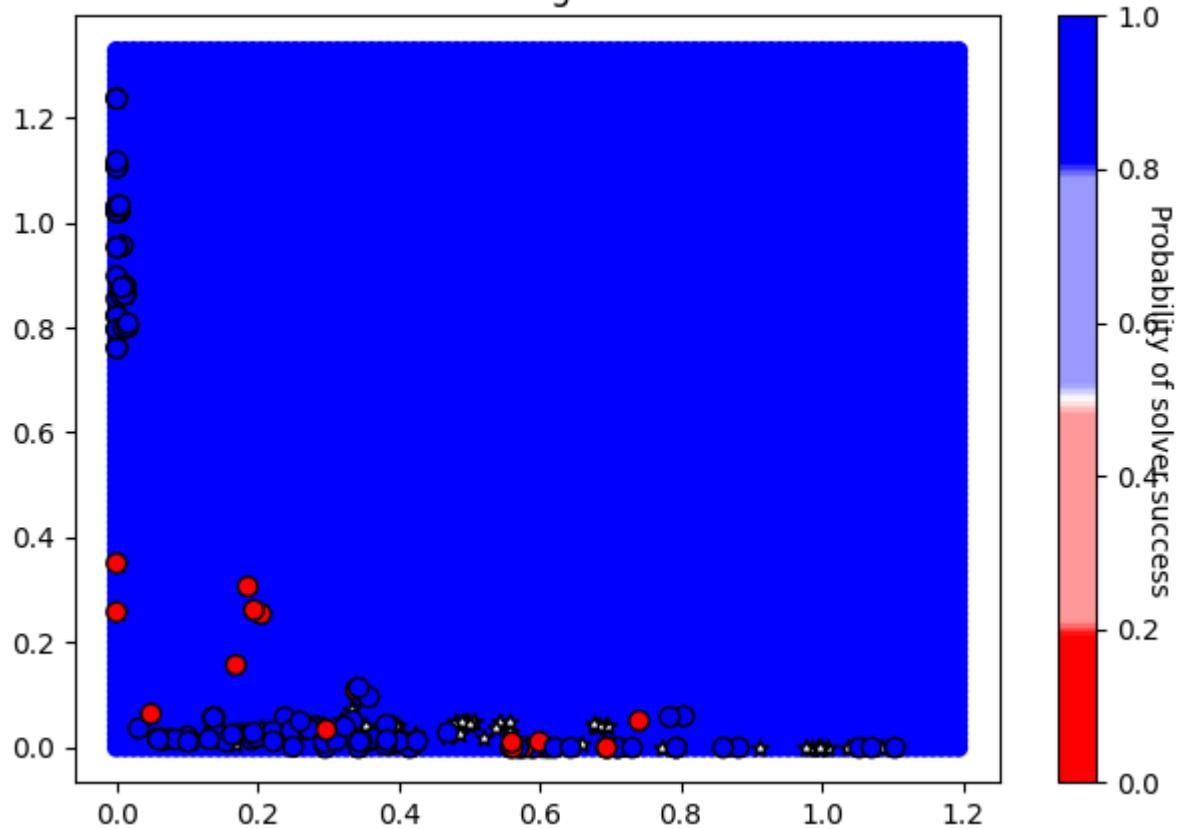
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



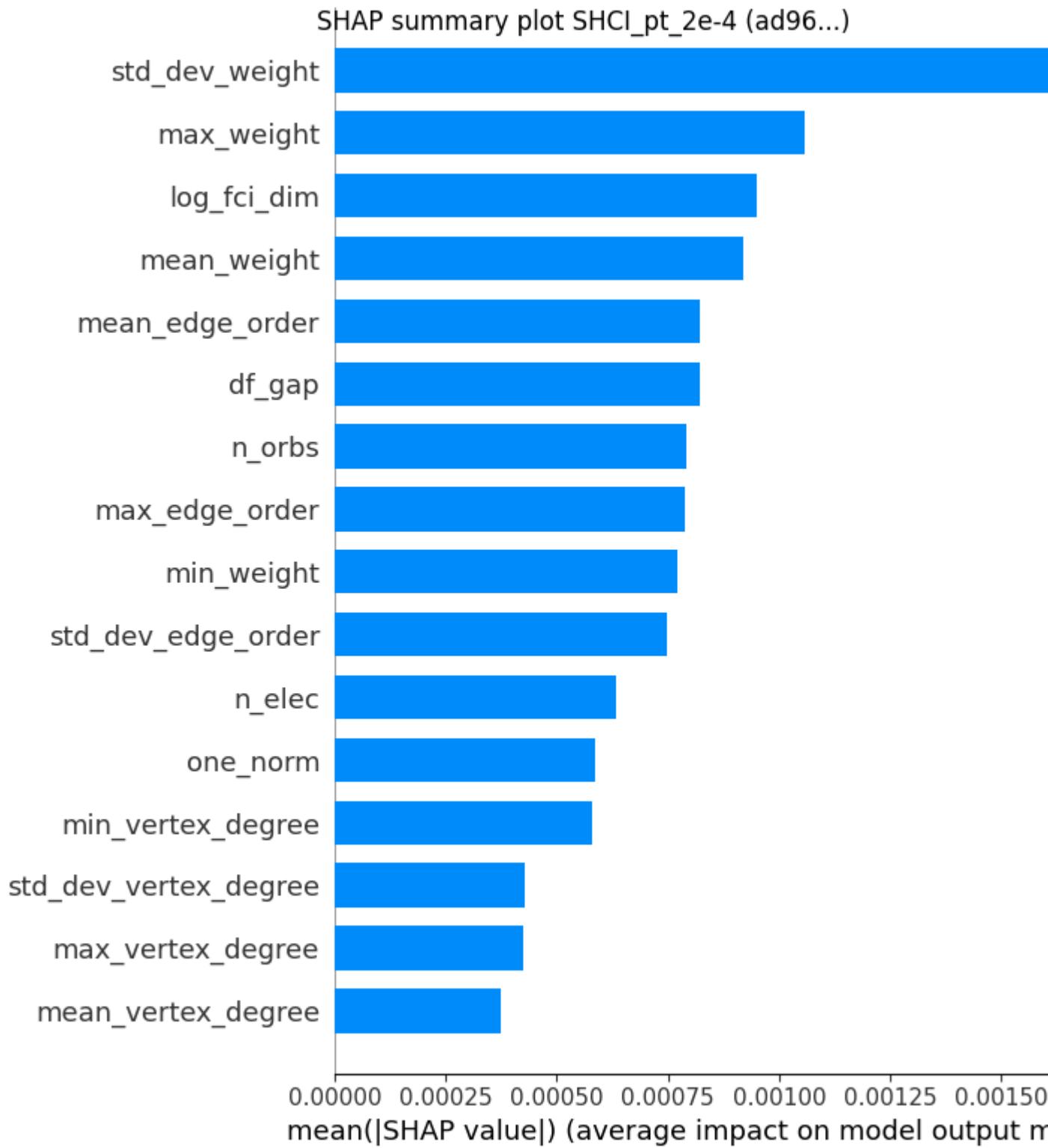
Solver SHCI_pt_2e-4 (ad96...)
Embedding: PCA



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.



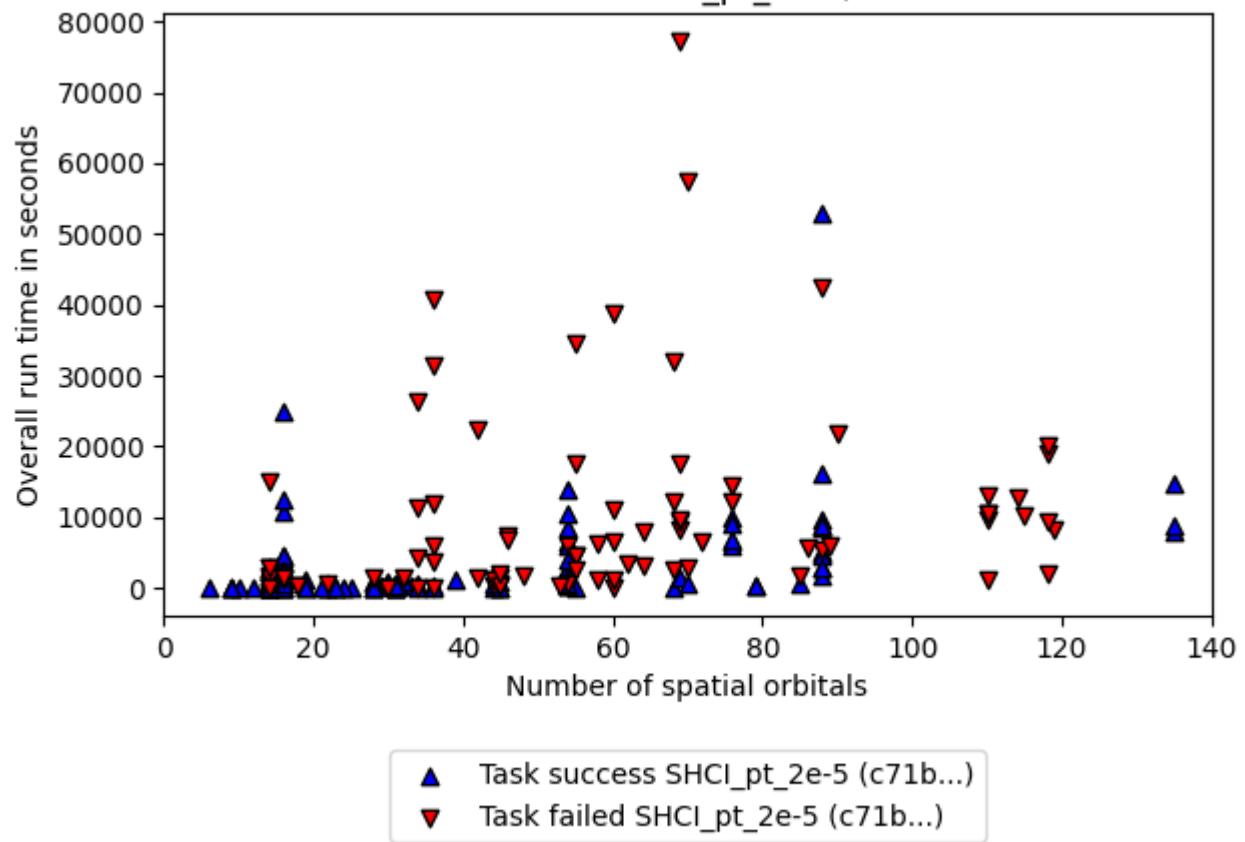
Solver SHCI_pt_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6

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

solver_short_name:SHCI_pt_2e-5

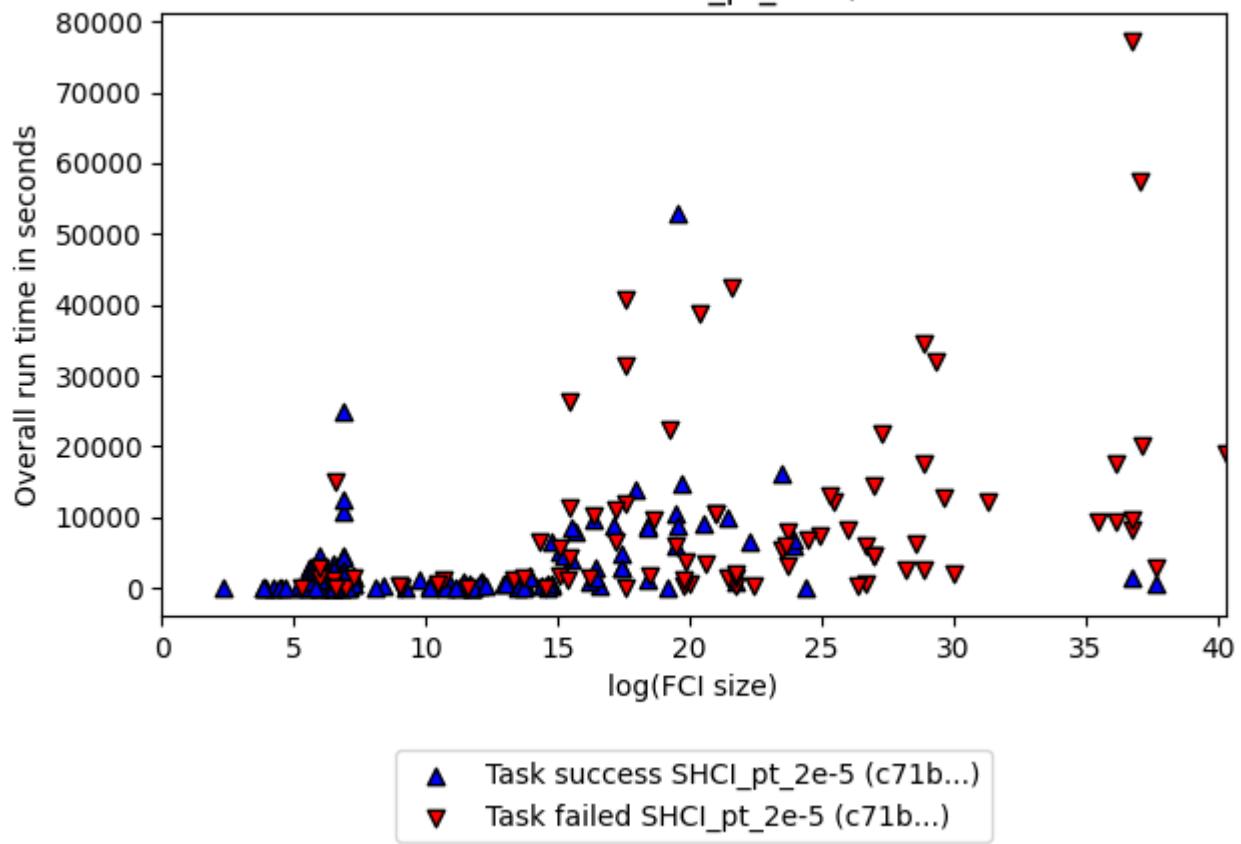
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-5 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: d8fc853e-919b-4635-a03b-eedb9c97449f
creation.timestamp: 2025-02-24T20:41:03.349036+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.

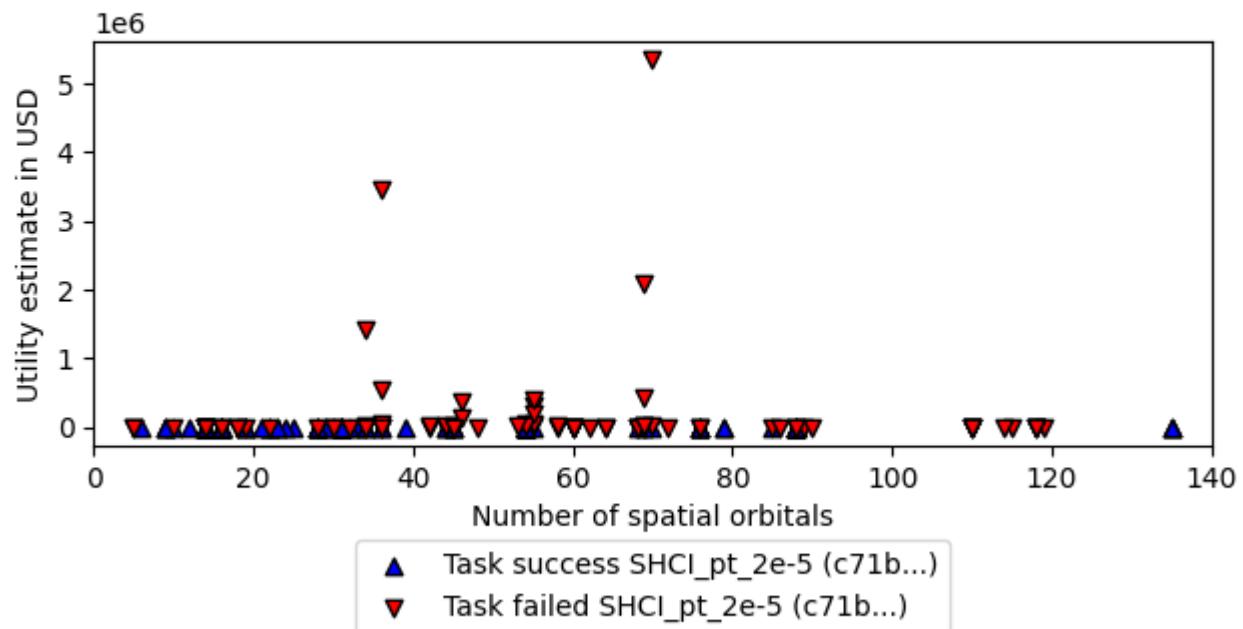
Run time for SHCI_pt_2e-5/c71b...



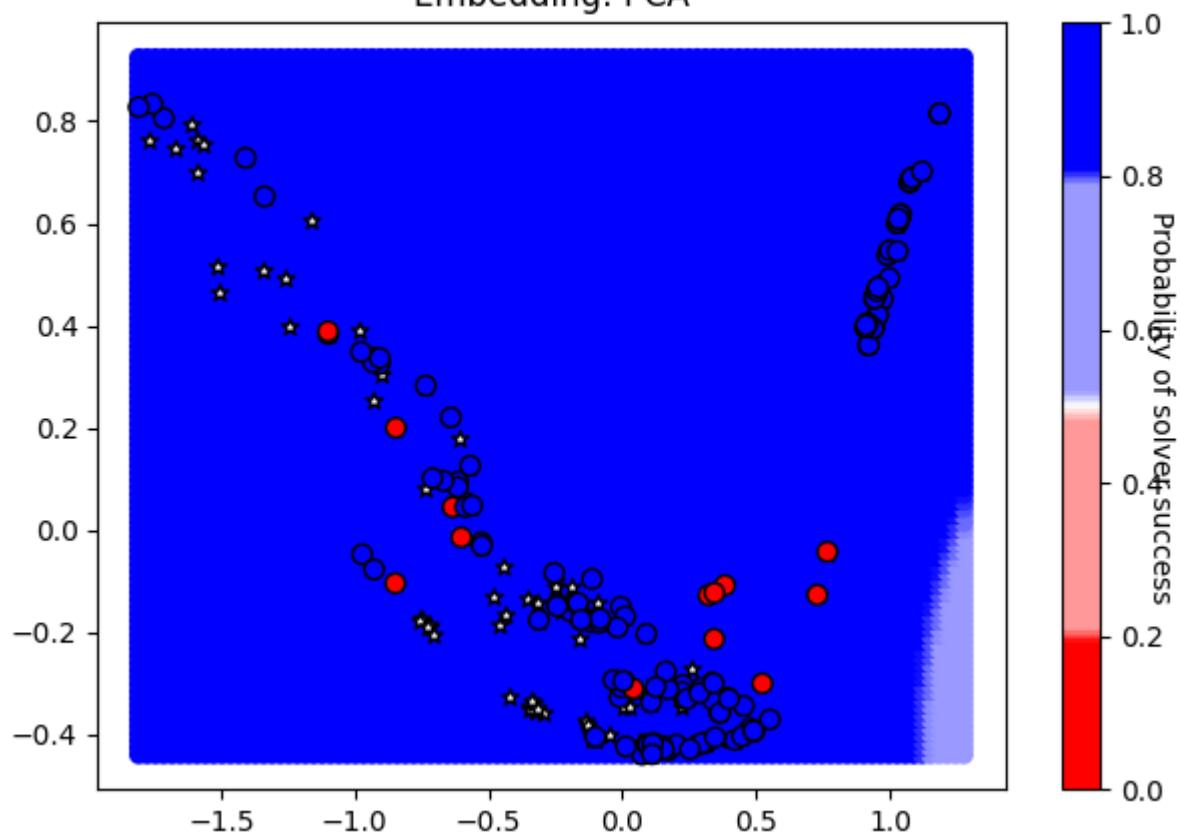
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-5/c71b...

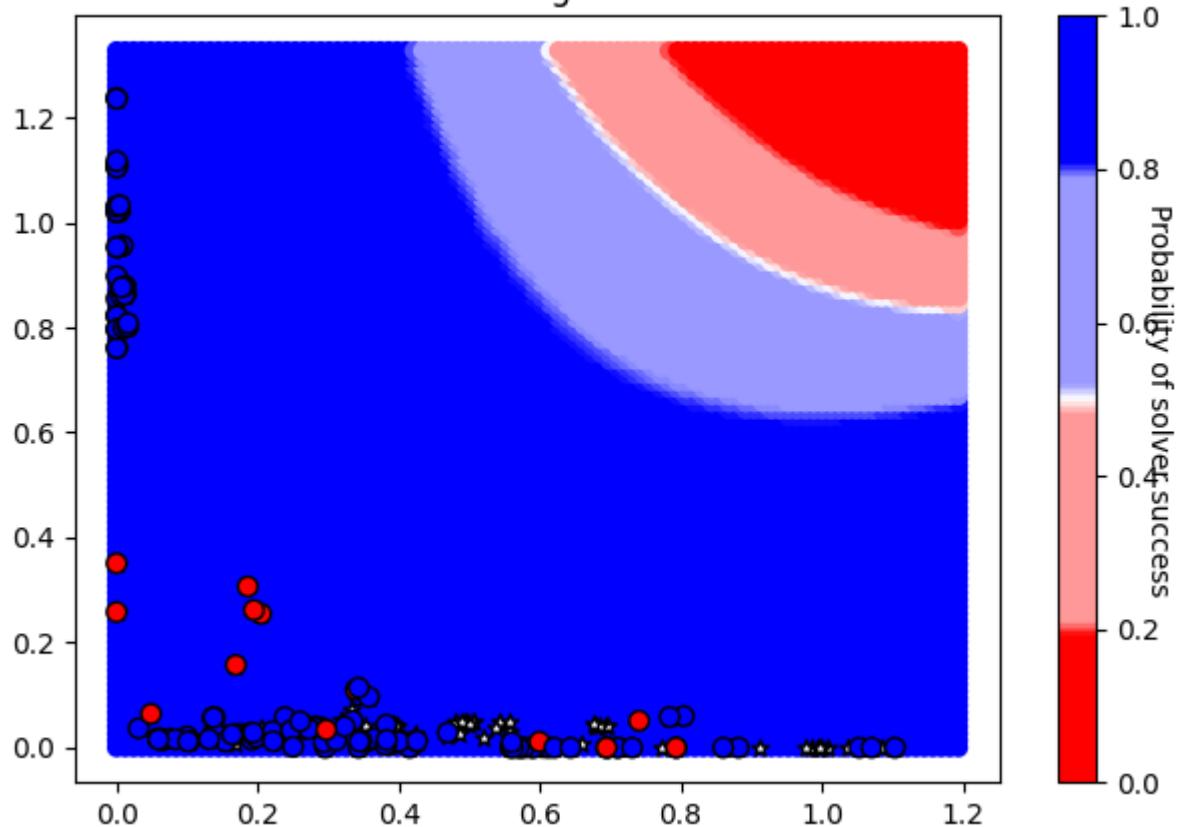
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



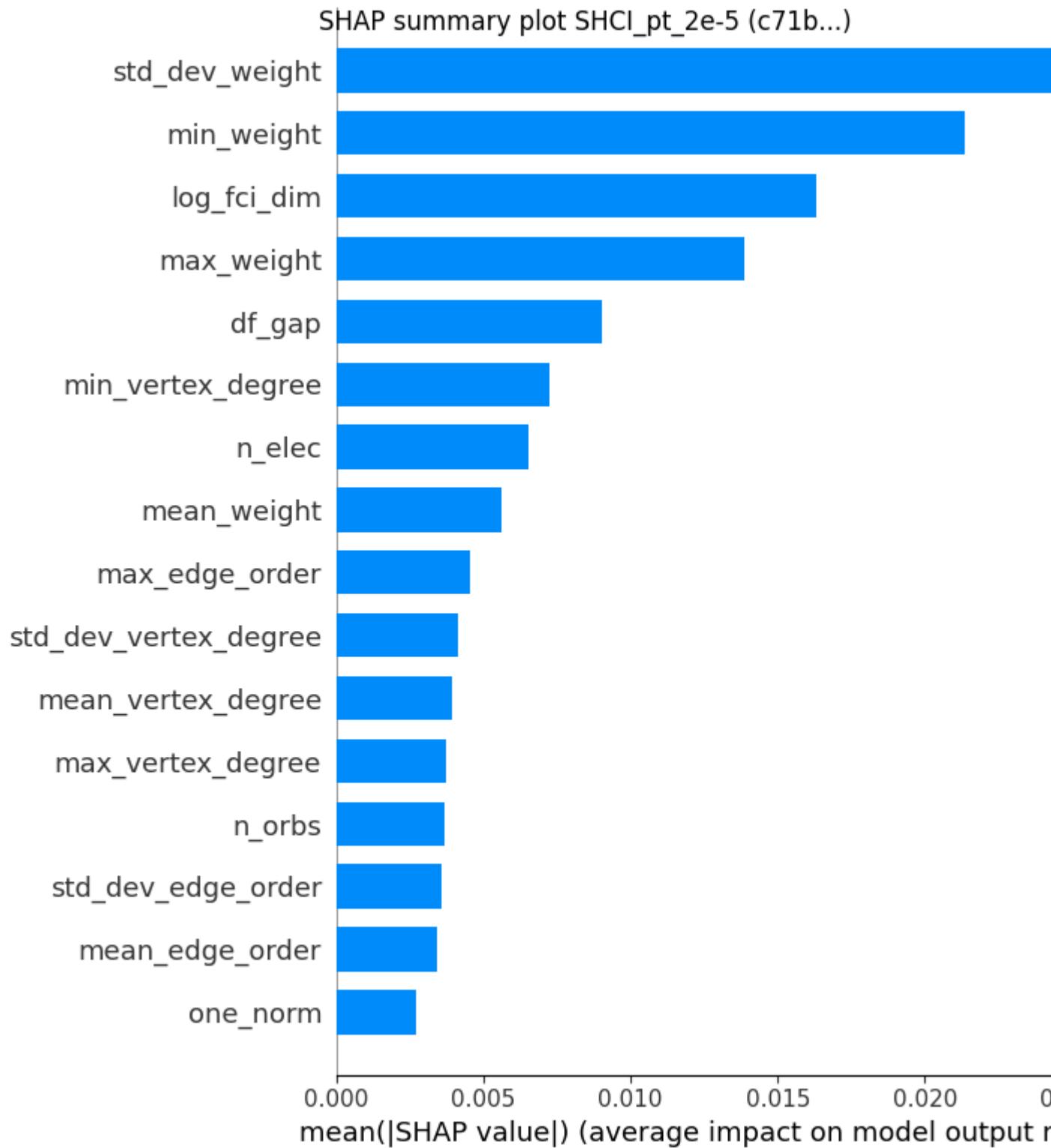
Solver SHCI_pt_2e-5 (c71b...)
Embedding: PCA



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.

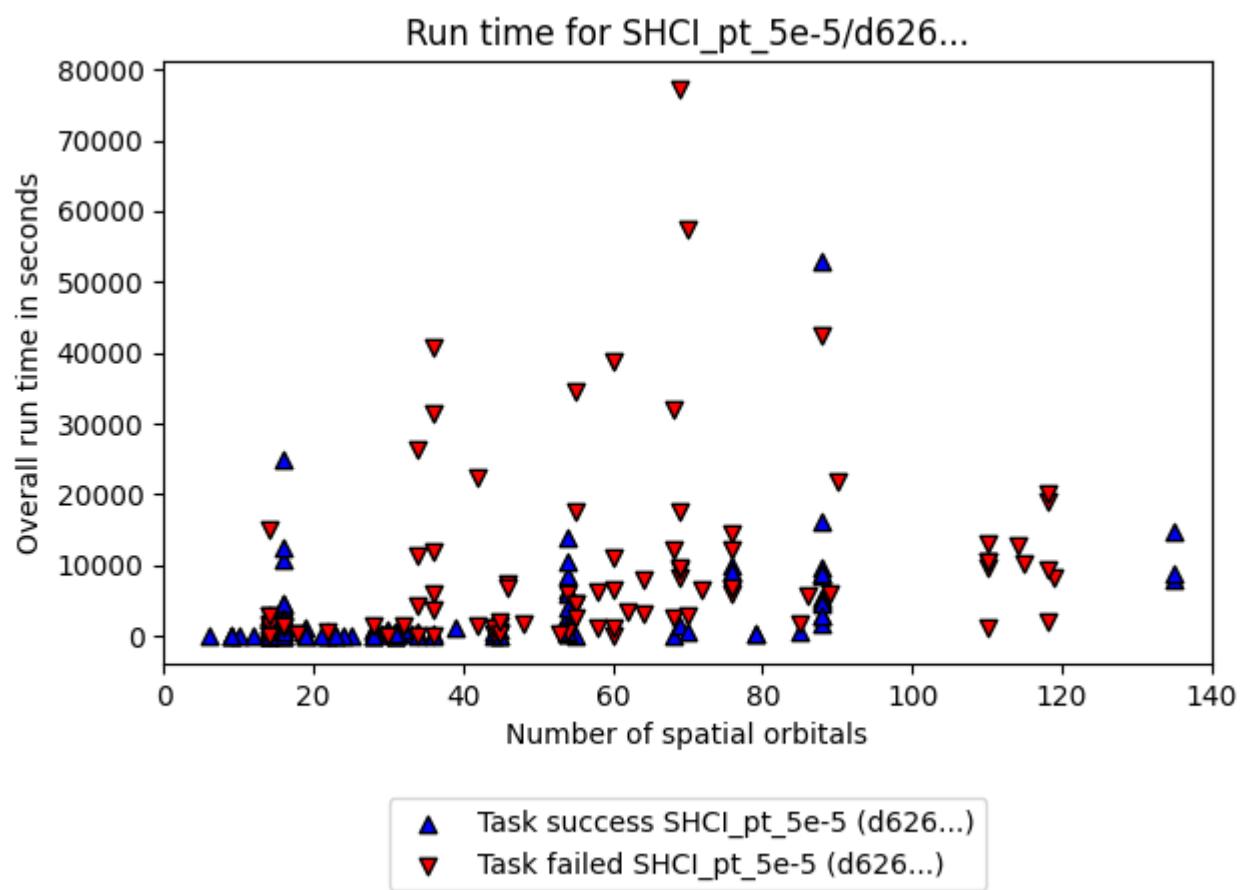


Solver SHCI_pt_5e-5, d626506c-7aae-4ad6-802a-b29af5f2bb93

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

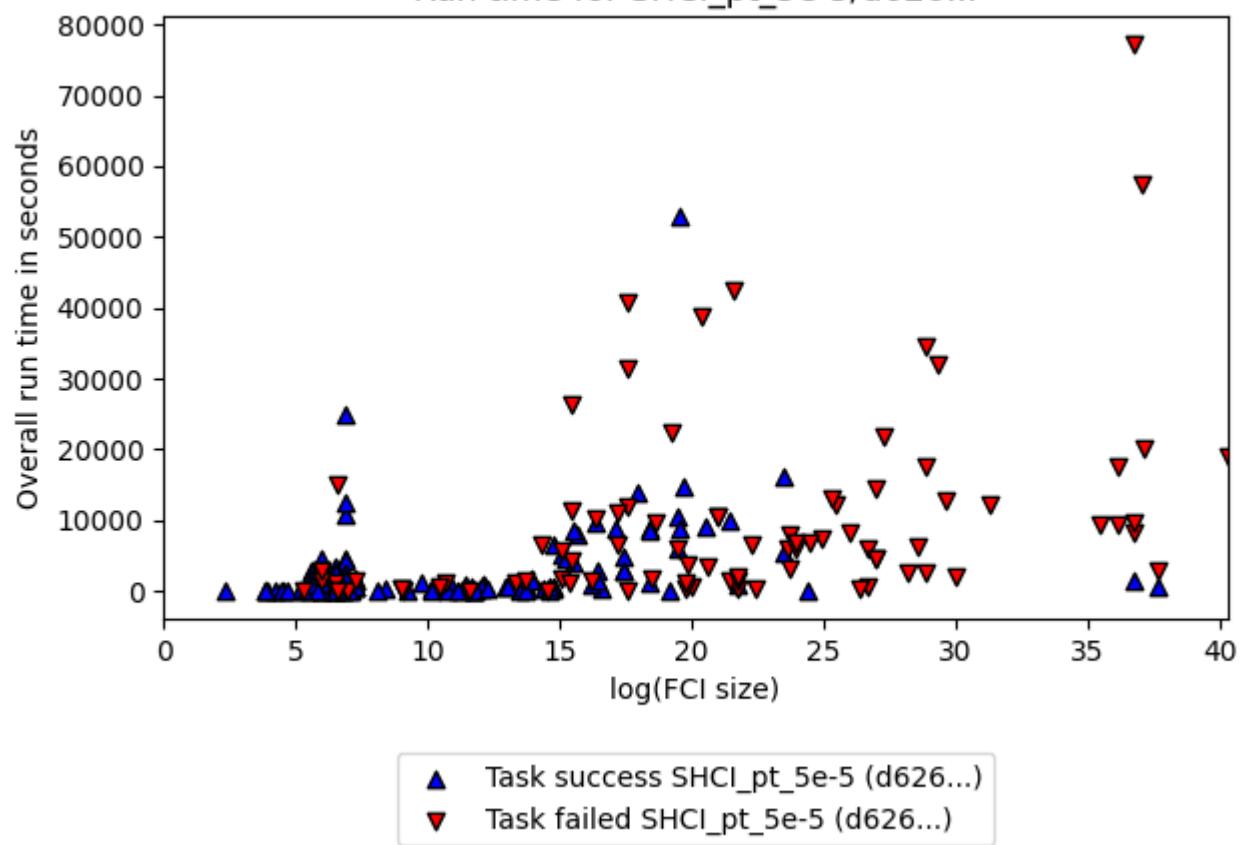
solver_short_name:SHCI_pt_5e-5

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: 60f4198c-01c5-4753-94d2-e417ca07abc7
creation.timestamp: 2025-02-24T20:41:03.349036+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.

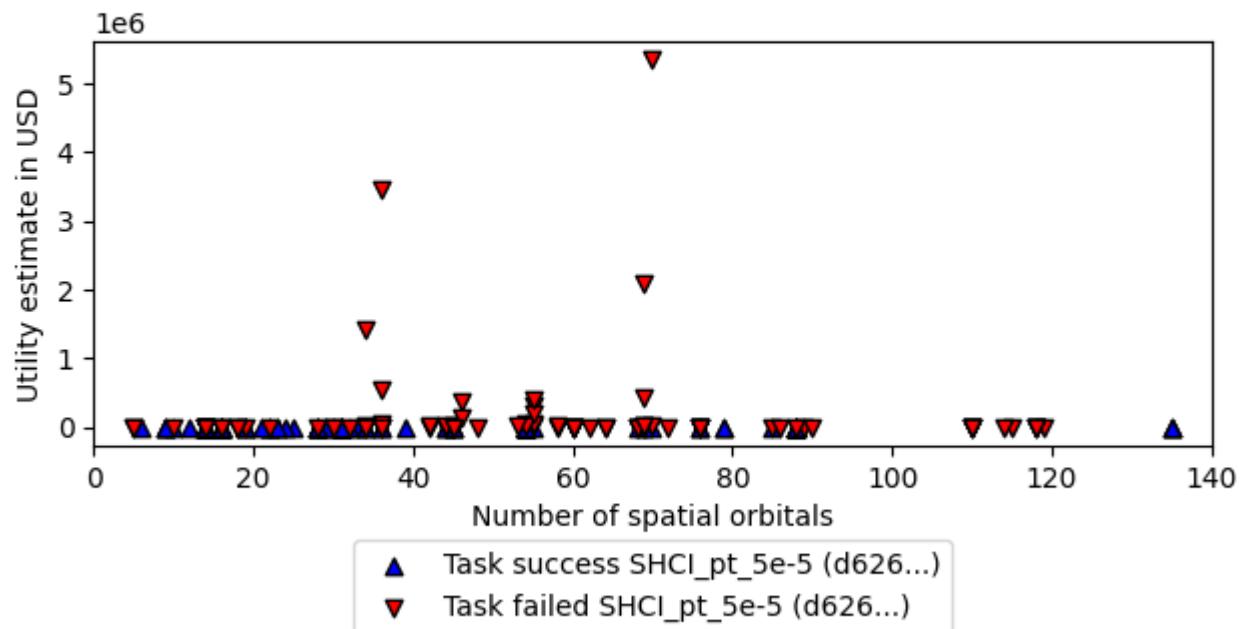
Run time for SHCI_pt_5e-5/d626...



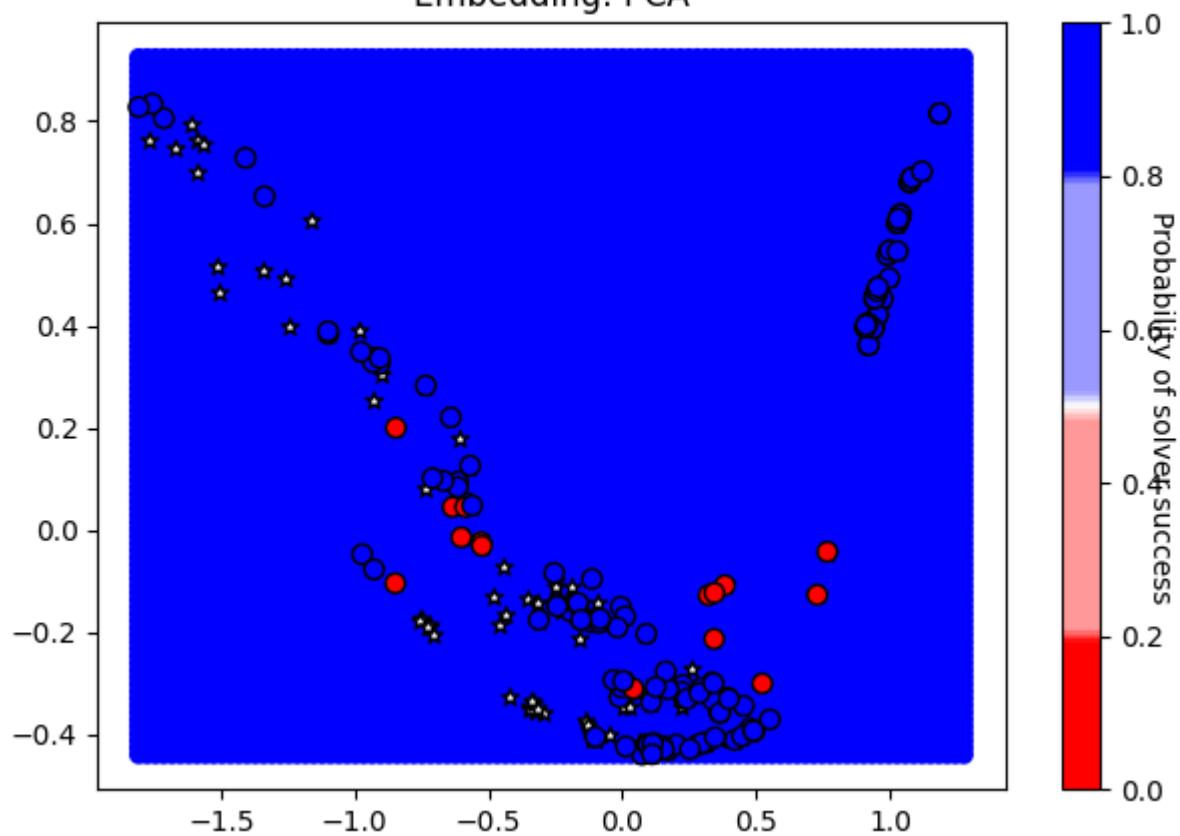
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_5e-5/d626...

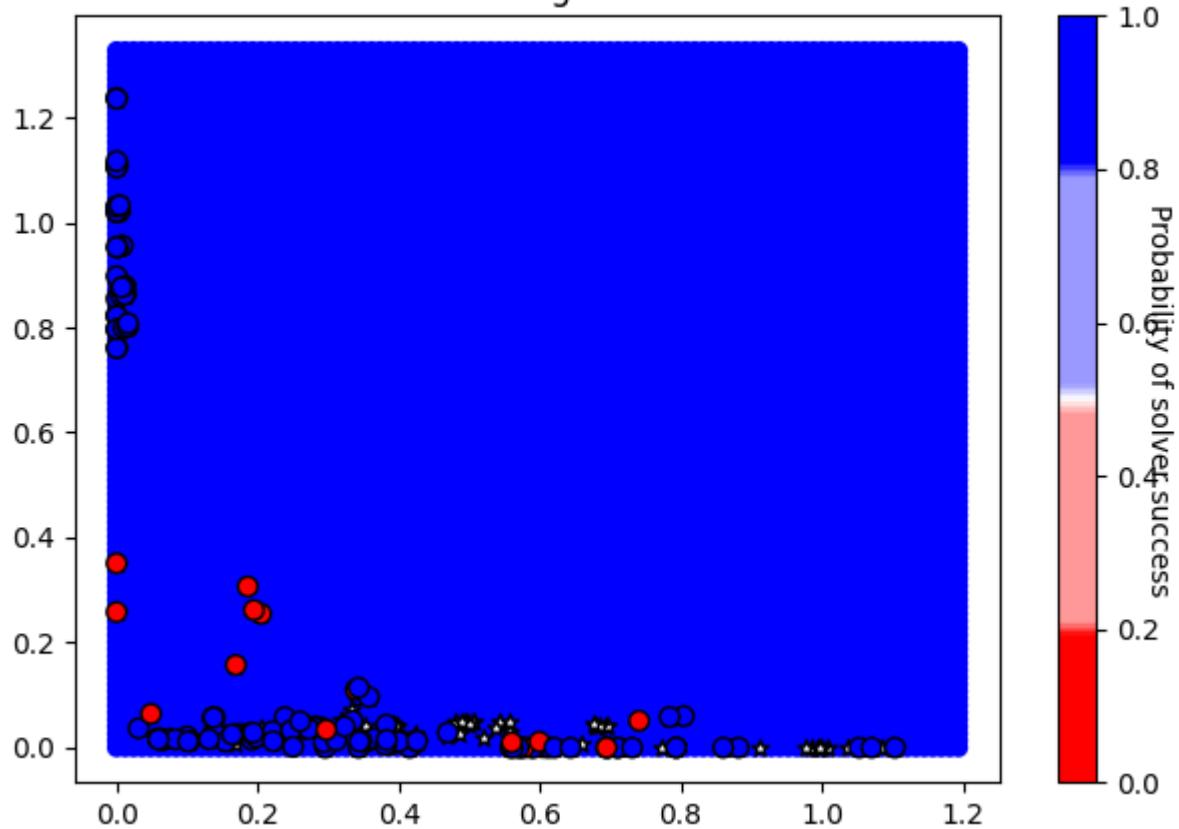
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



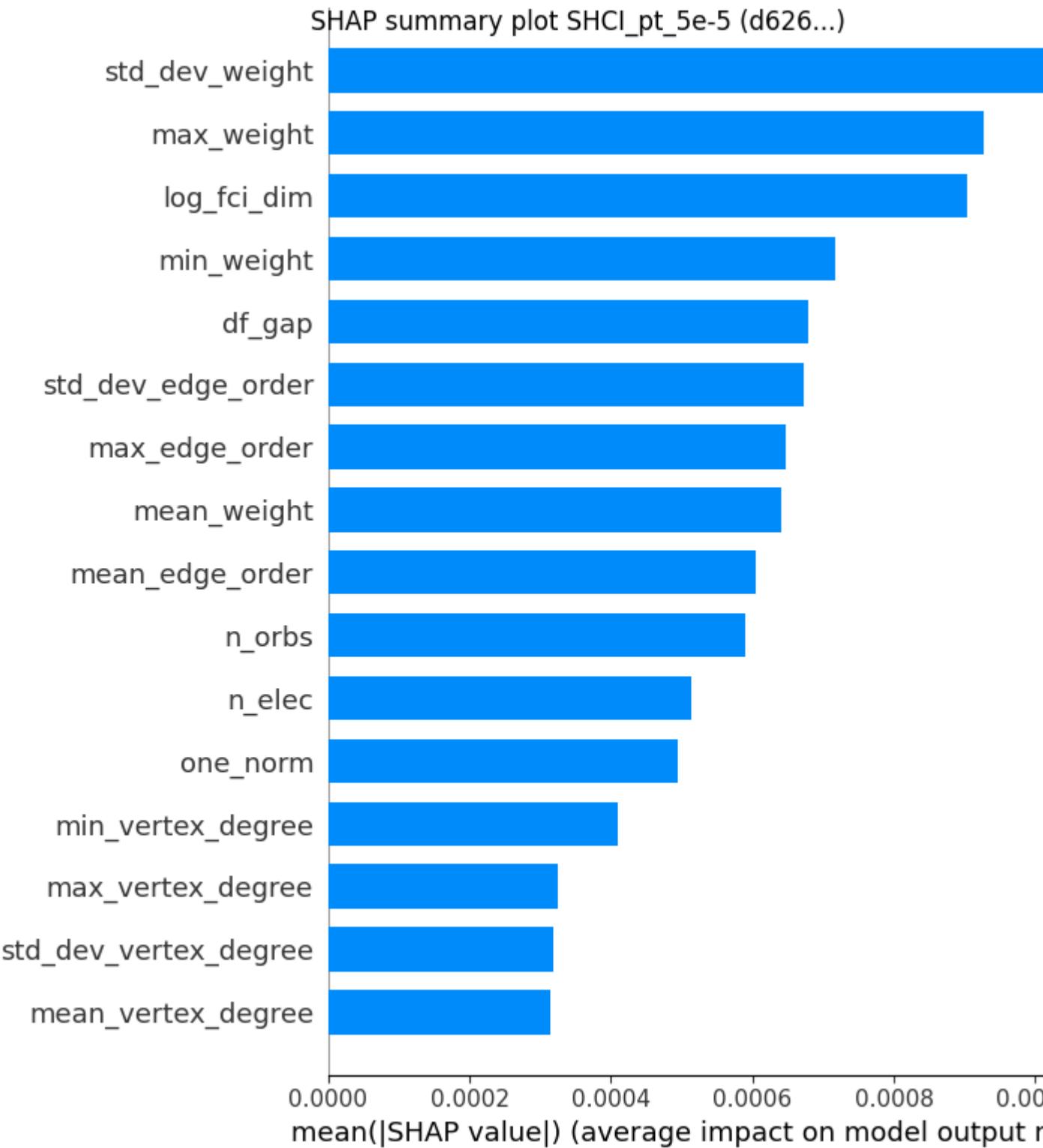
Solver SHCI_pt_5e-5 (d626...)
Embedding: PCA



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.

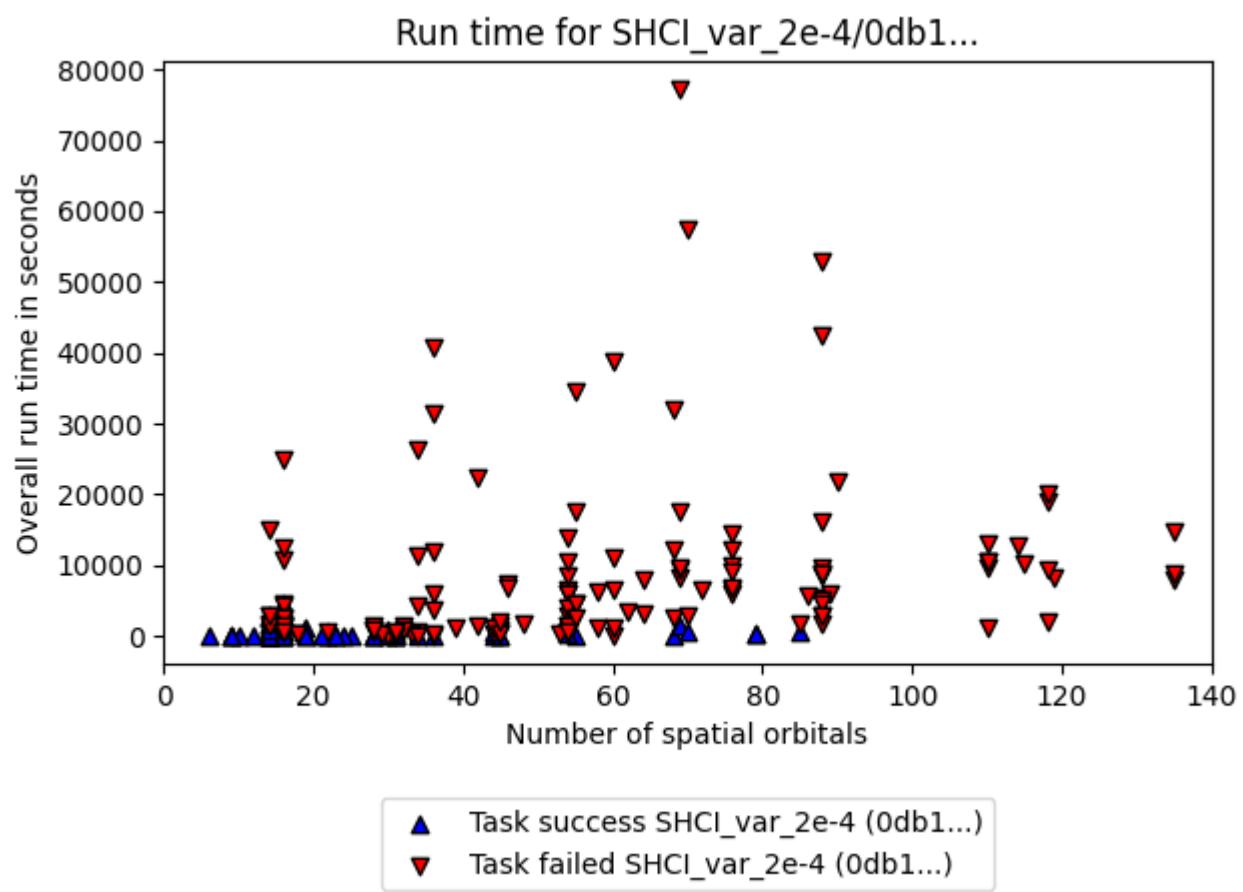


Solver SHCI_var_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a

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

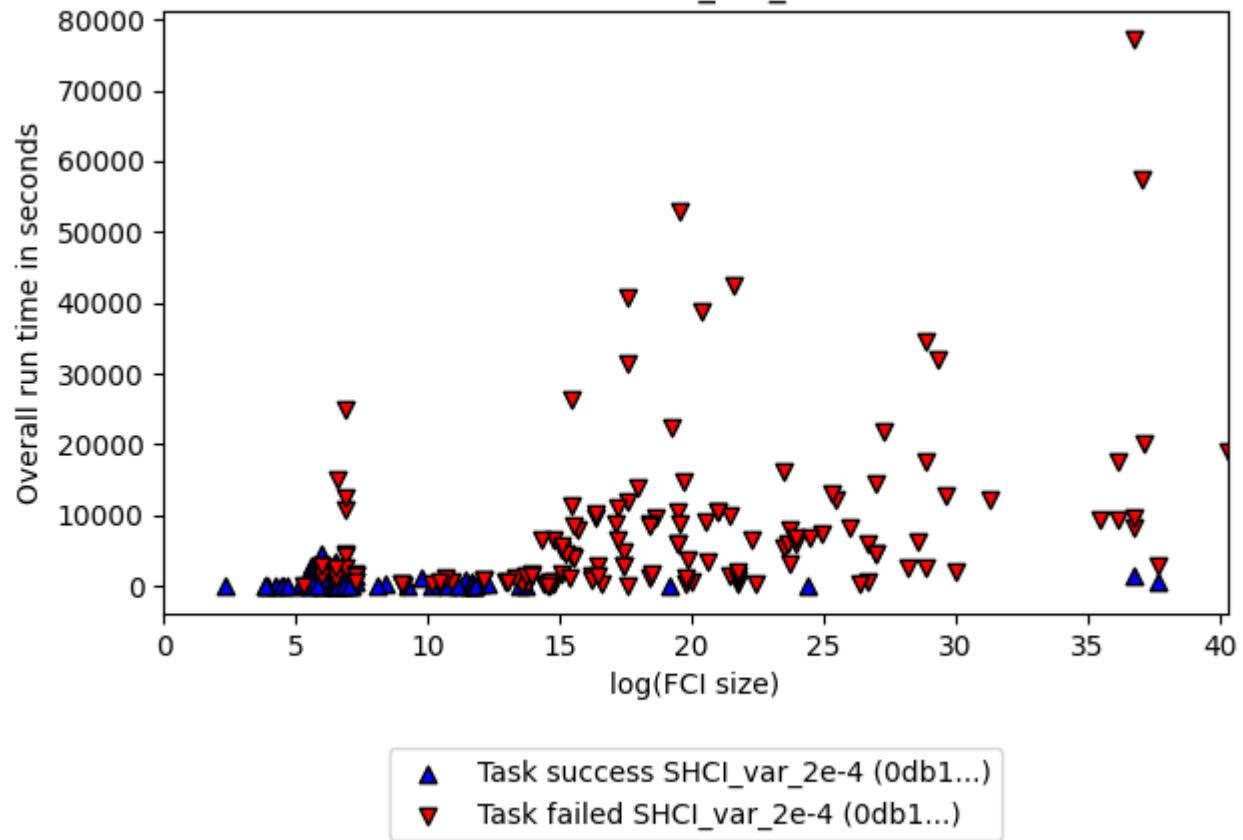
solver_short_name:SHCI_var_2e-4

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: cd5ec27a-fd46-4e4b-9a20-7598267424ee
creation.timestamp: 2025-02-24T20:41:03.349036+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.

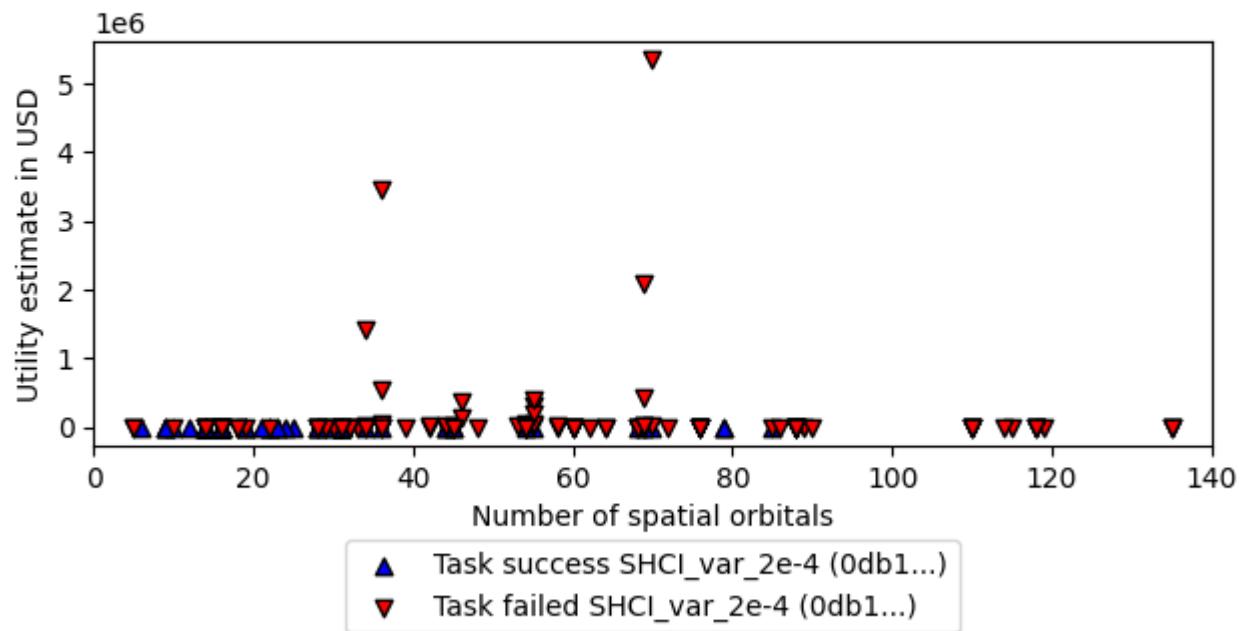
Run time for SHCI_var_2e-4/0db1...



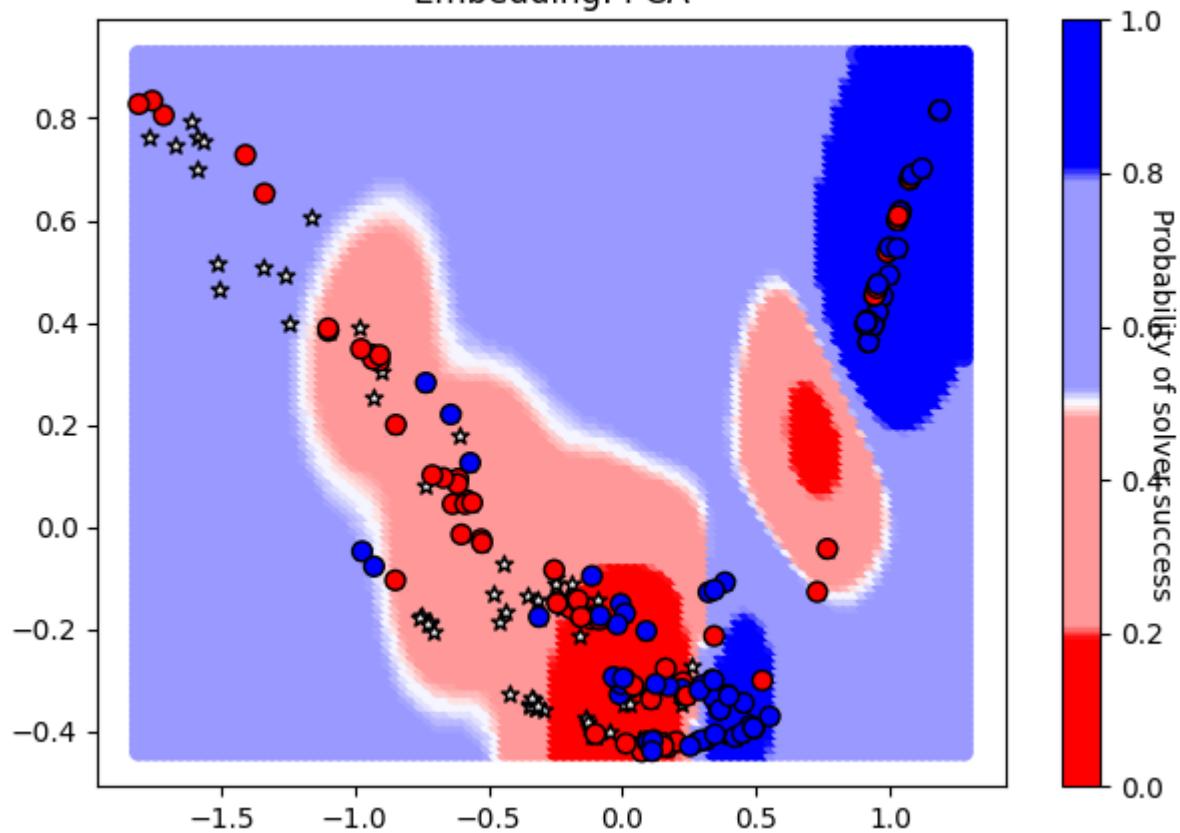
Note: plot only contains attempted tasks.

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

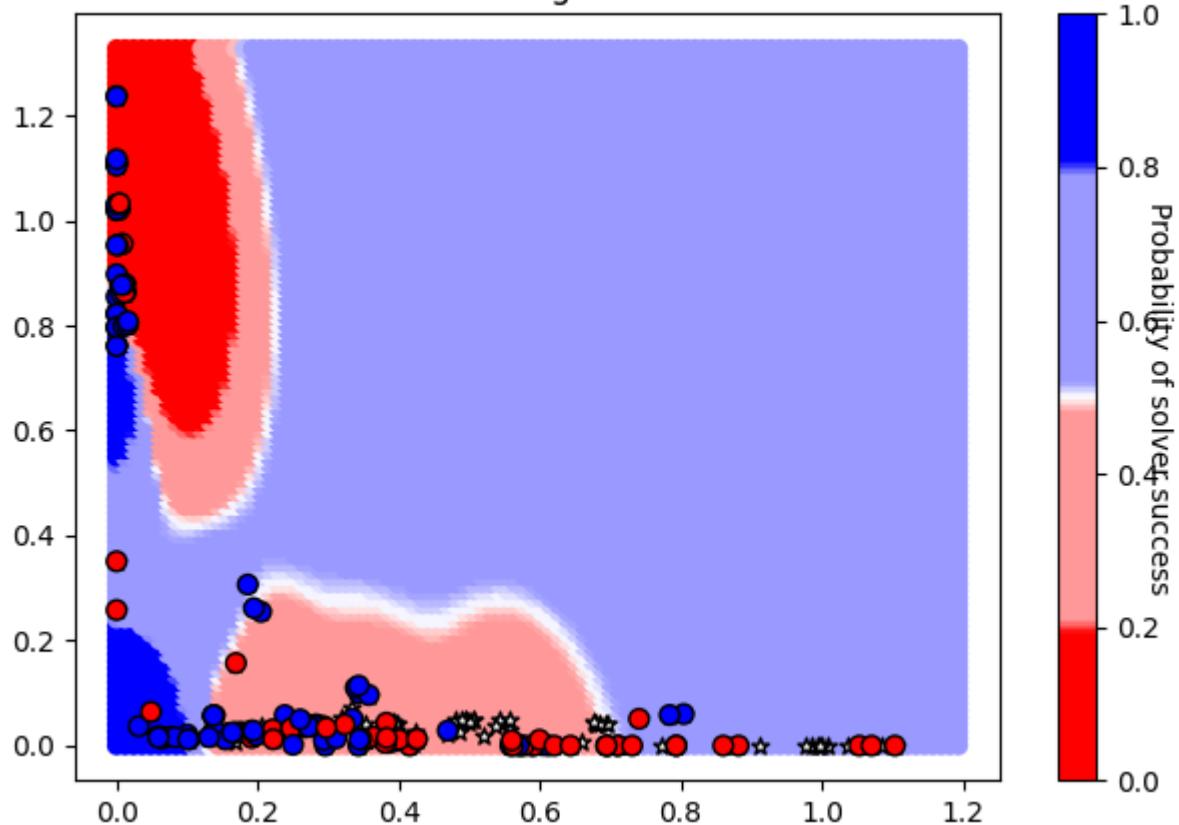
(captured: $\$8.6\text{e+}01/1.5\text{e+}07$, approximately $5.8\text{e-}04\%$)



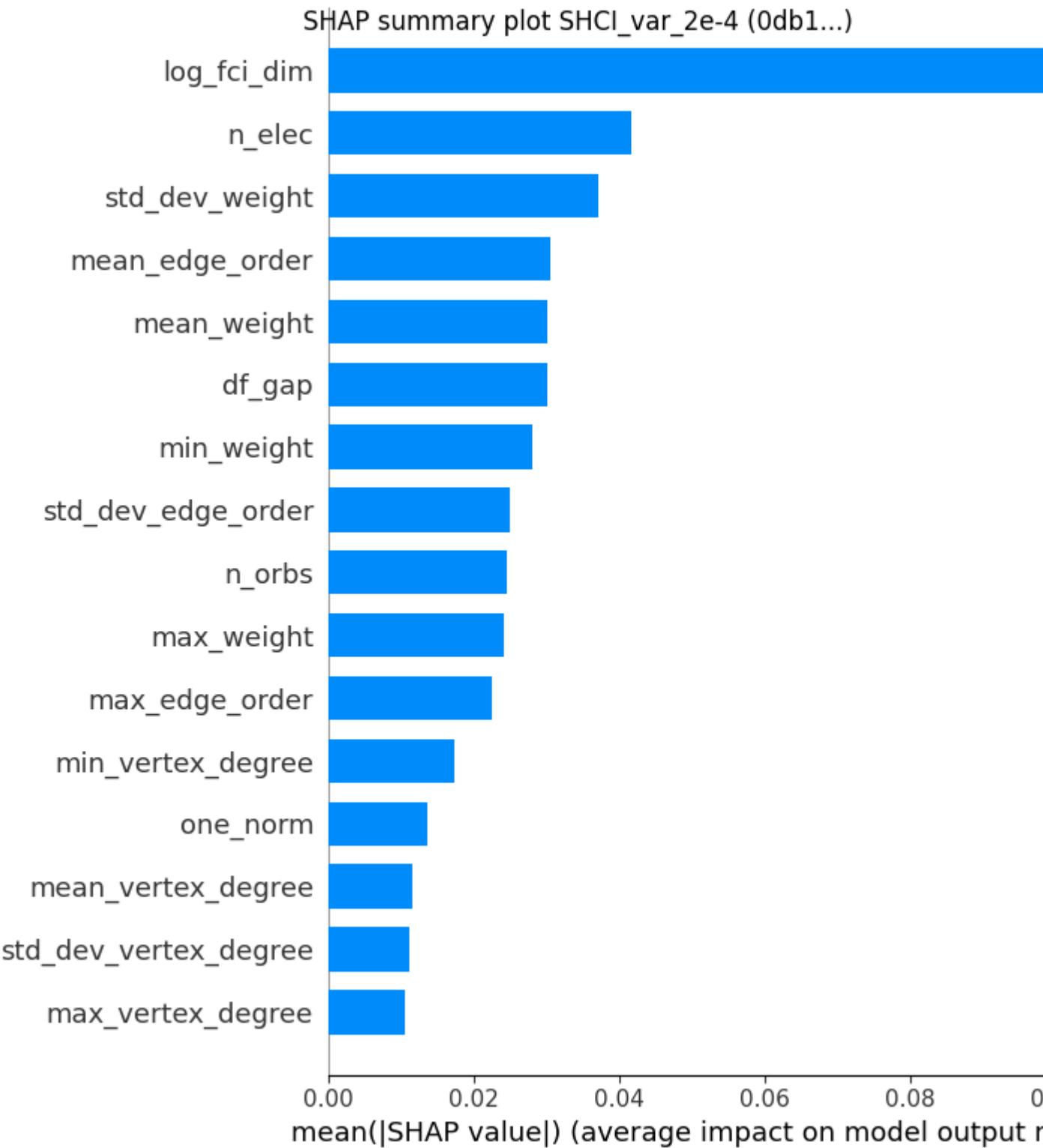
Solver SHCI_var_2e-4 (0db1...)
Embedding: PCA



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.

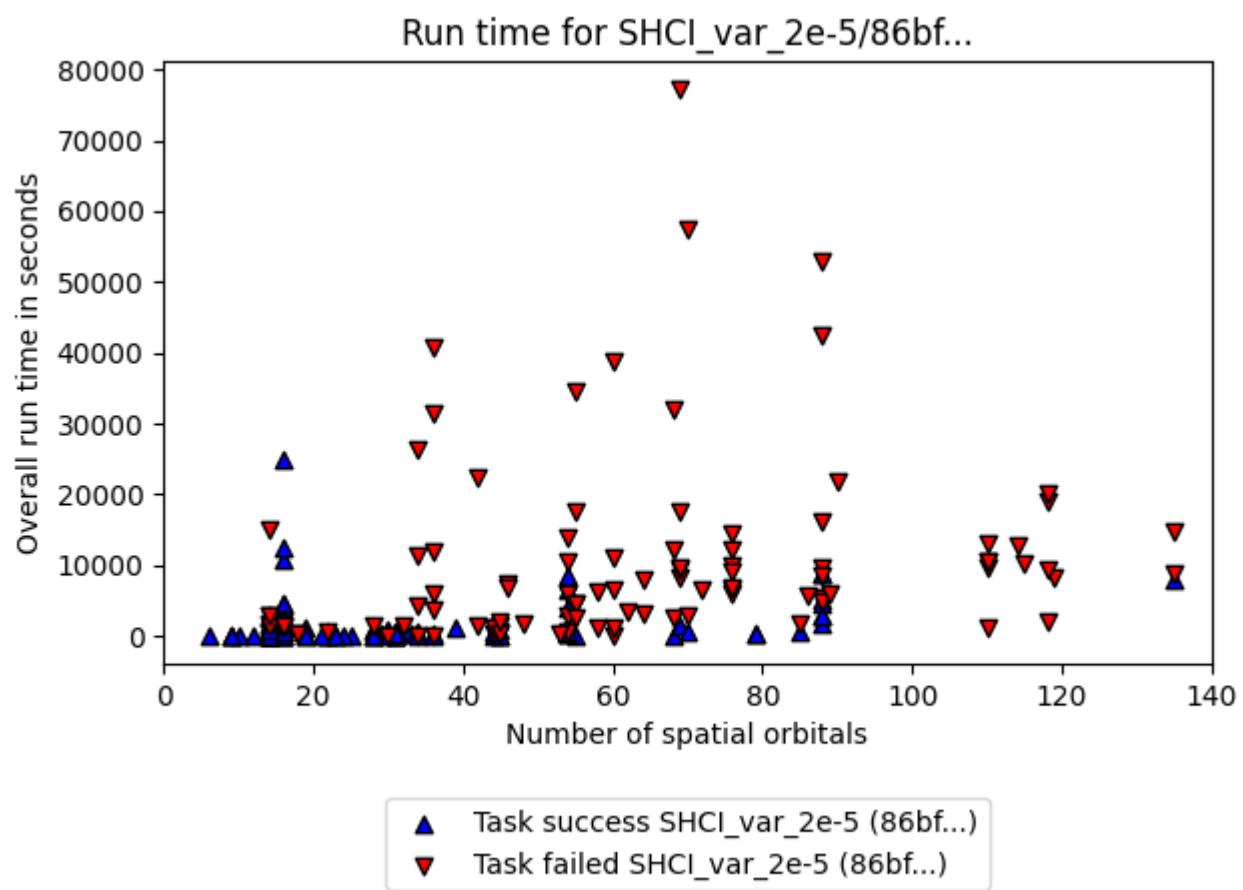


Solver SHCI_var_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688

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

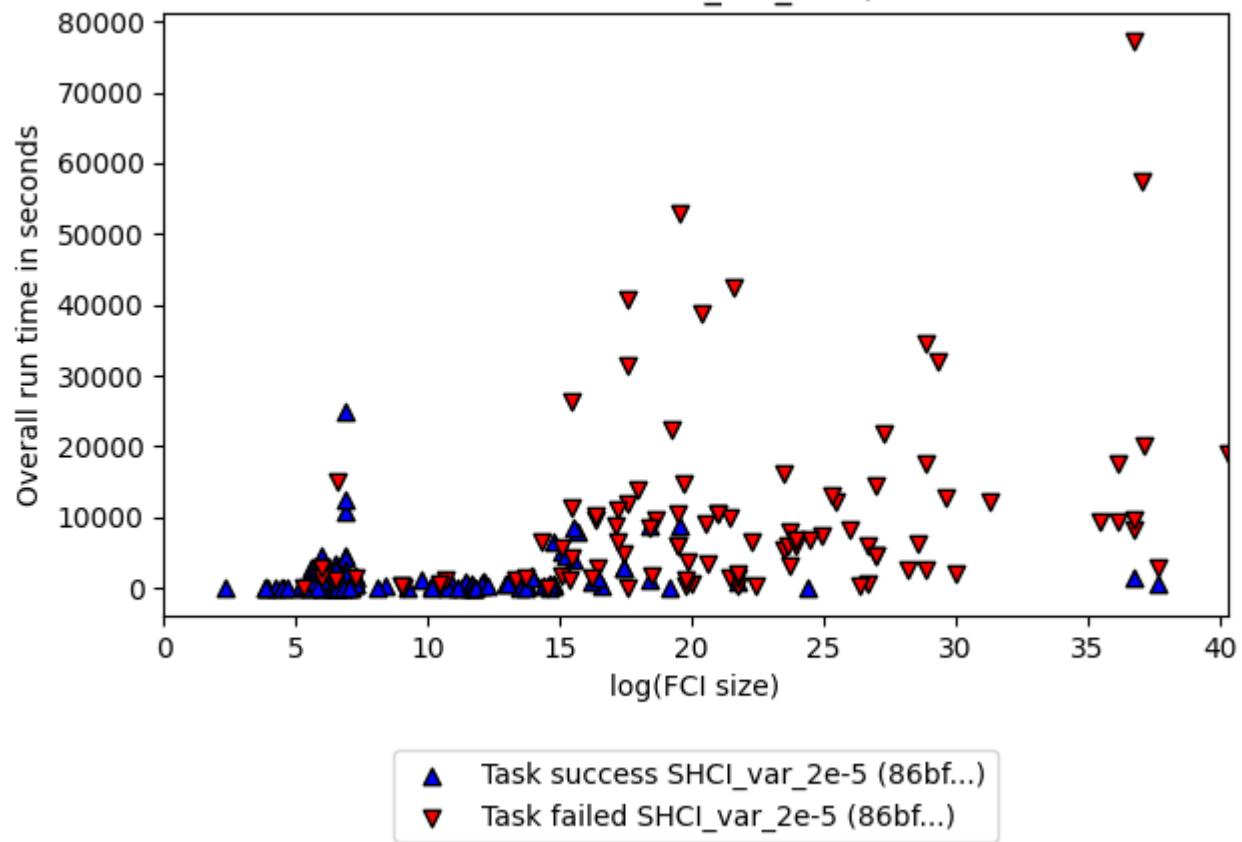
solver_short_name:SHCI_var_2e-5

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: ff1b052f-4cb0-4fe8-a7be-b034d2968b77
creation_timestamp: 2025-02-24T20:41:03.349036+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.

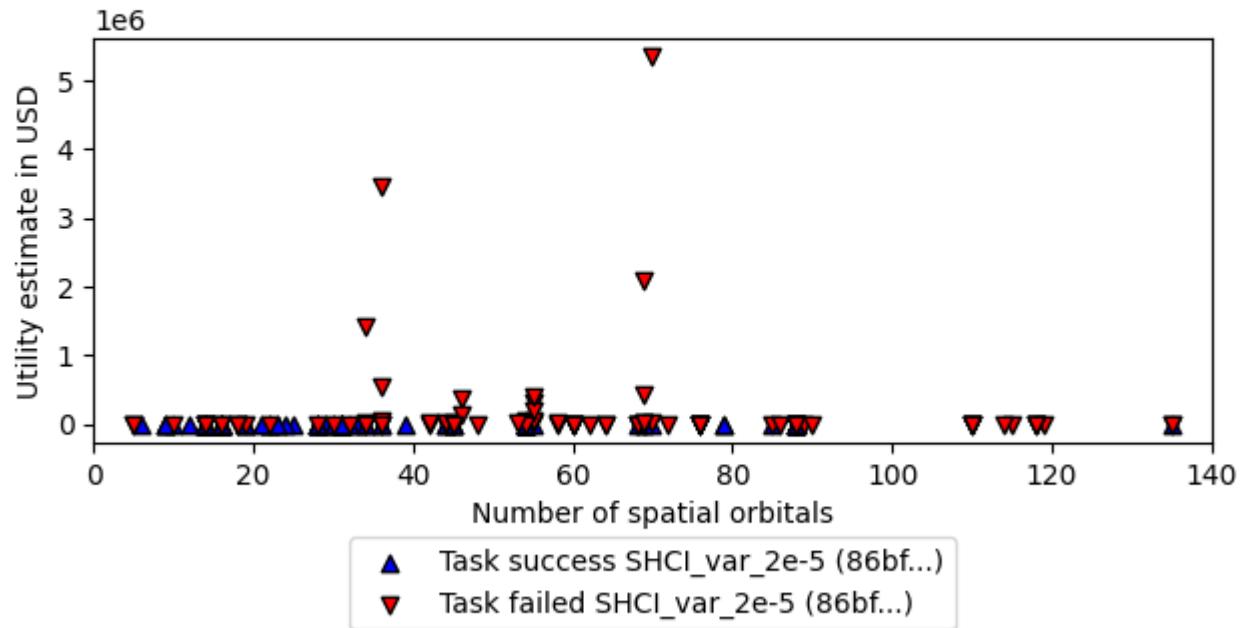
Run time for SHCI_var_2e-5/86bf...



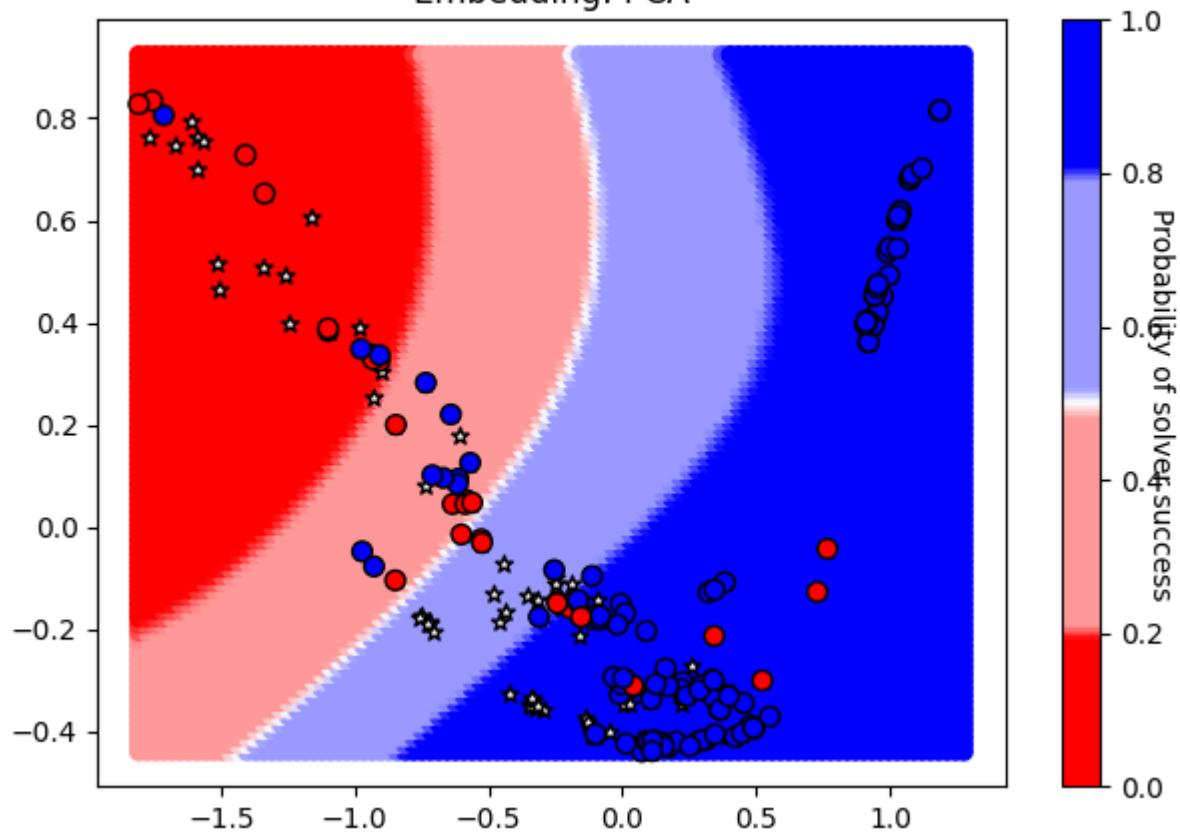
Note: plot only contains attempted tasks.

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

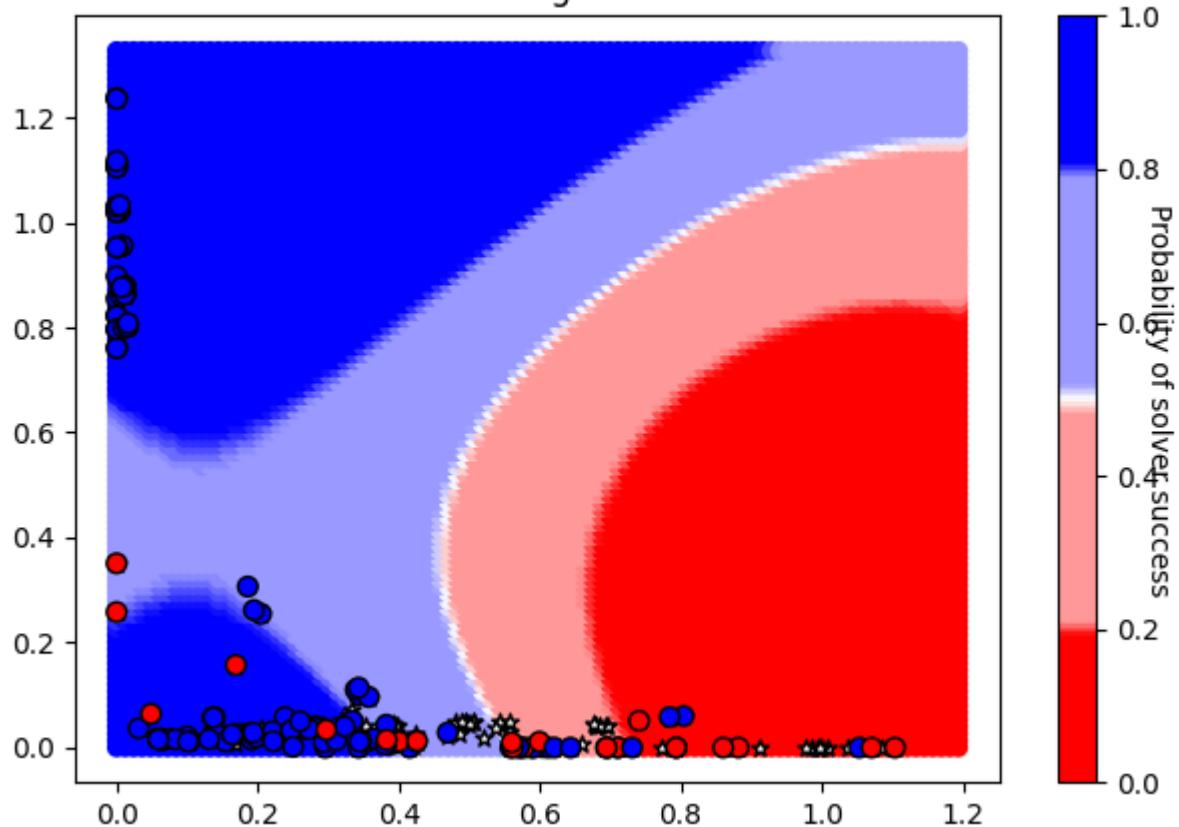
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



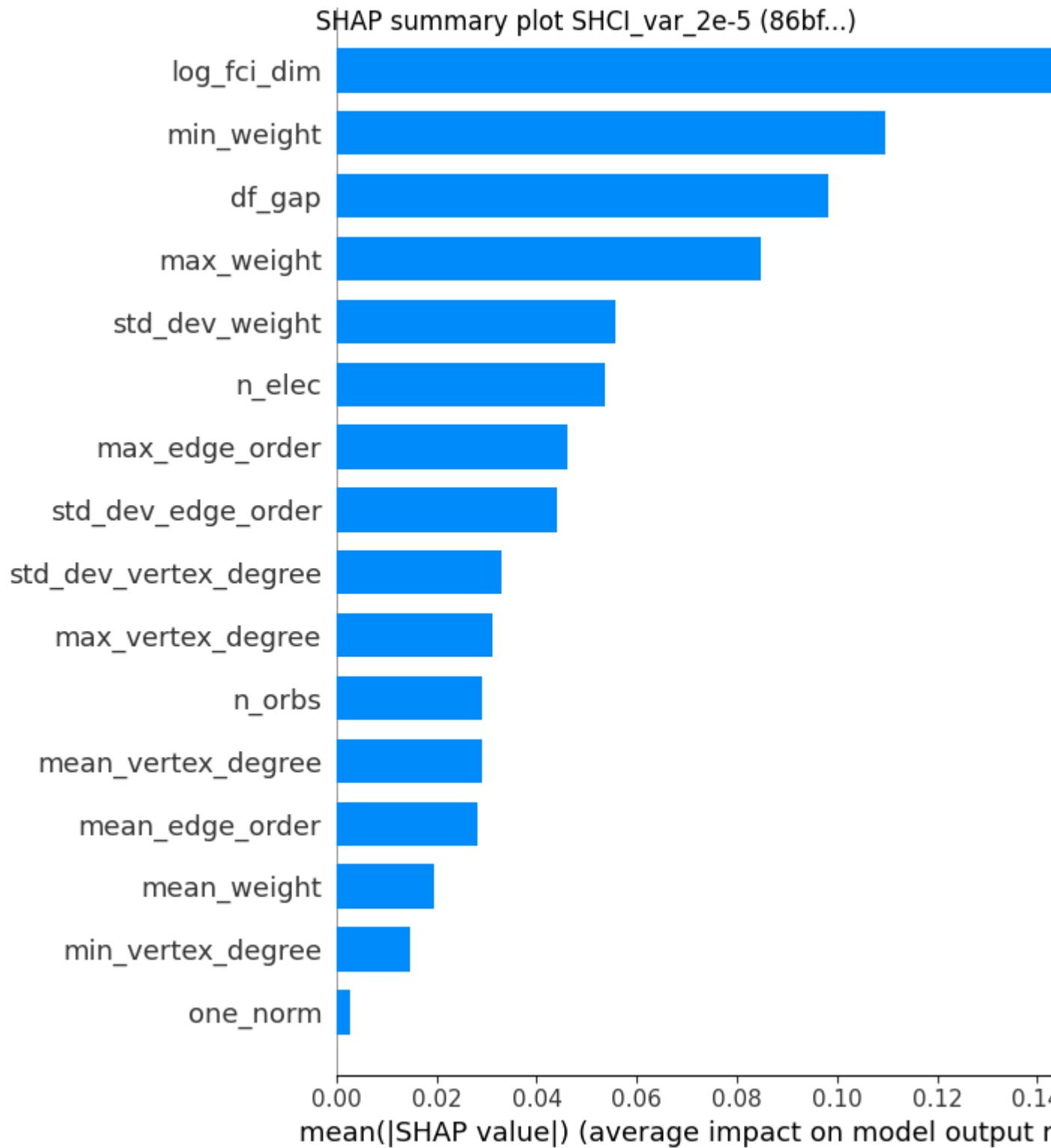
Solver SHCI_var_2e-5 (86bf...)
Embedding: PCA



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.

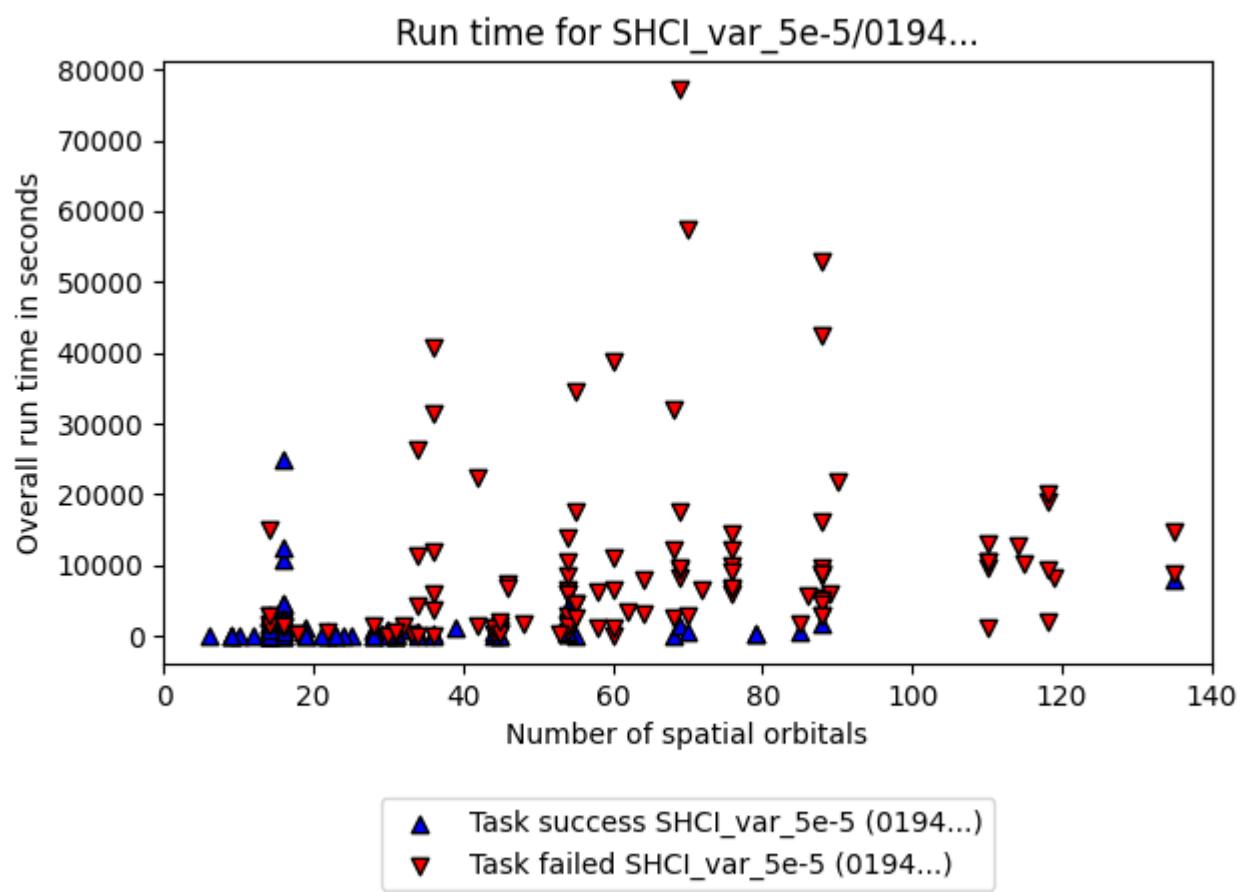


Solver SHCI_var_5e-5, 01949b95-c427-4693-9134-01f47f688c09

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

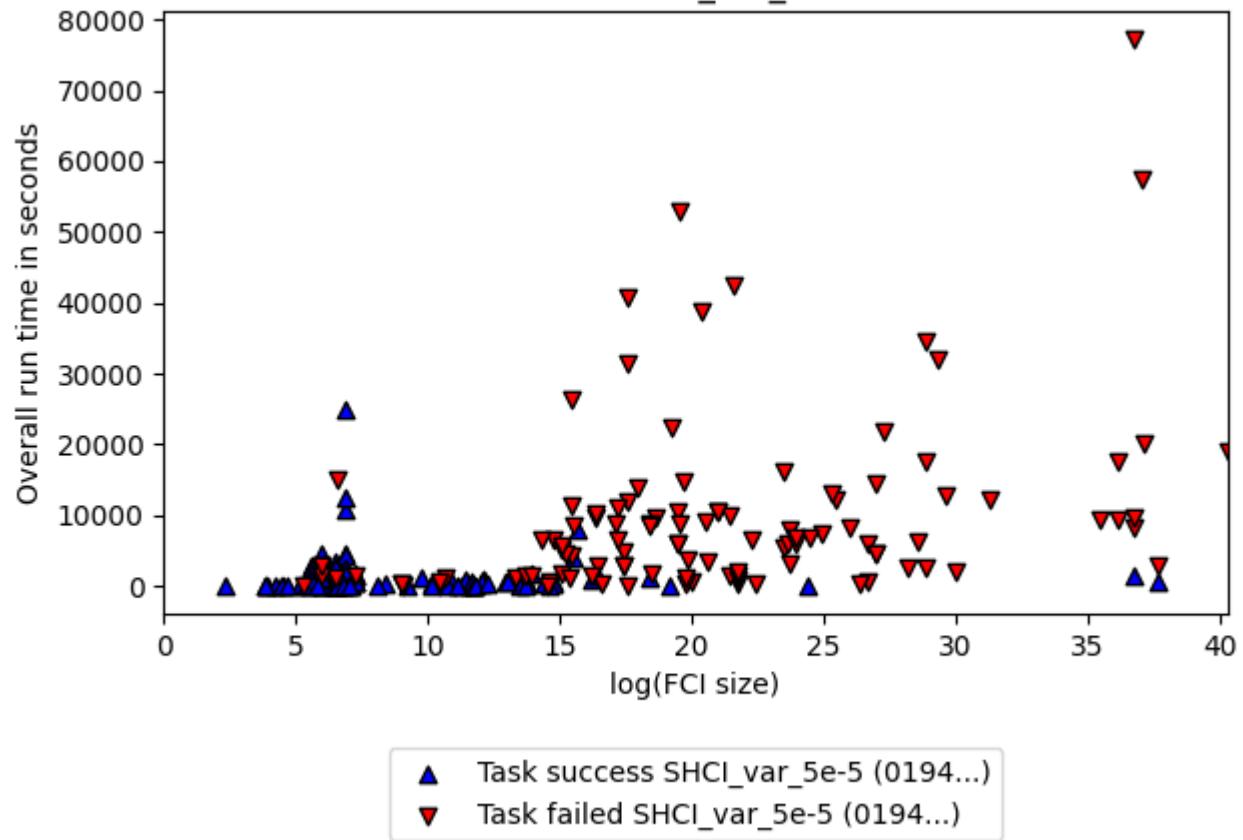
solver_short_name:SHCI_var_5e-5

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: 47ddbf8c-3195-4a58-b3ce-36862dd198bc
creation.timestamp: 2025-02-24T20:41:03.349036+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.

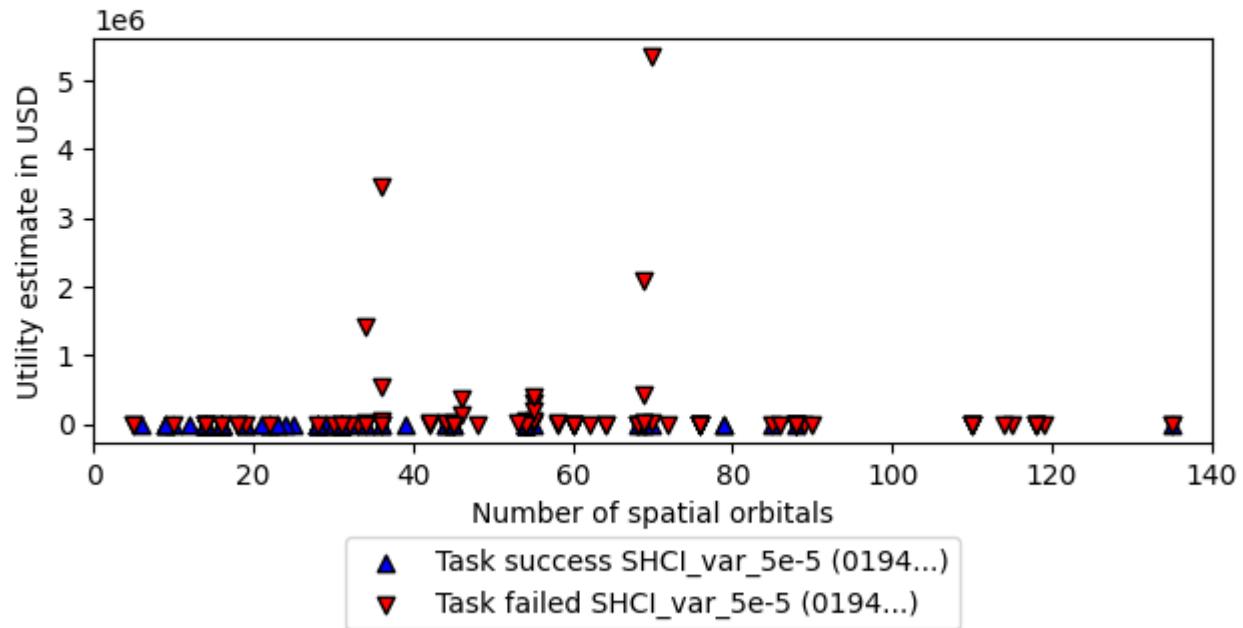
Run time for SHCI_var_5e-5/0194...



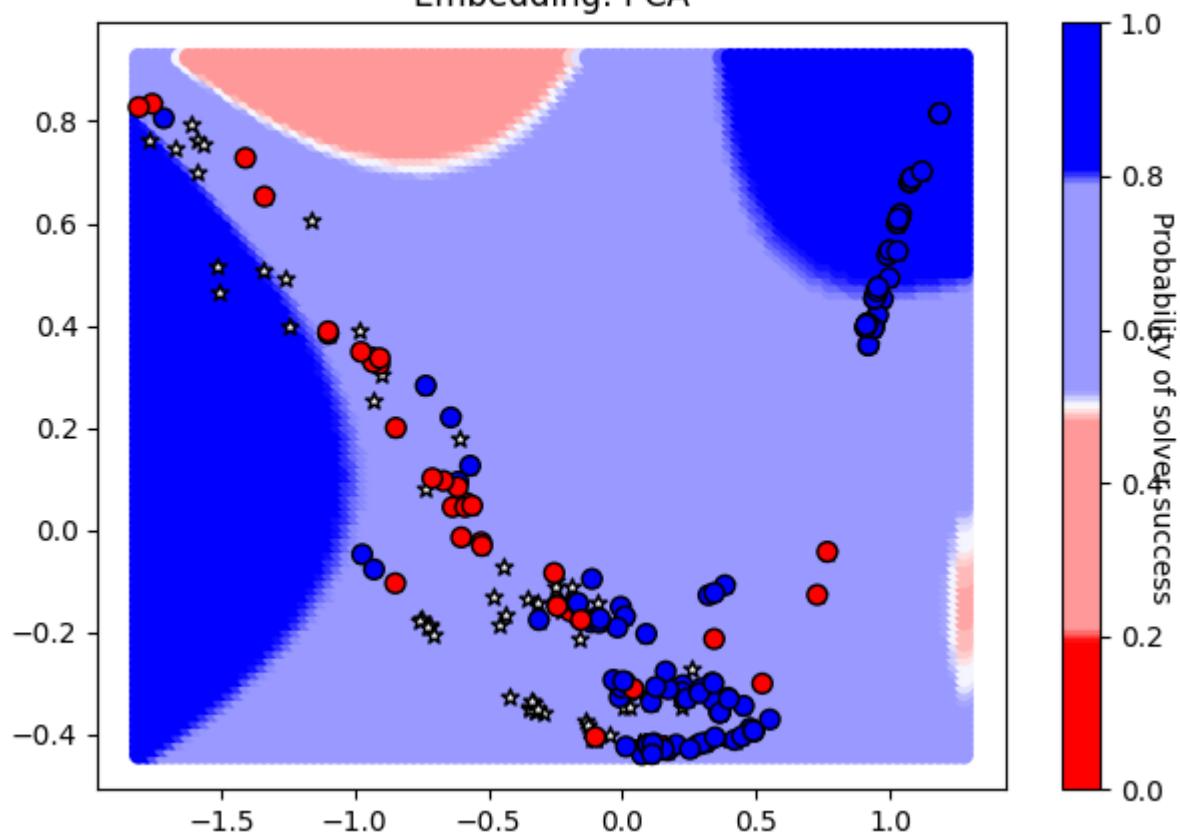
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_5e-5/0194...

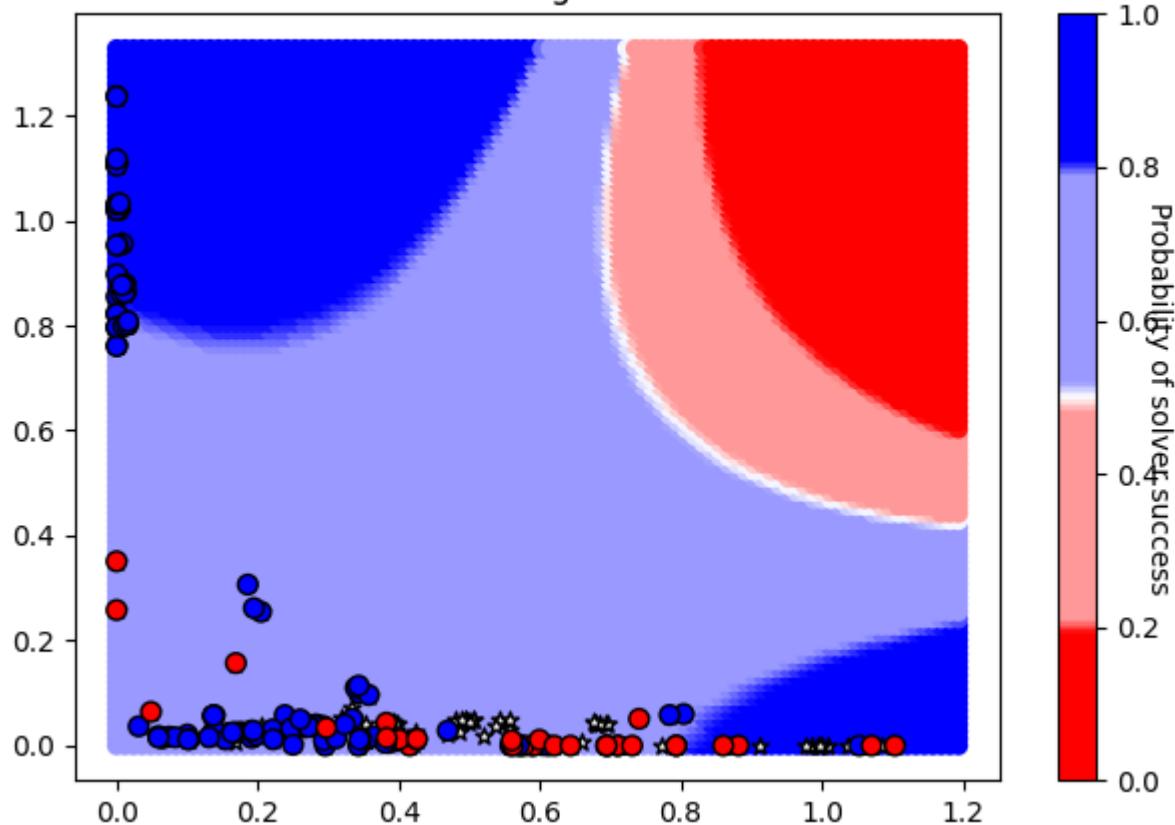
(captured: $\$4.5\text{e+}02/1.5\text{e+}07$, approximately $3.0\text{e-}03\%$)



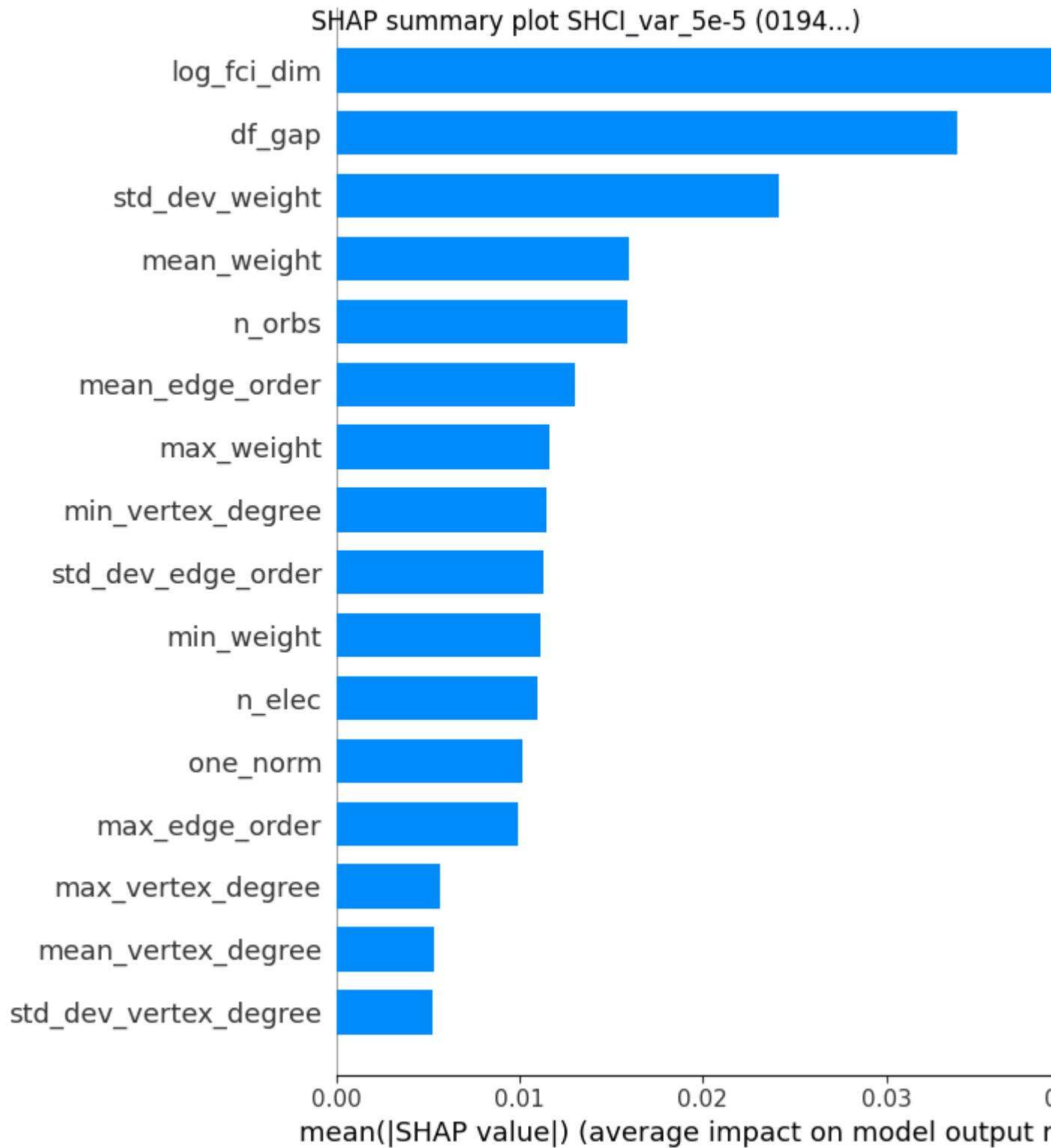
Solver SHCI_var_5e-5 (0194...)
Embedding: PCA



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: 6d1111d9-39ea-44a7-a57c-410c6bcd1bc

creation_timestamp: 2025-02-24T20:41:03.349036+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

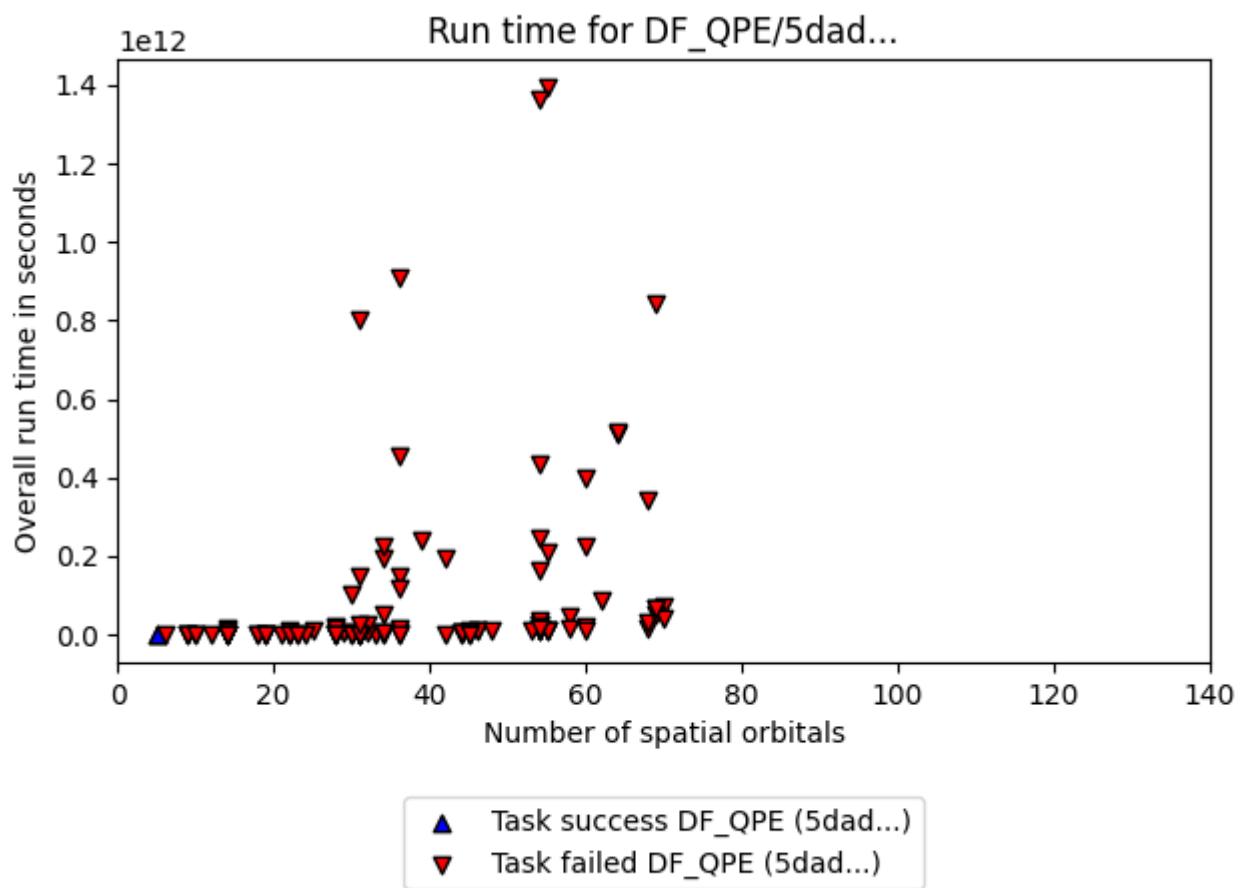
sum_of_run_time_of_attempted_tasks: 11314745416246.352

solvability_ratio: 0.0394

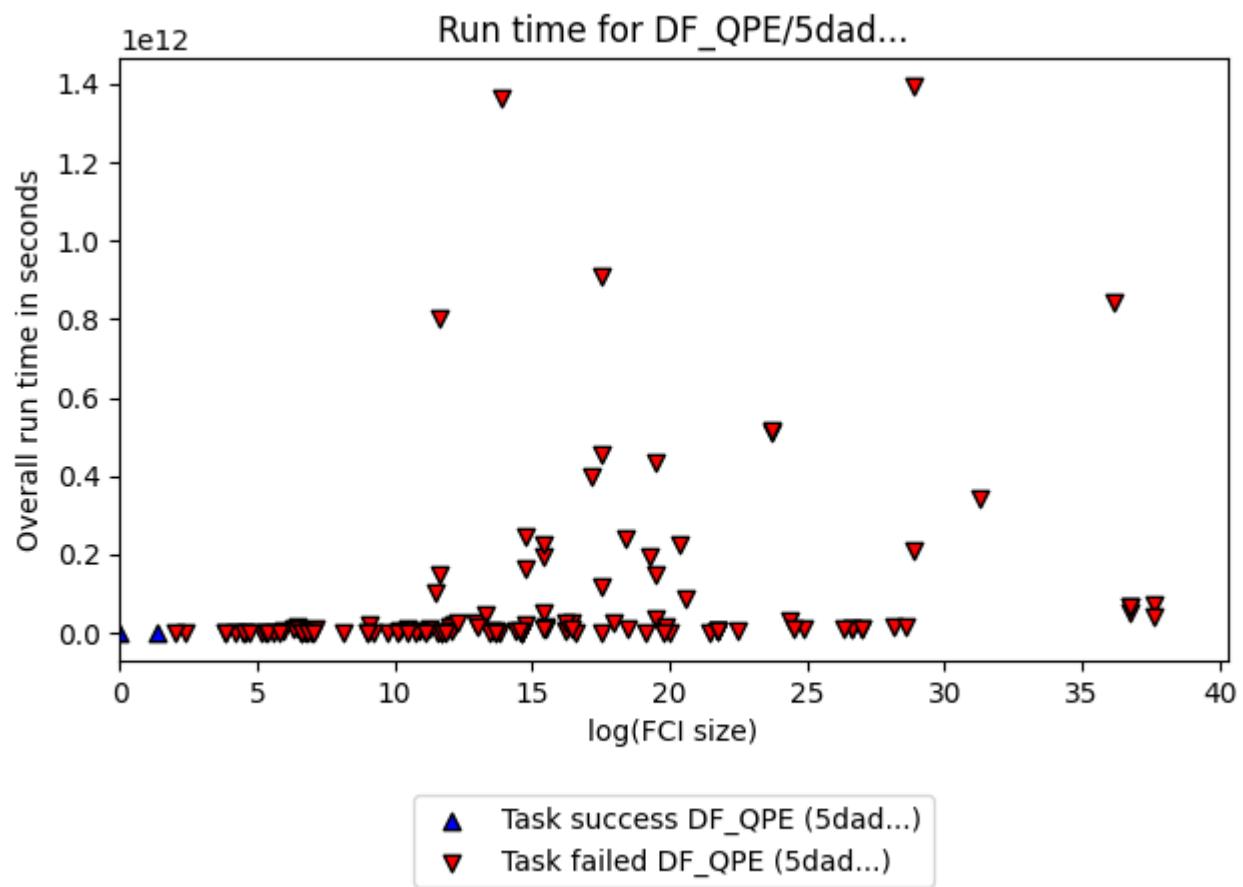
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



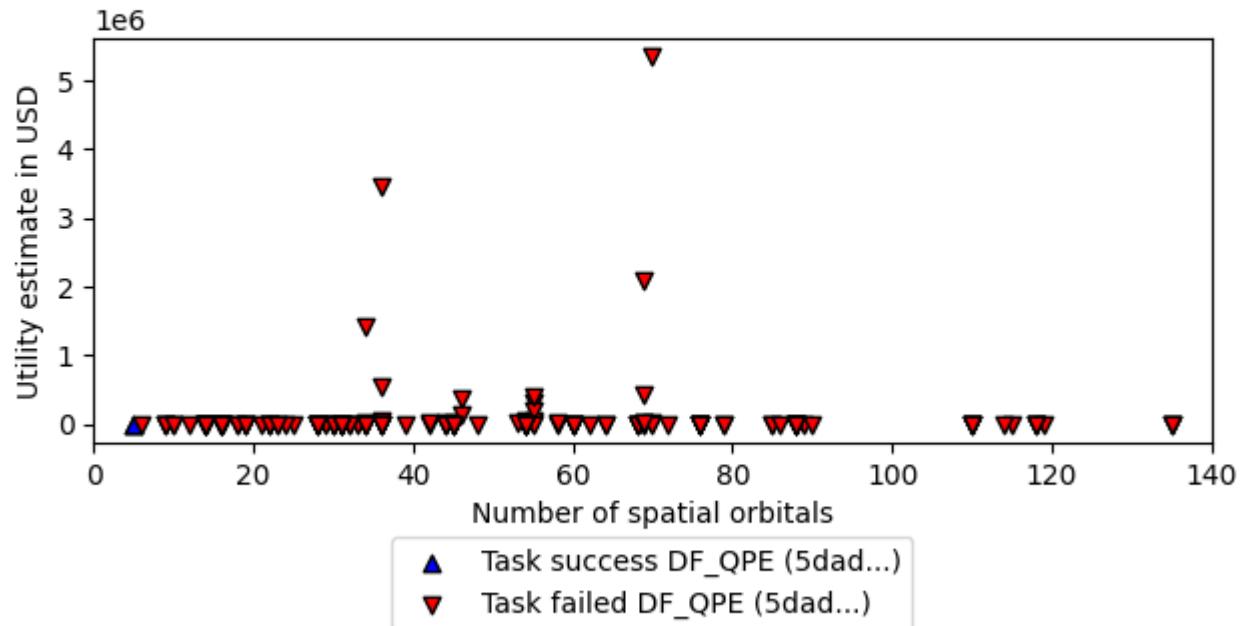
Note: plot only contains attempted tasks.



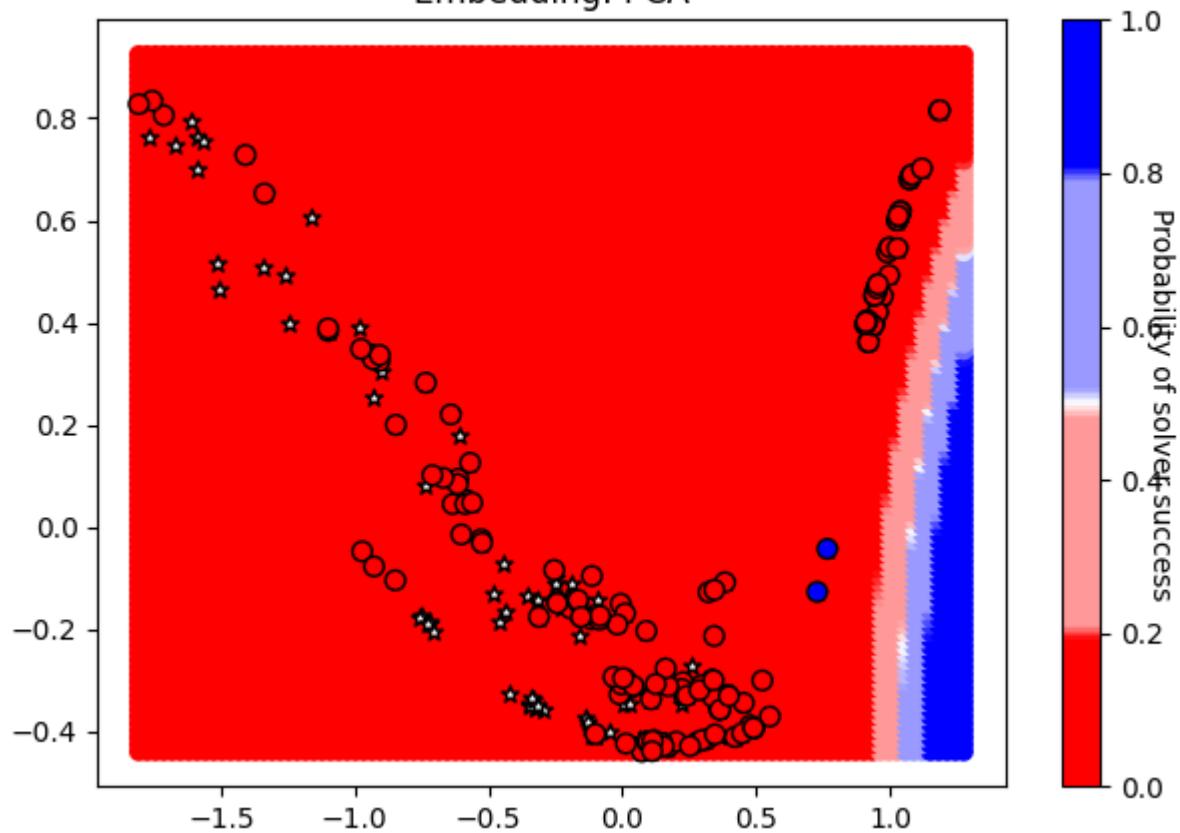
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5dad...

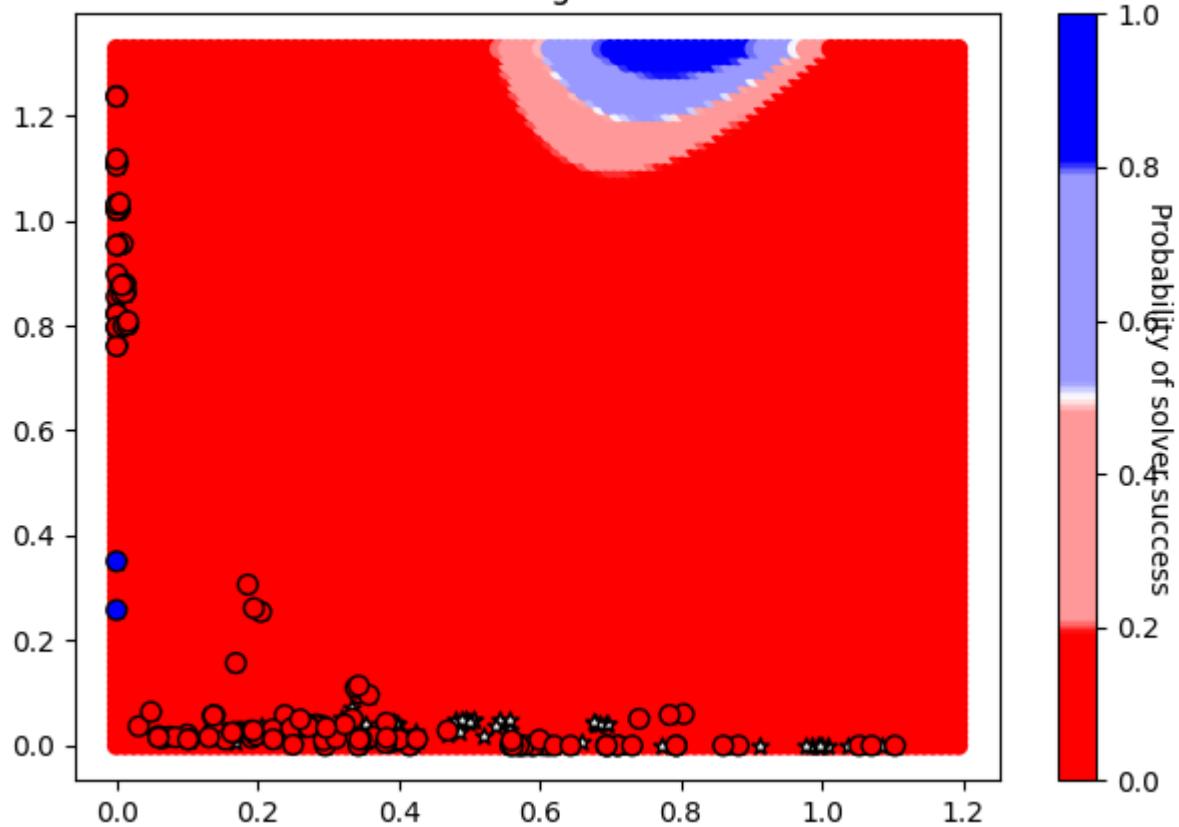
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



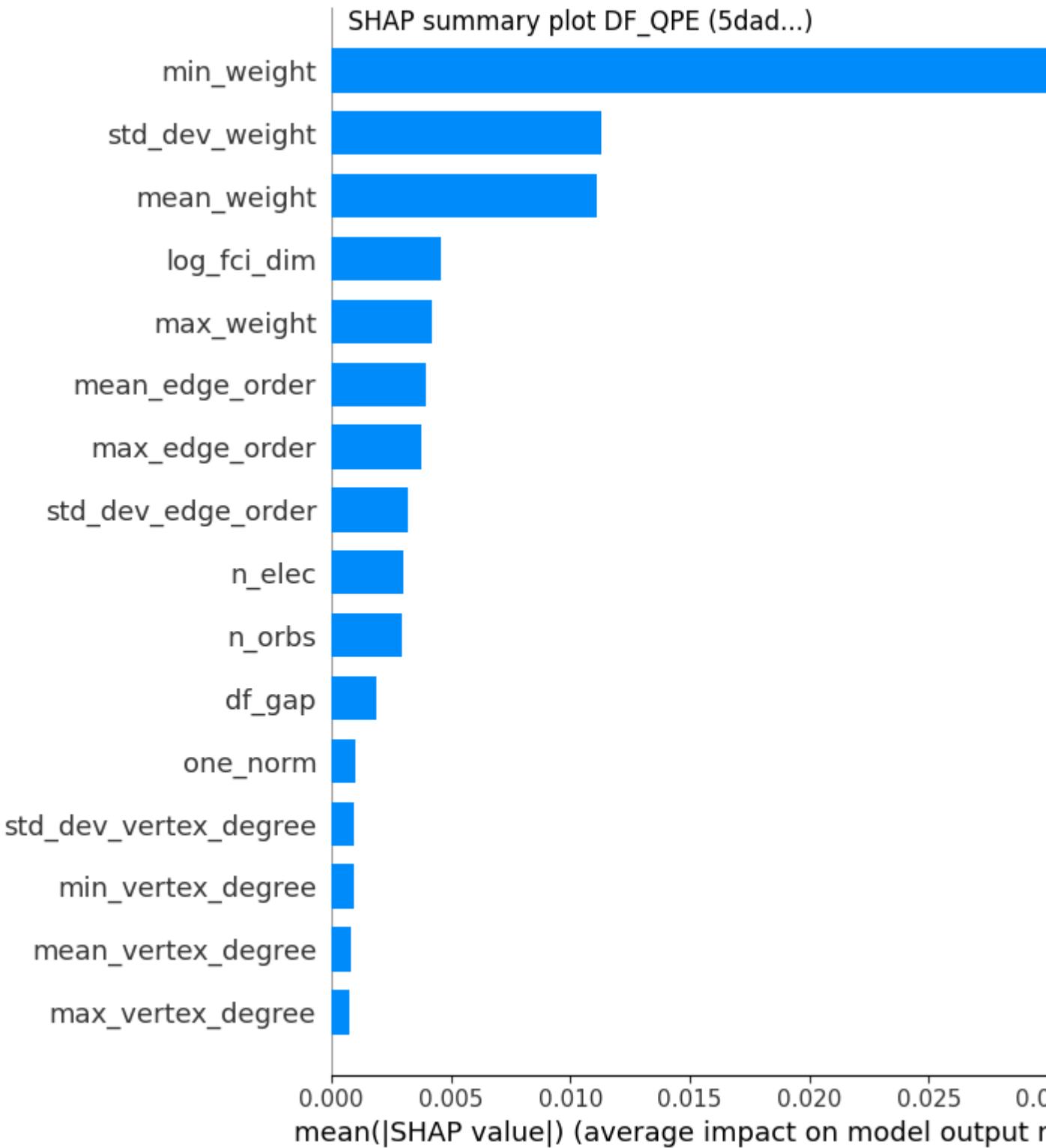
Solver DF_QPE (5dad...)
Embedding: PCA



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.



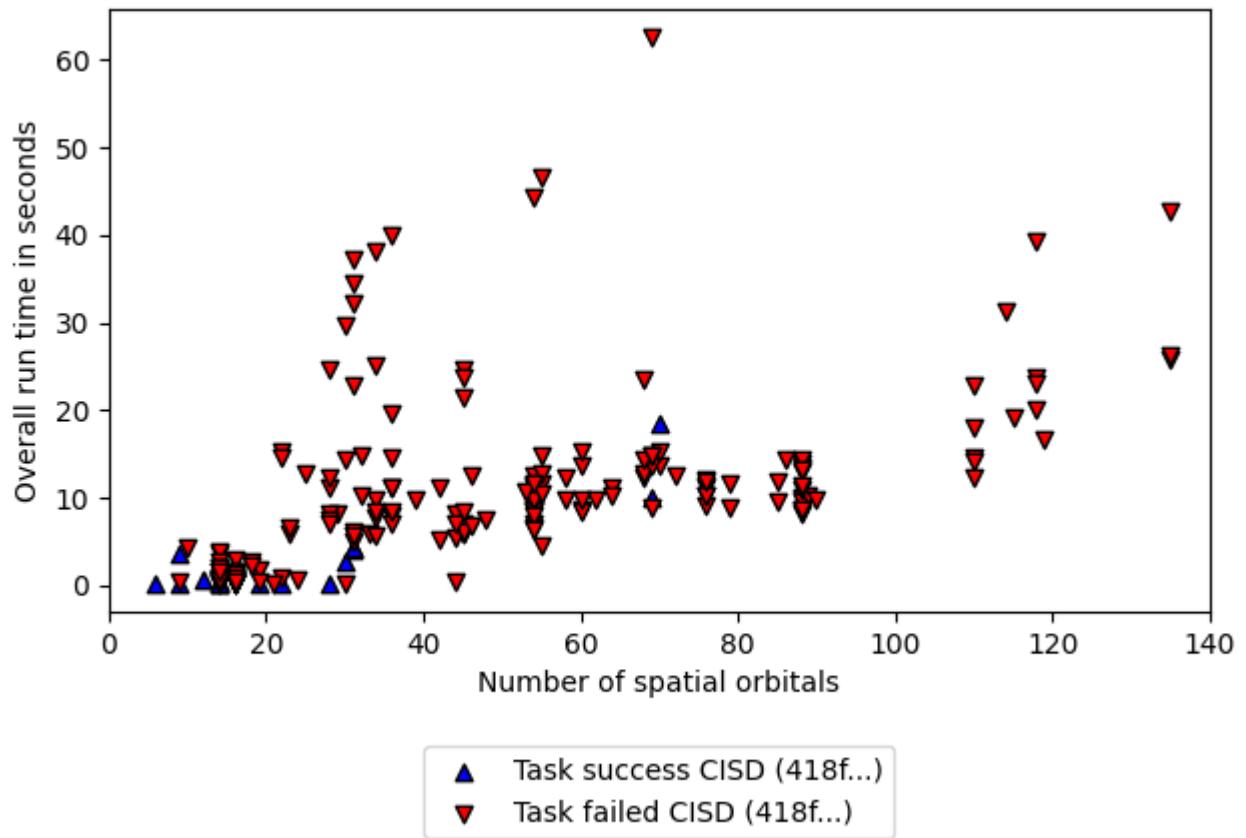
Solver CISD, **418f060e-496b-4024-8d2d-9b1f8791e76d**

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

solver_short_name:CISD

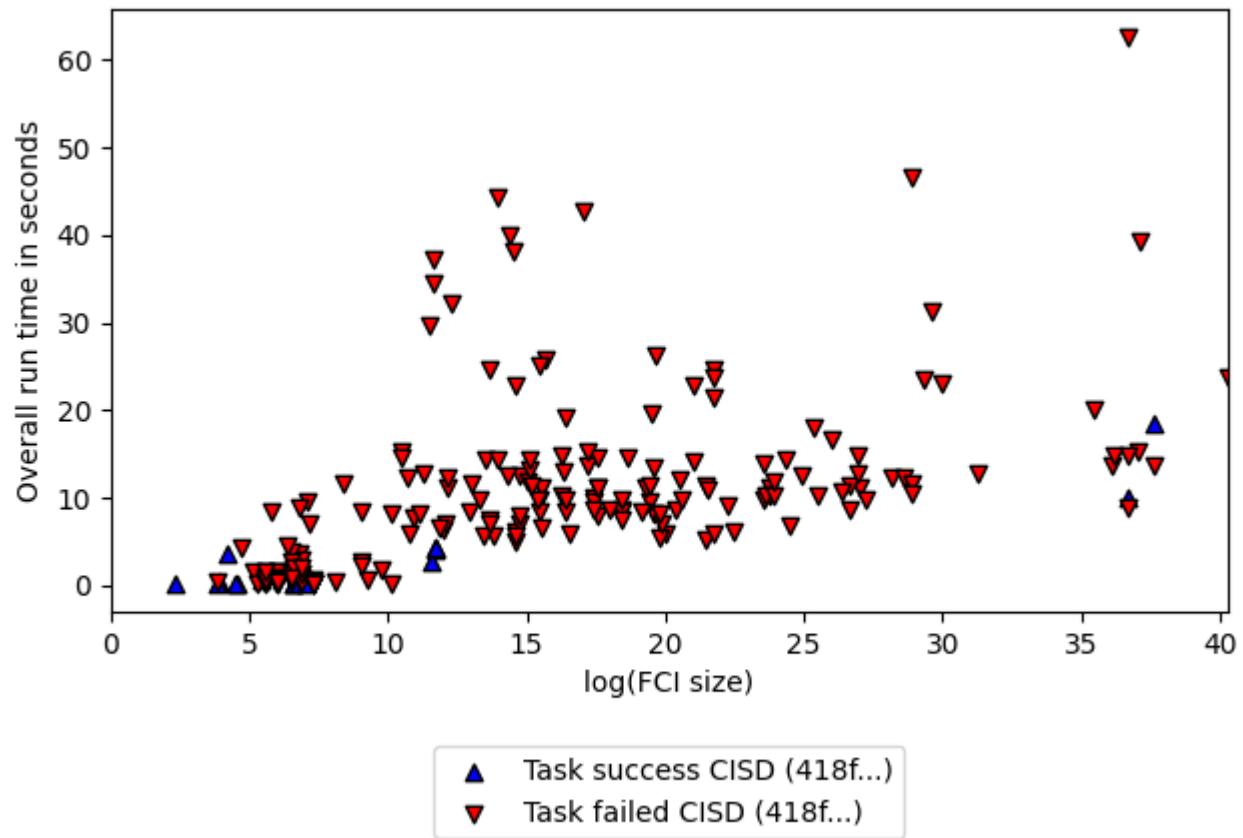
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CISD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 0a5c9d8b-baf9-4438-bdf9-7b85c9960130
creation_timestamp: 2025-02-24T20:41:03.349036+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.

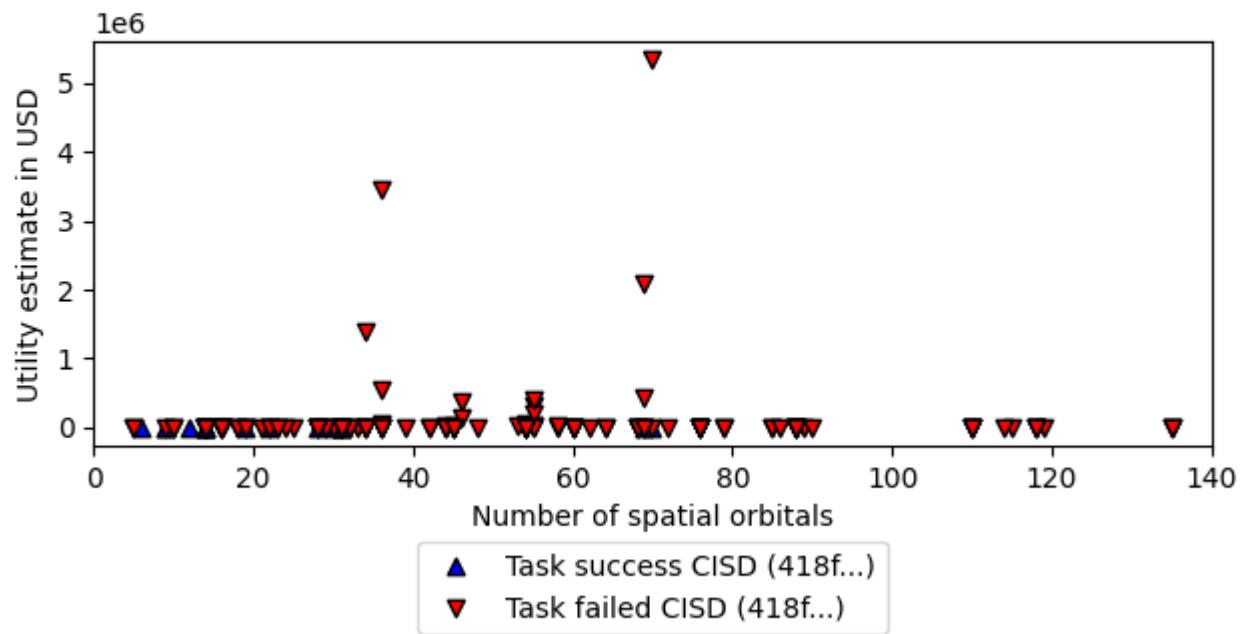
Run time for CISD/418f...



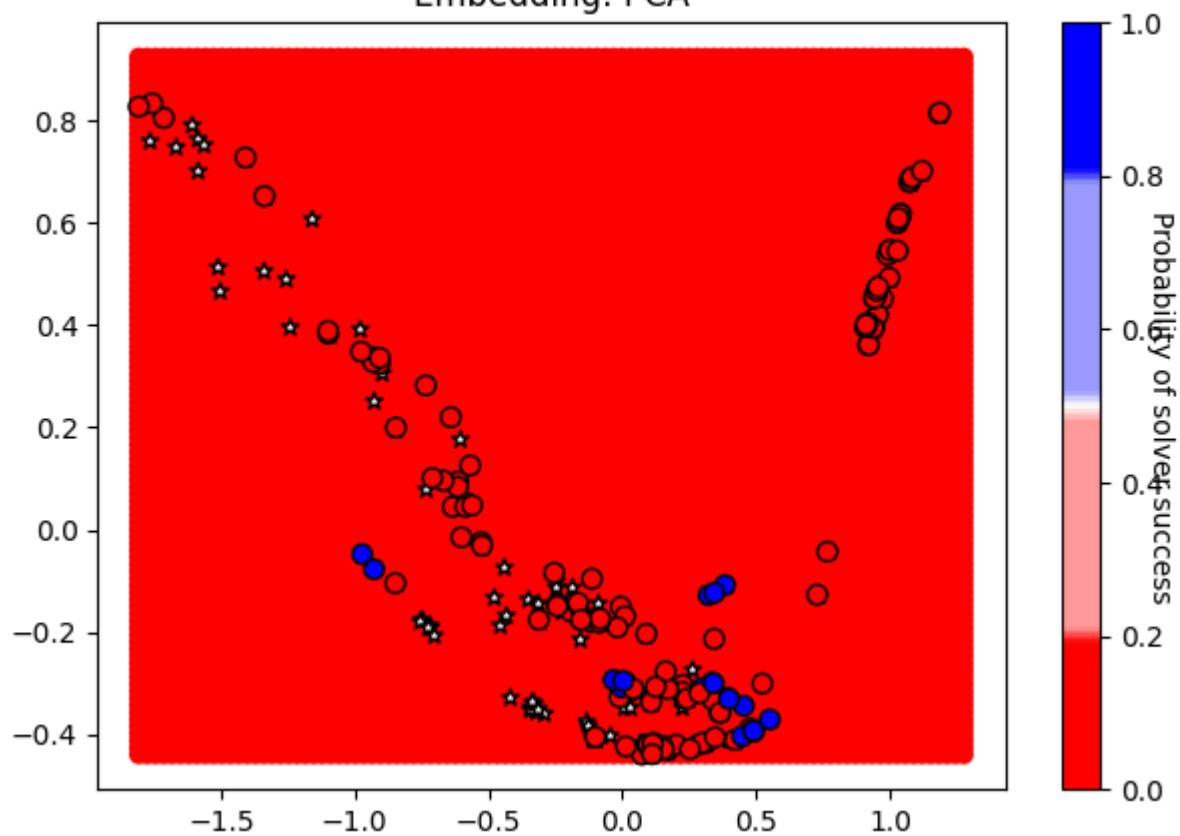
Note: plot only contains attempted tasks.

Utility capture from CISD/418f...

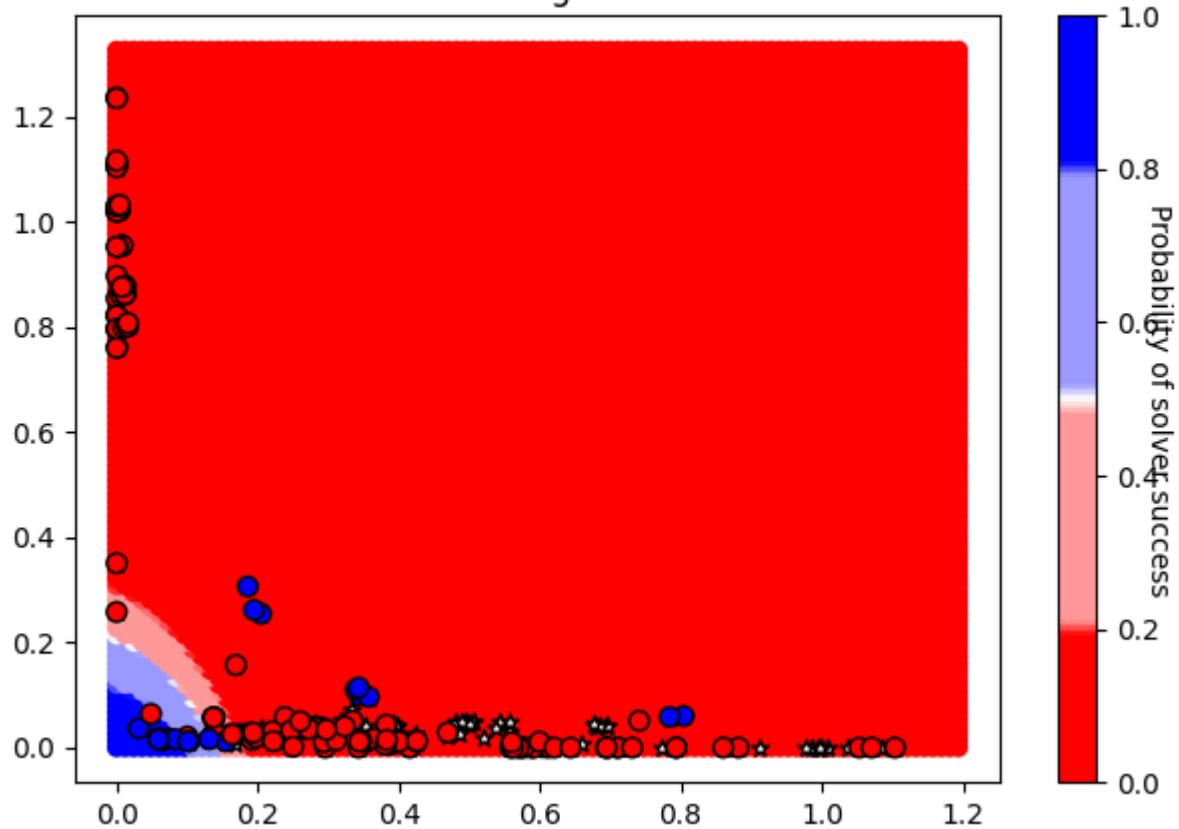
(captured: \$4.8e-03/1.5e+07, approximately 3.2e-08%)



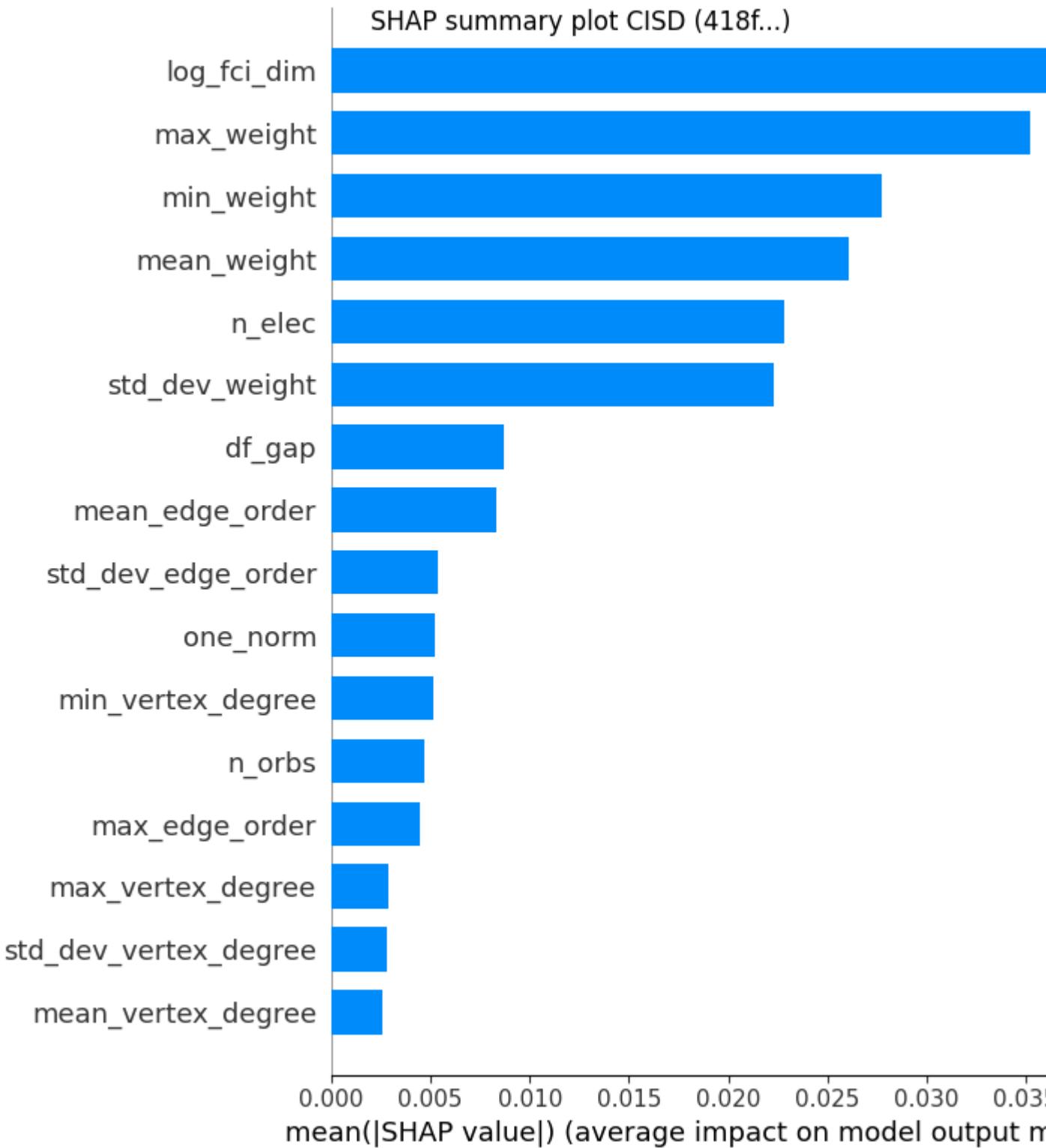
Solver CISD (418f...)
Embedding: PCA



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.



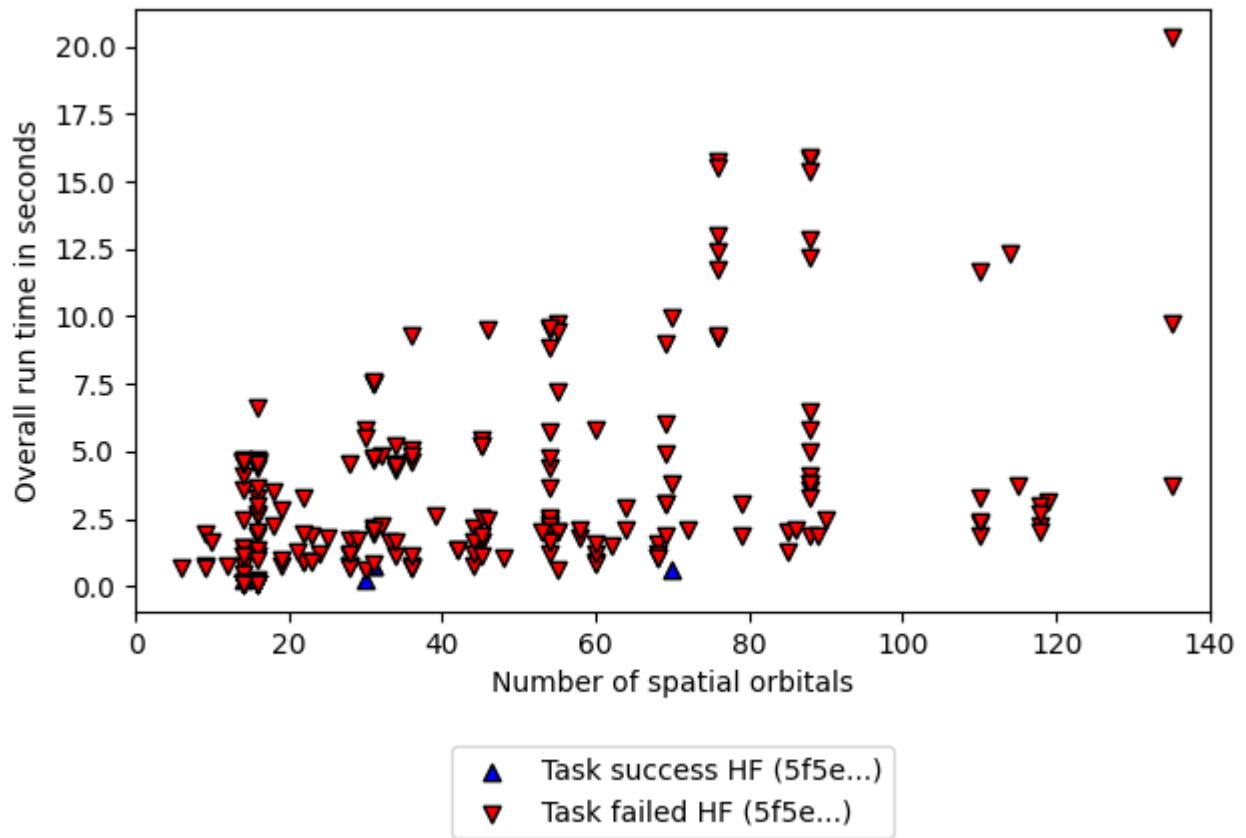
Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

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

solver_short_name:HF

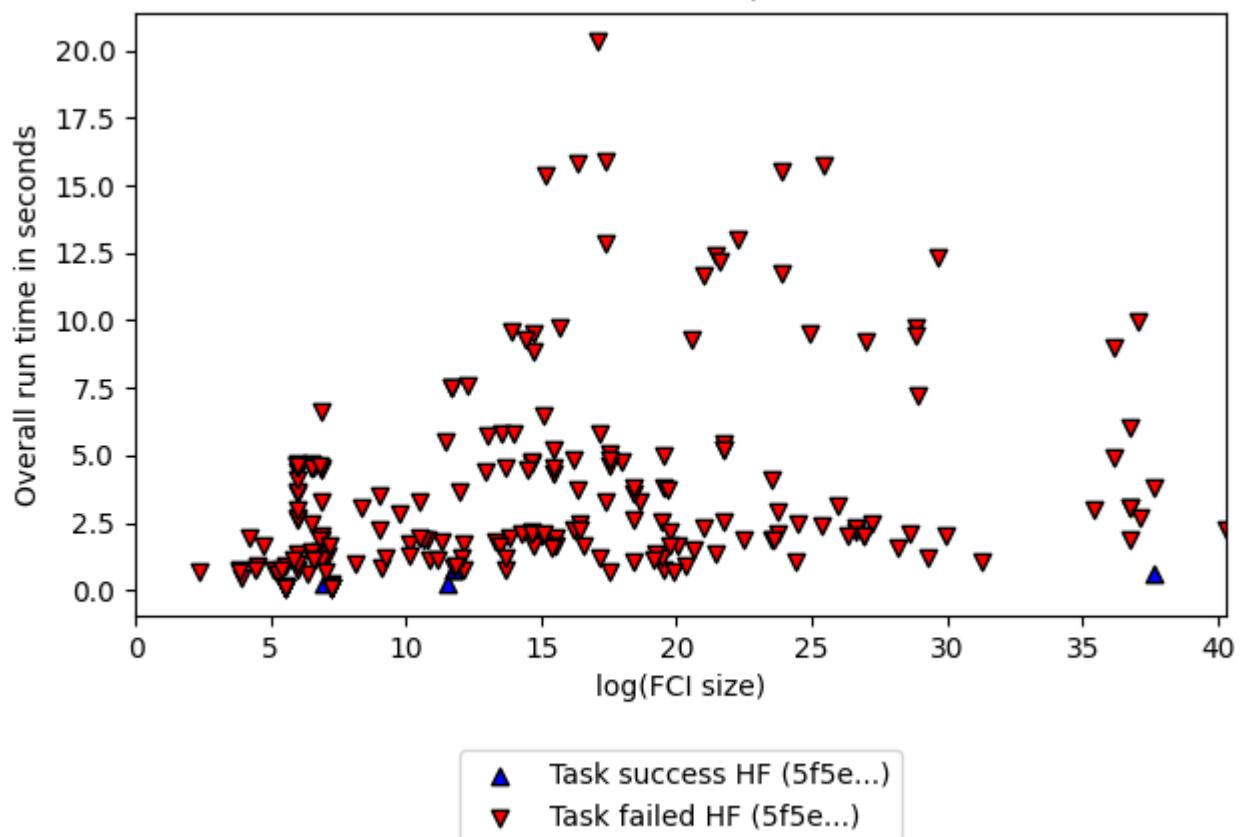
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:Hartree Fock
software.details:pyscf (<https://github.com/pyscf/pyscf>).
performance.metrics.uuid: 428a4869-d721-40d2-8409-92b803e029e4
creation.timestamp: 2025-02-24T20:41:03.349036+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.

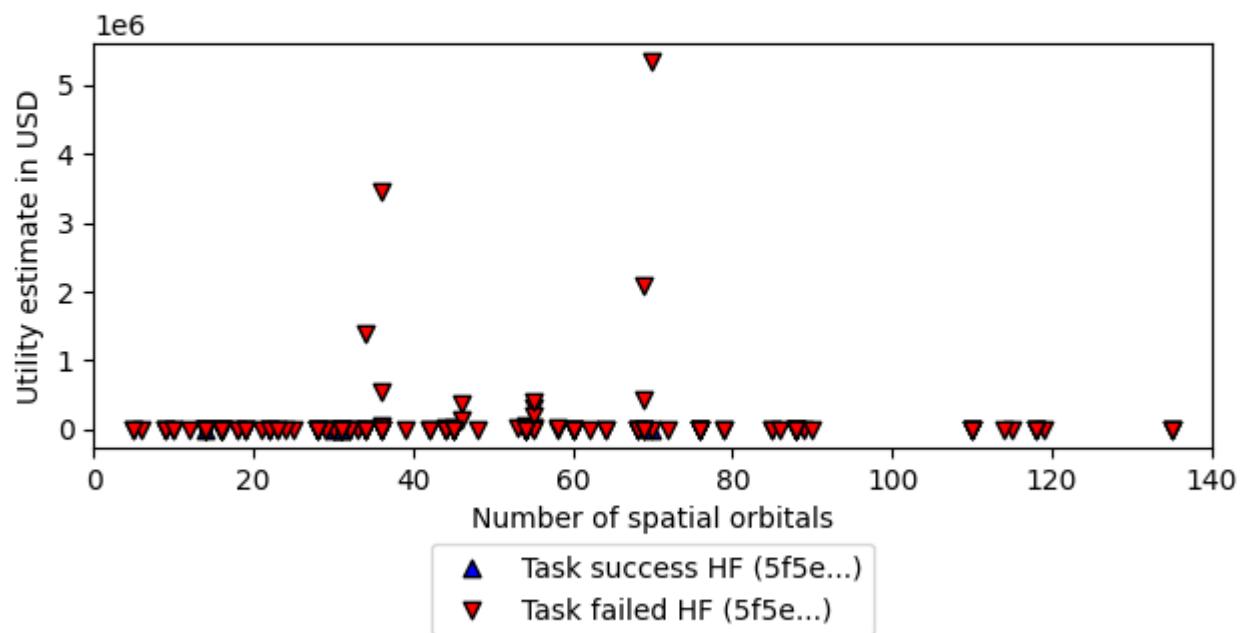
Run time for HF/5f5e...



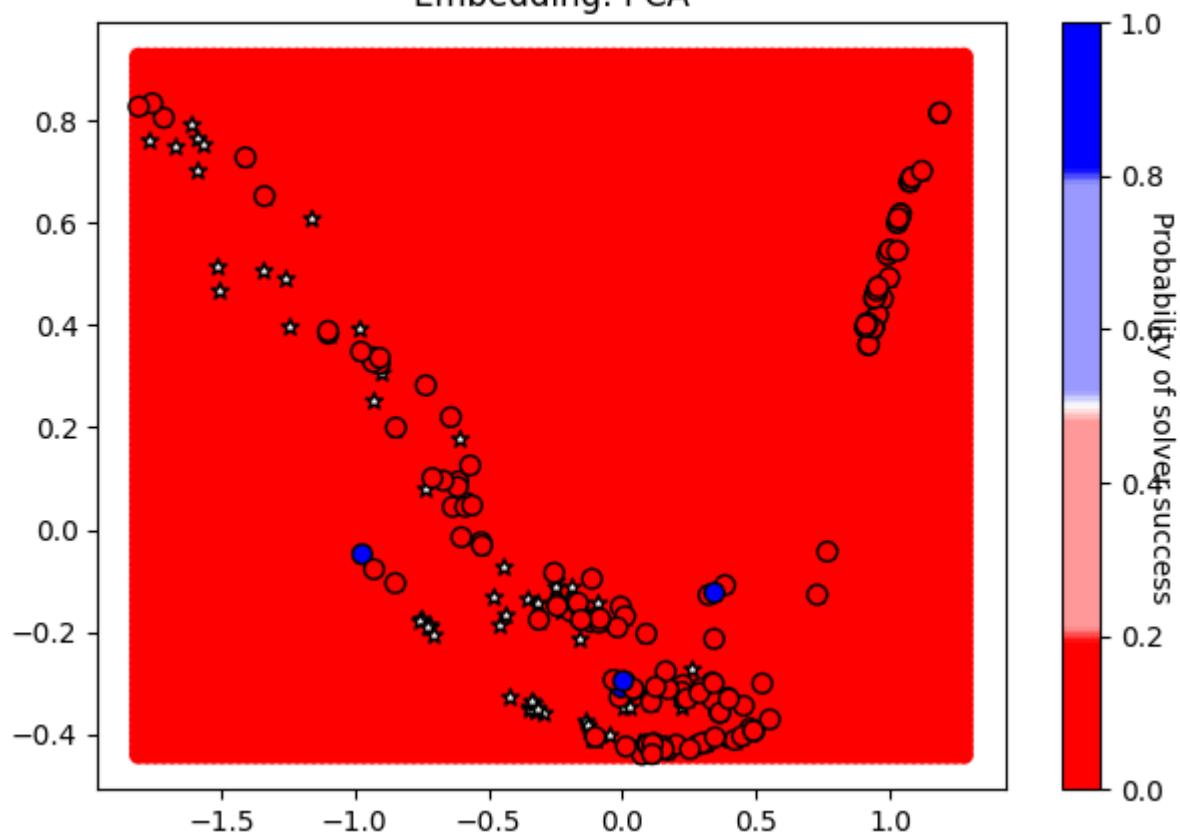
Note: plot only contains attempted tasks.

Utility capture from HF/5f5e...

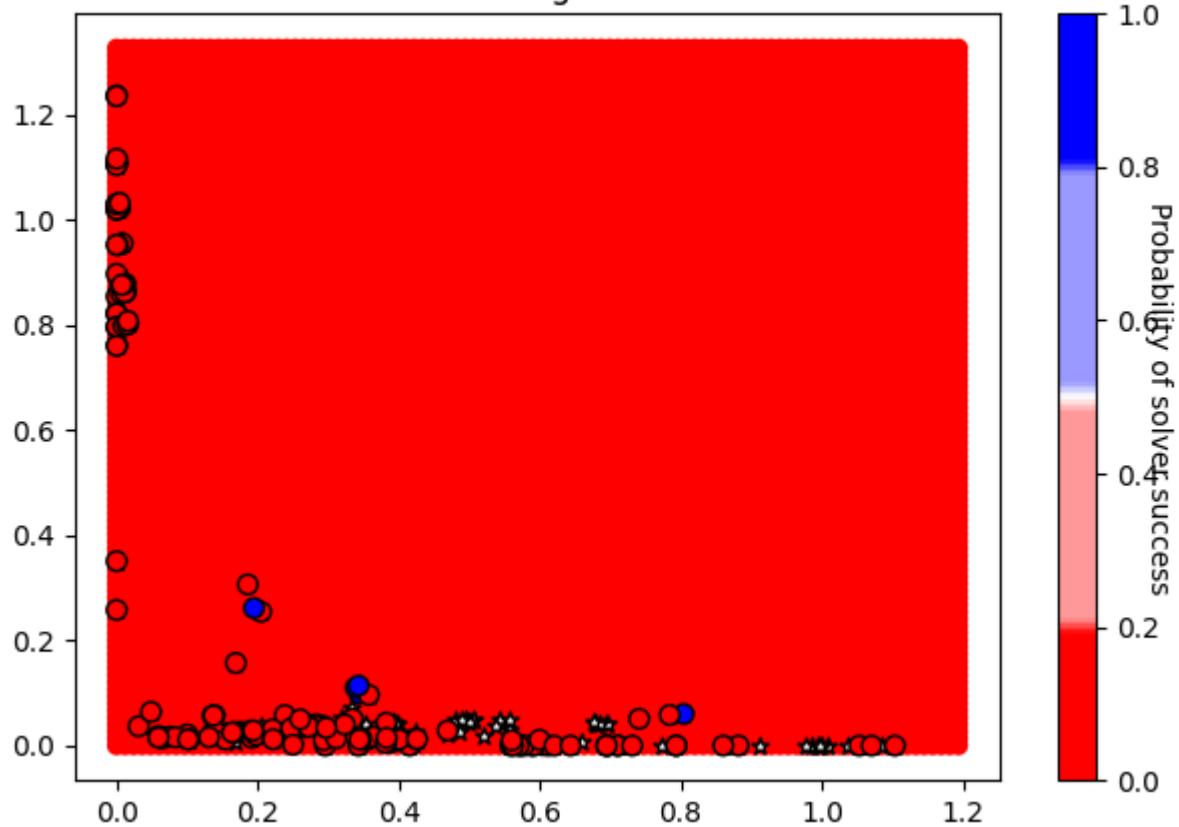
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



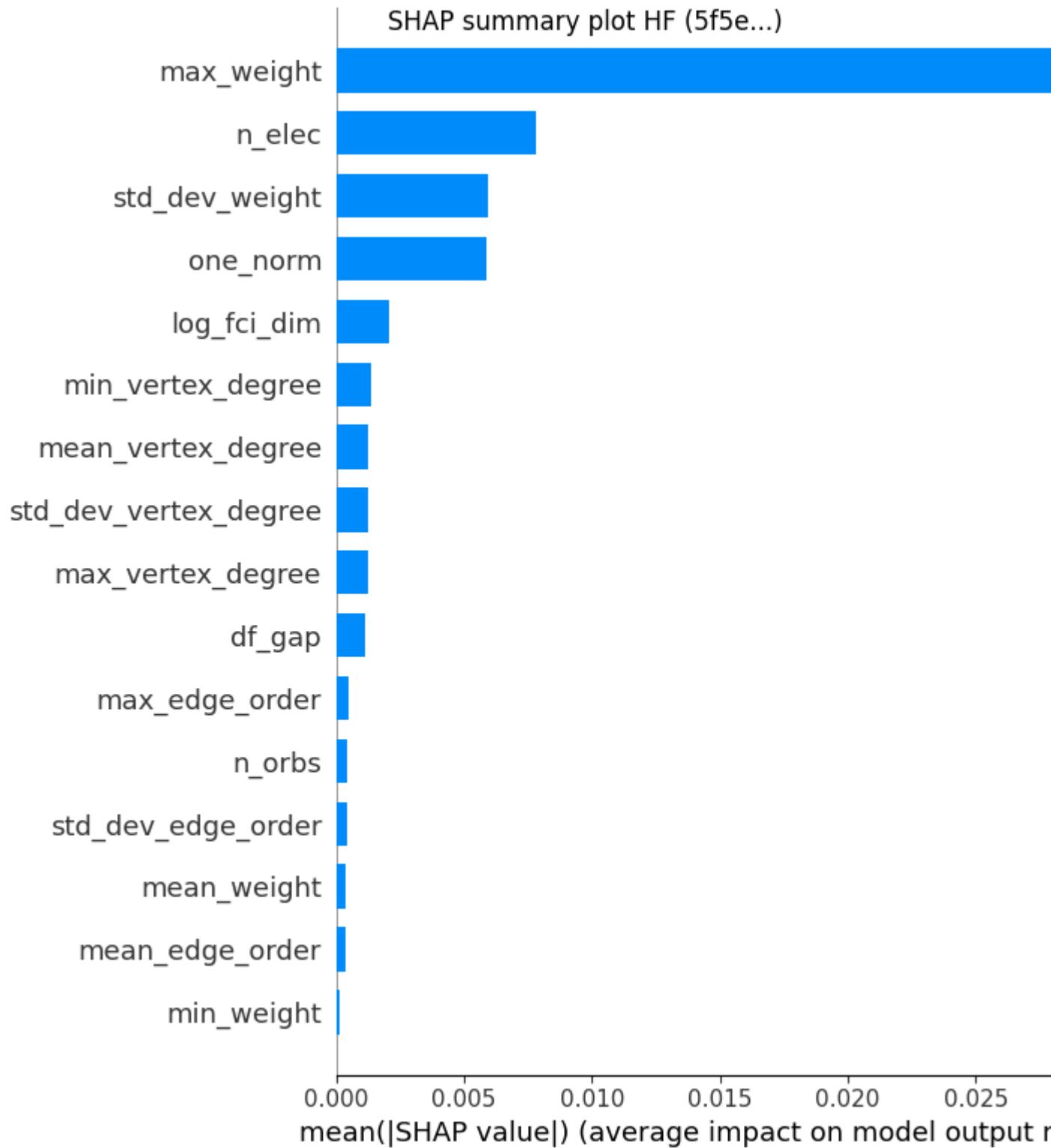
Solver HF (5f5e...)
Embedding: PCA



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.



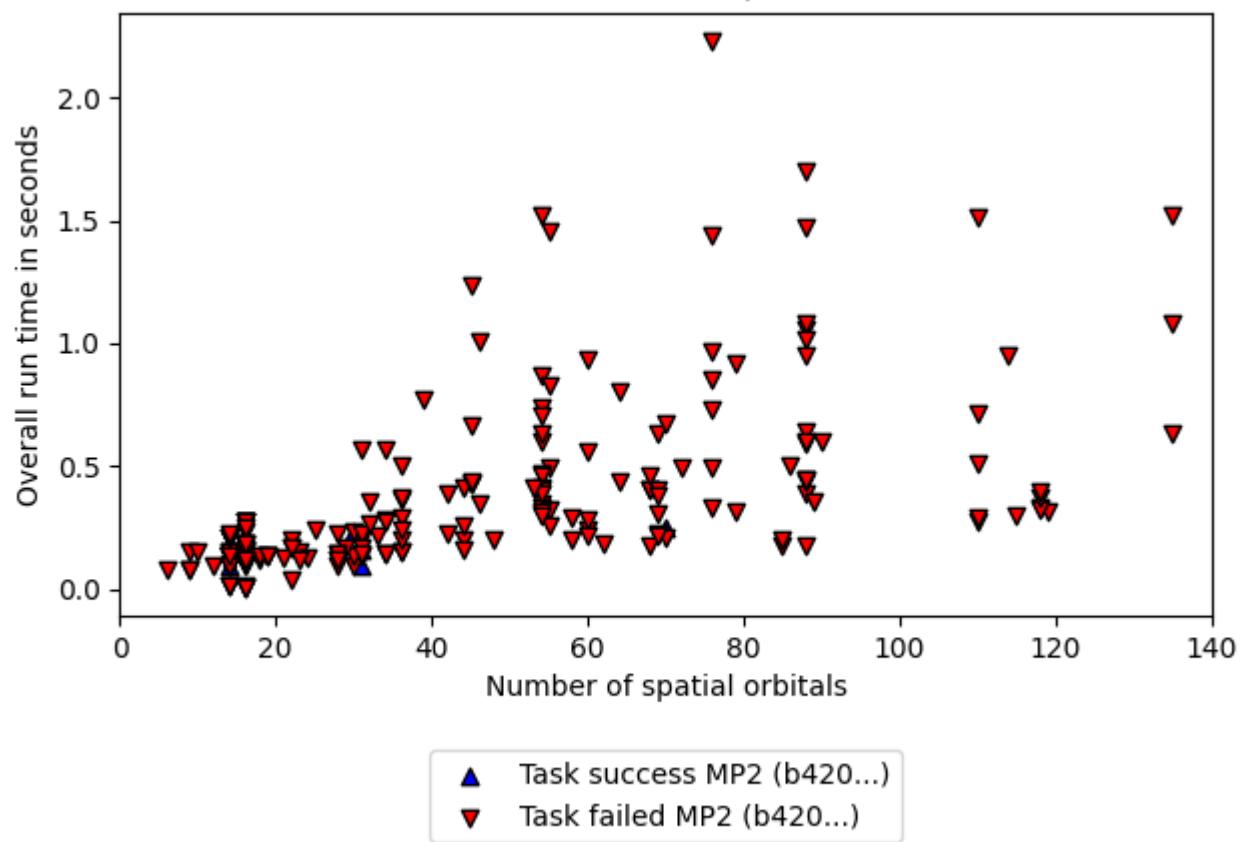
Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aecd2

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

solver_short_name:MP2

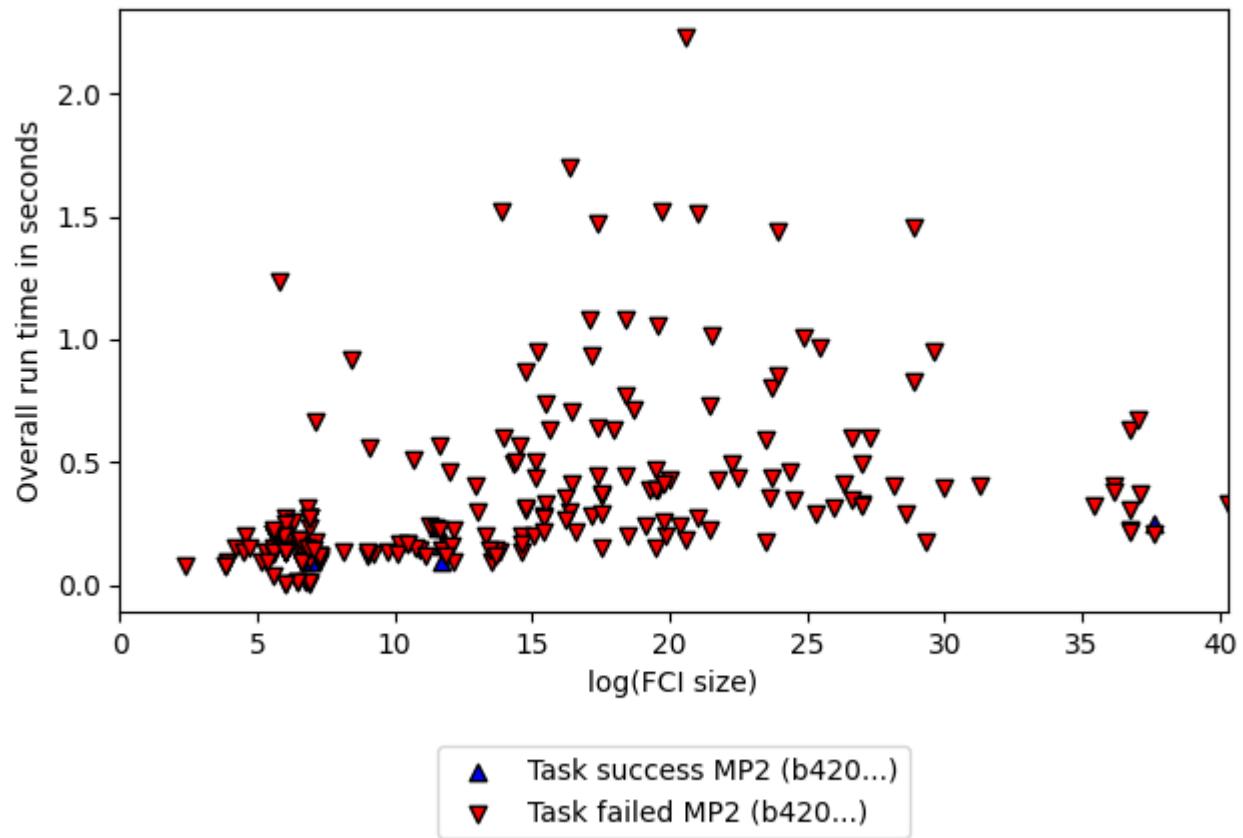
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:MP2
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 6d5f0bee-b9ce-4f5a-9ab7-bc3ead209aa5
creation_timestamp: 2025-02-24T20:41:03.349036+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.

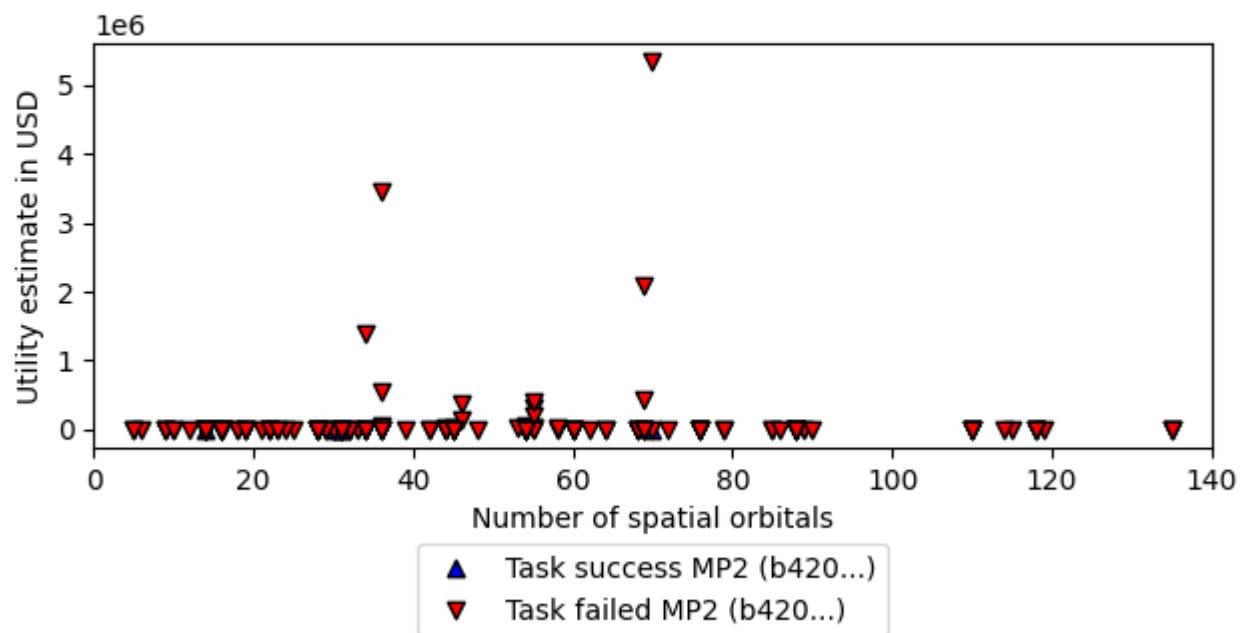
Run time for MP2/b420...



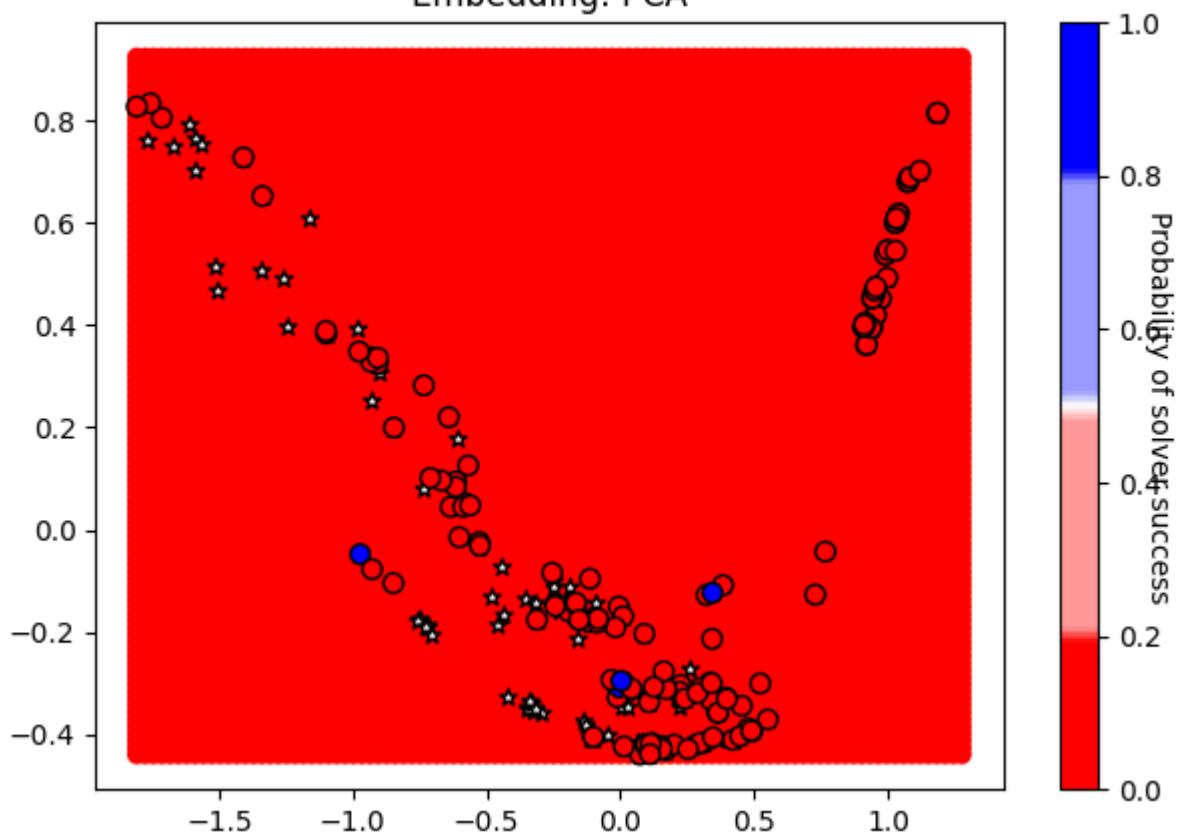
Note: plot only contains attempted tasks.

Utility capture from MP2/b420...

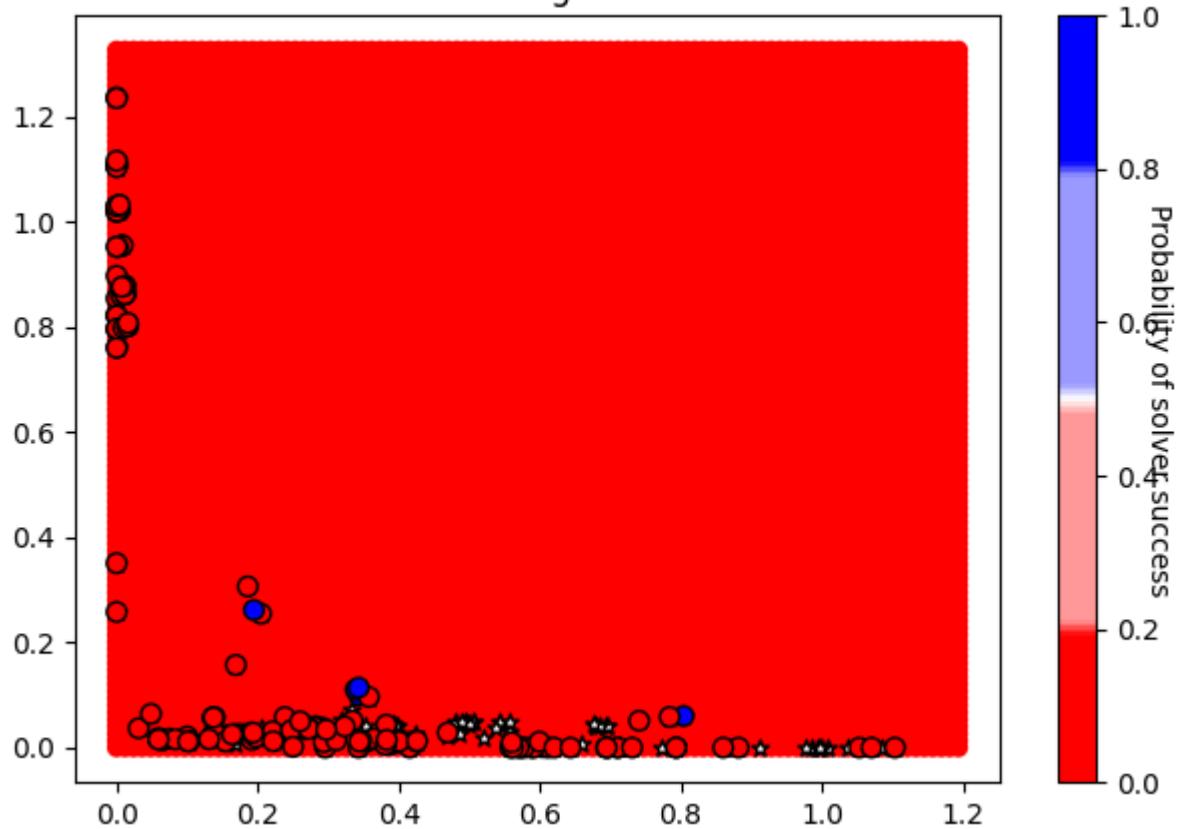
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



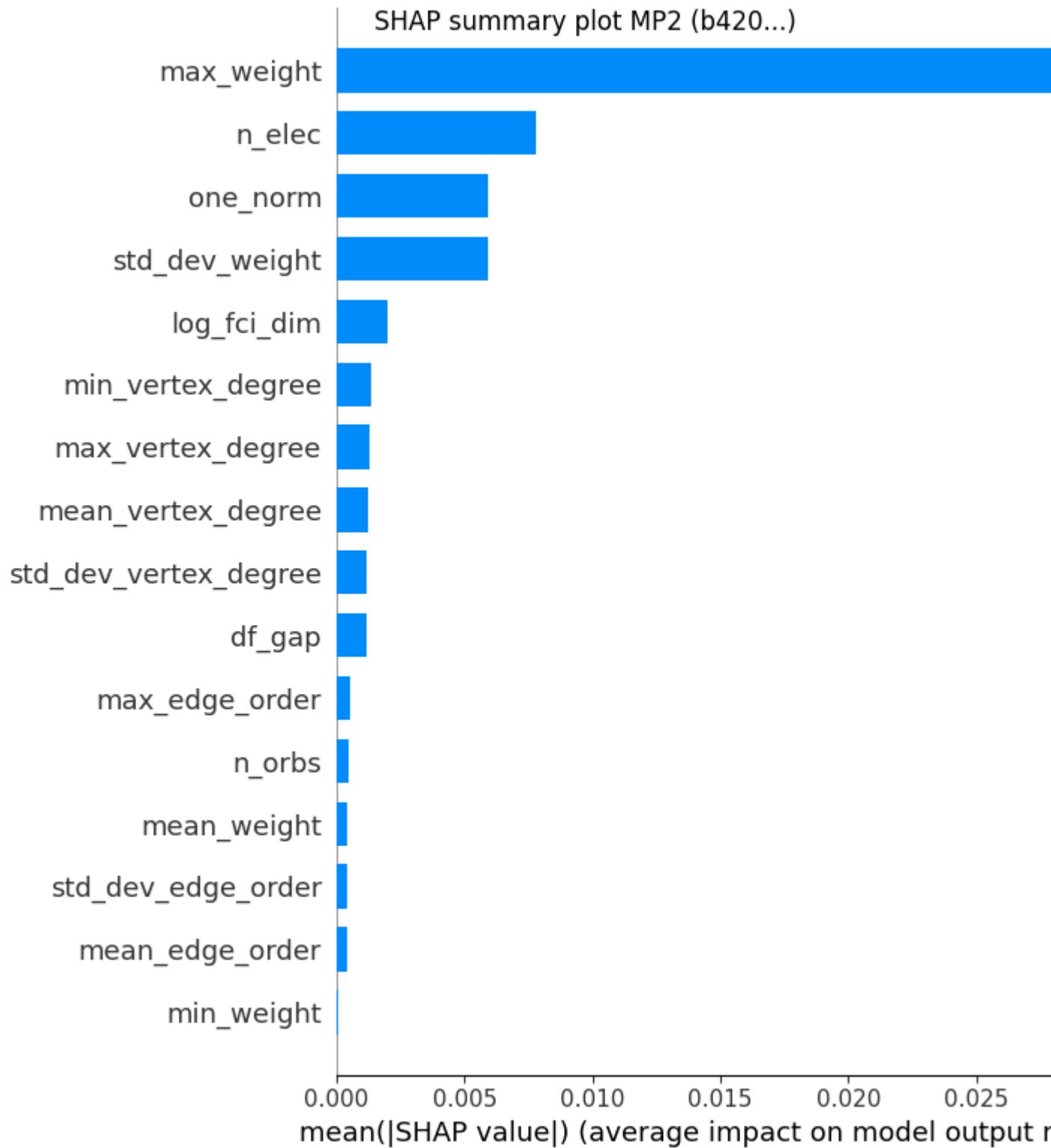
Solver MP2 (b420...)
Embedding: PCA



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.



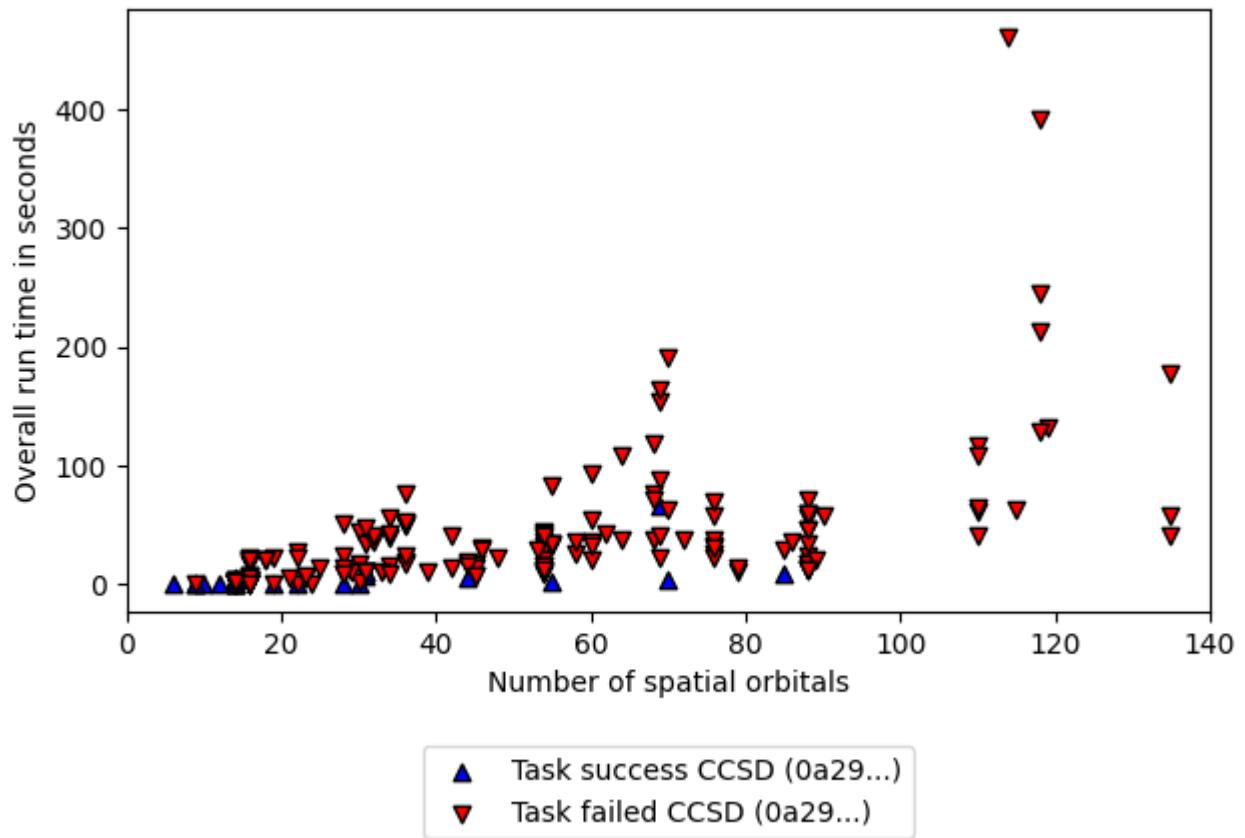
Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

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

solver_short_name:CCSD

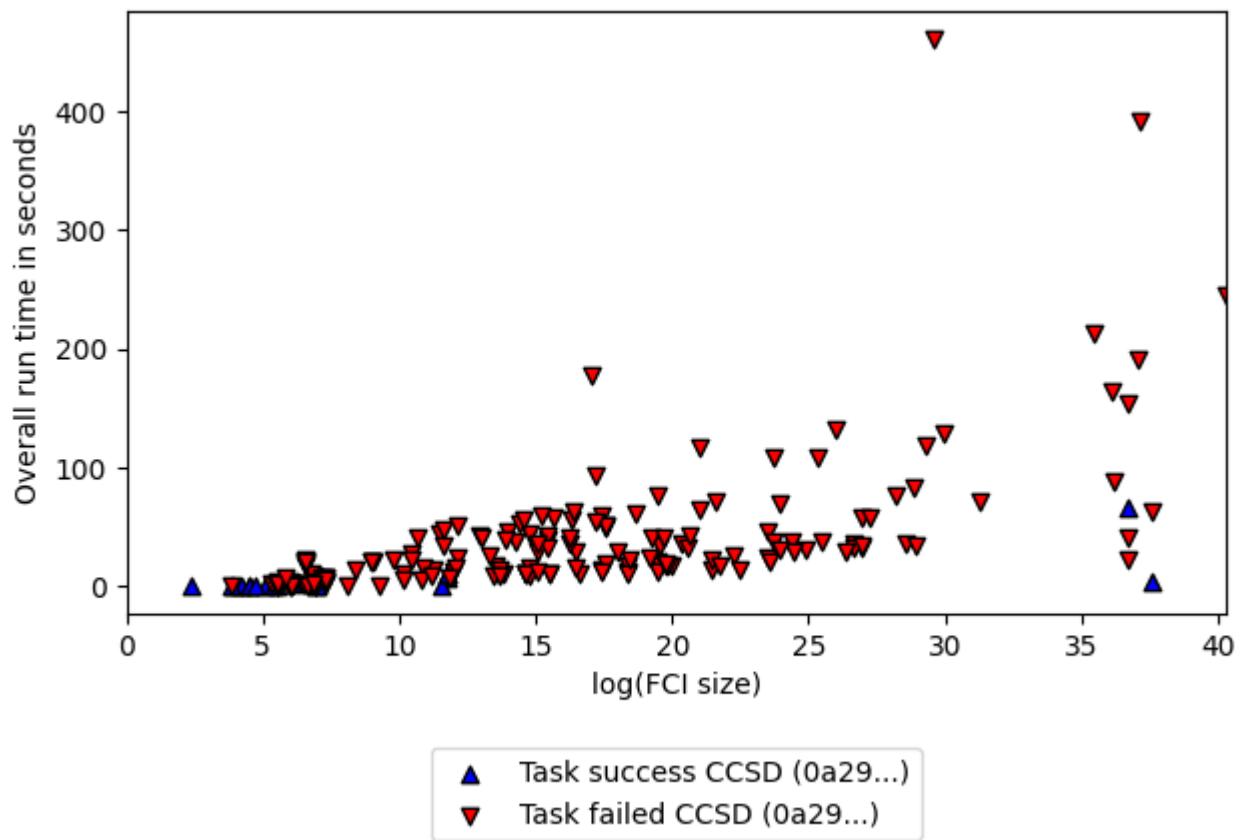
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: c7ae3036-7db4-4bc2-9bad-a7749598904a
creation_timestamp: 2025-02-24T20:41:03.349036+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.

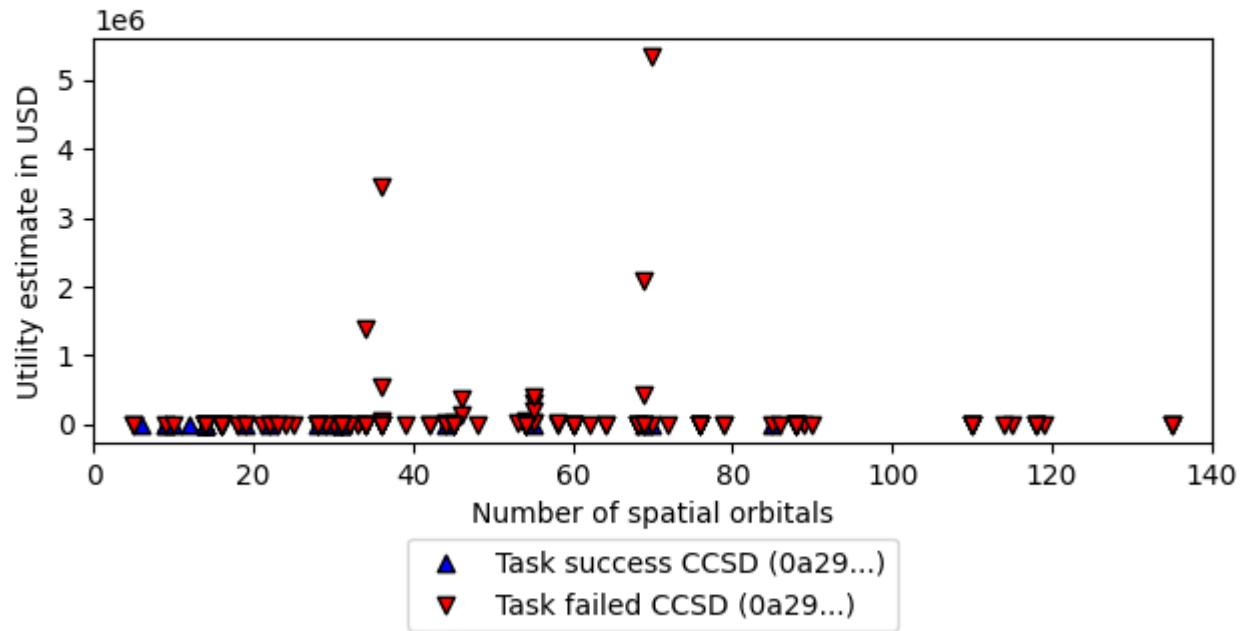
Run time for CCSD/0a29...



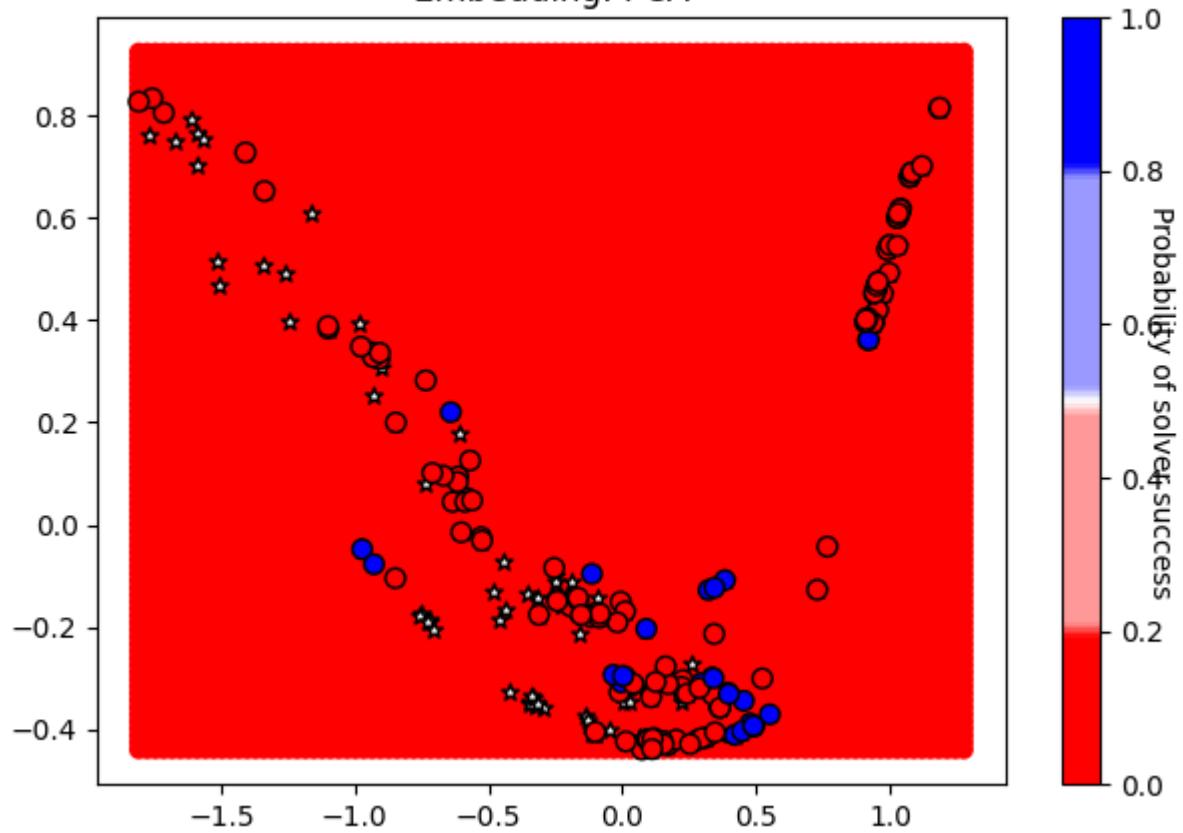
Note: plot only contains attempted tasks.

Utility capture from CCSD/0a29...

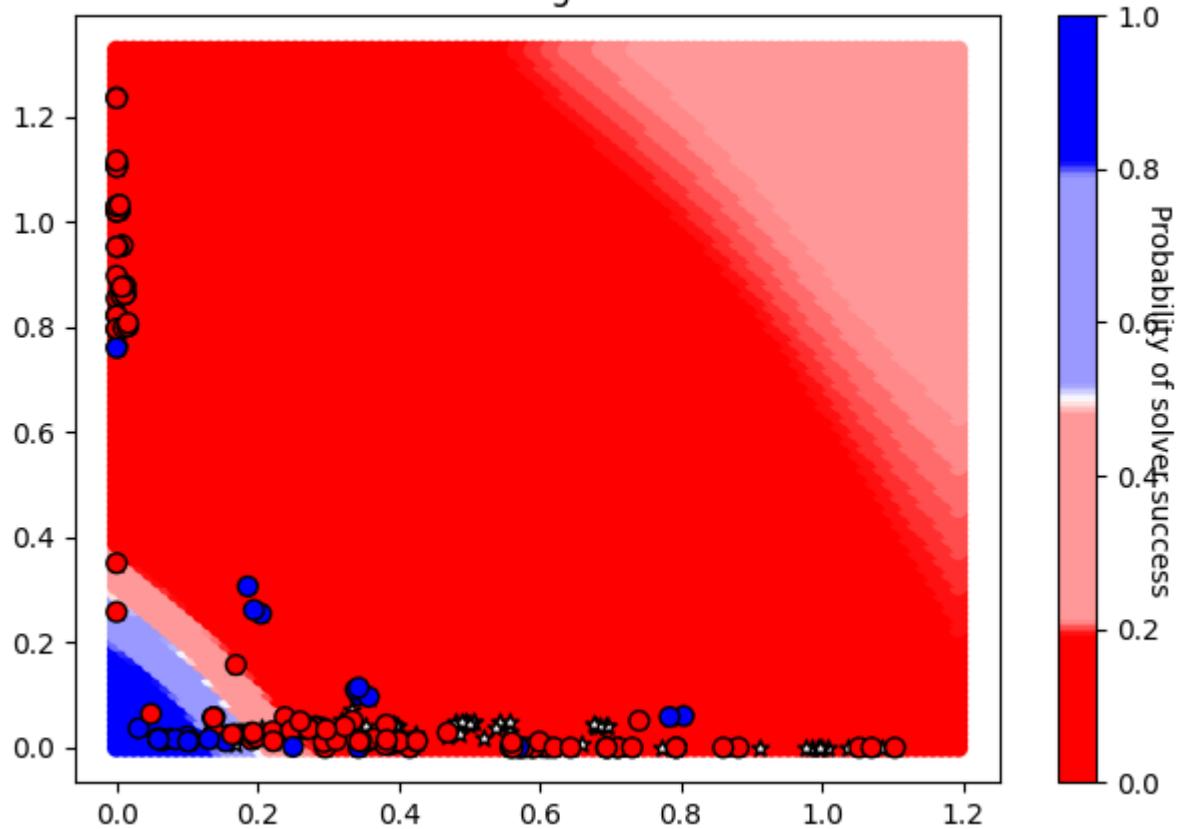
(captured: \$2.1e-02/1.5e+07, approximately 1.4e-07%)



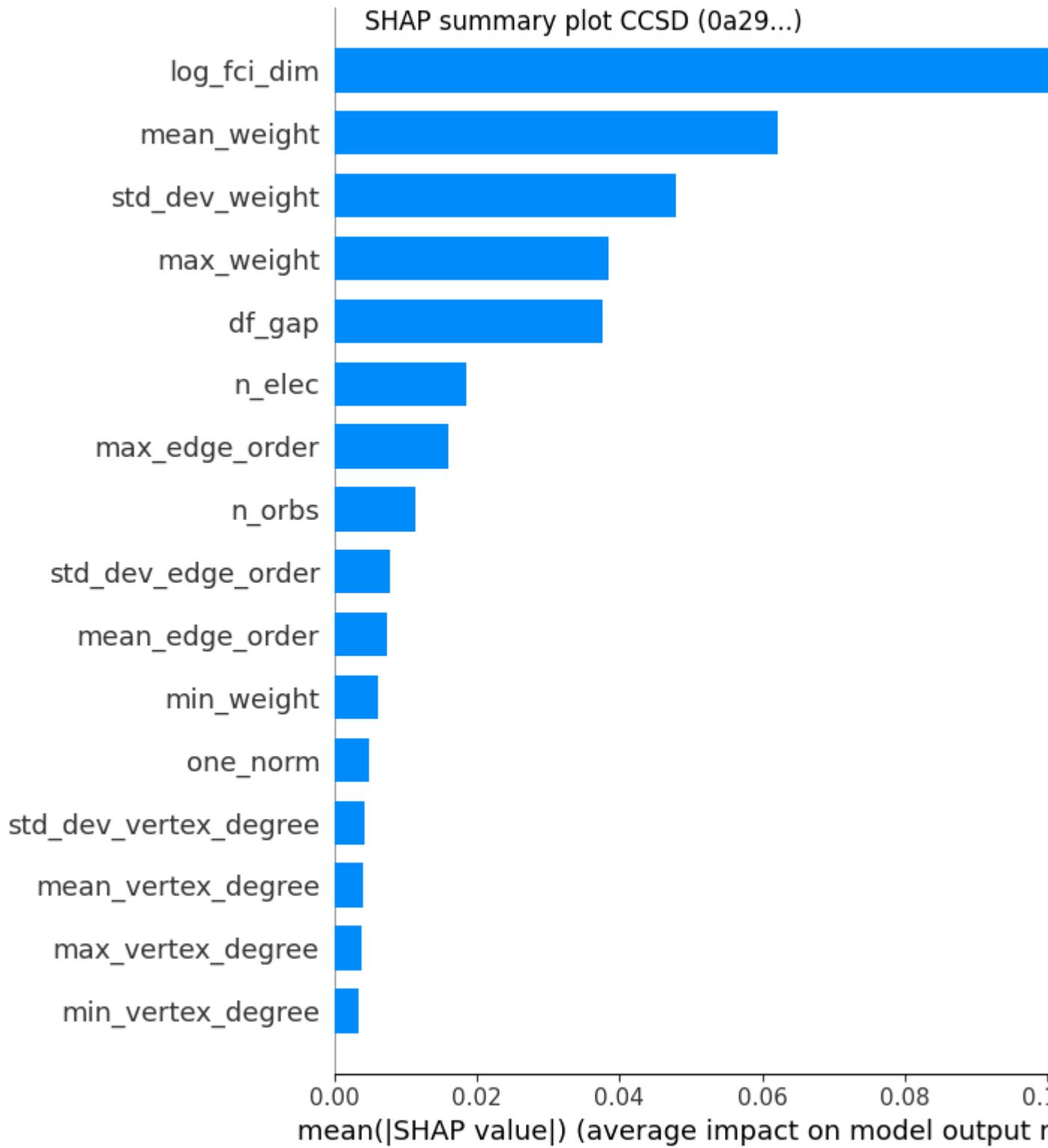
Solver CCSD (0a29...)
Embedding: PCA



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.



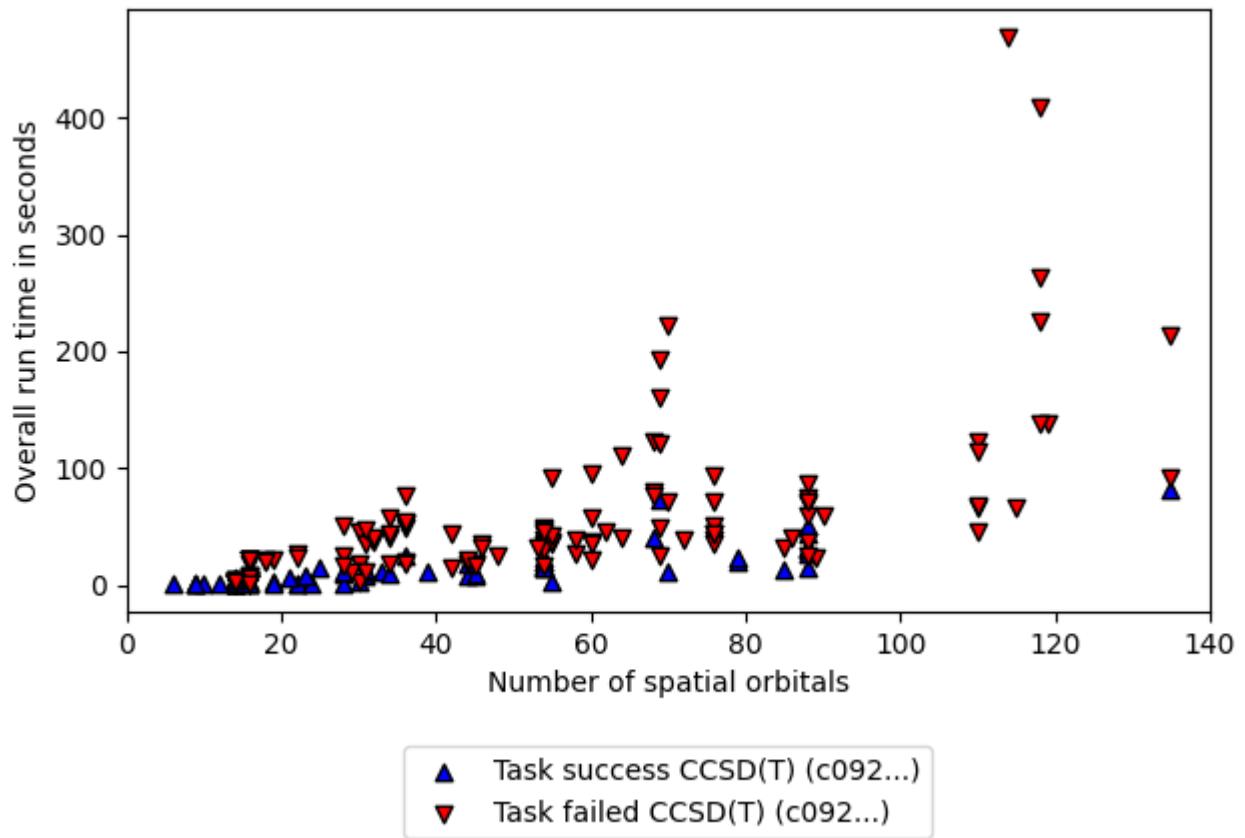
Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878

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

solver_short_name:CCSD(T)

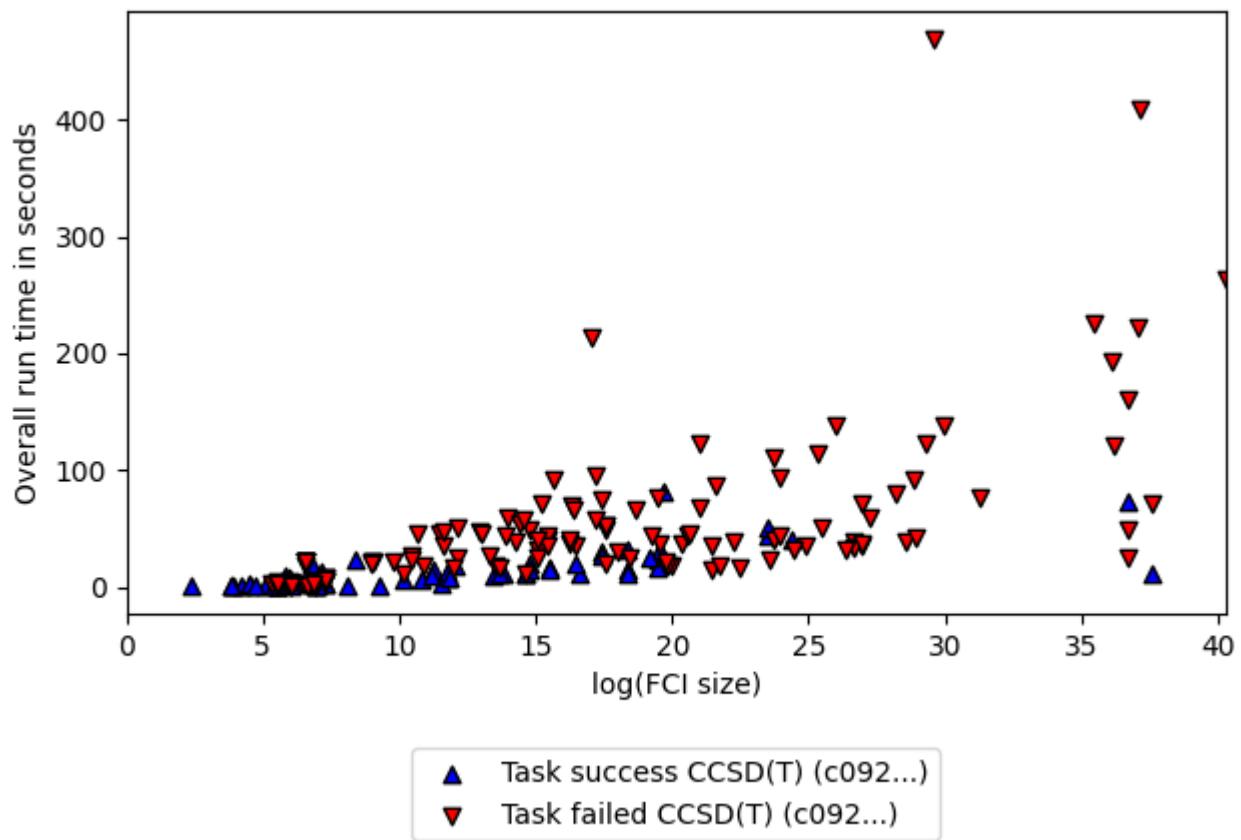
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD(T)
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 1f1018fb-0b50-4b5b-95b0-d9523d77e030
creation_timestamp: 2025-02-24T20:41:03.349036+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.

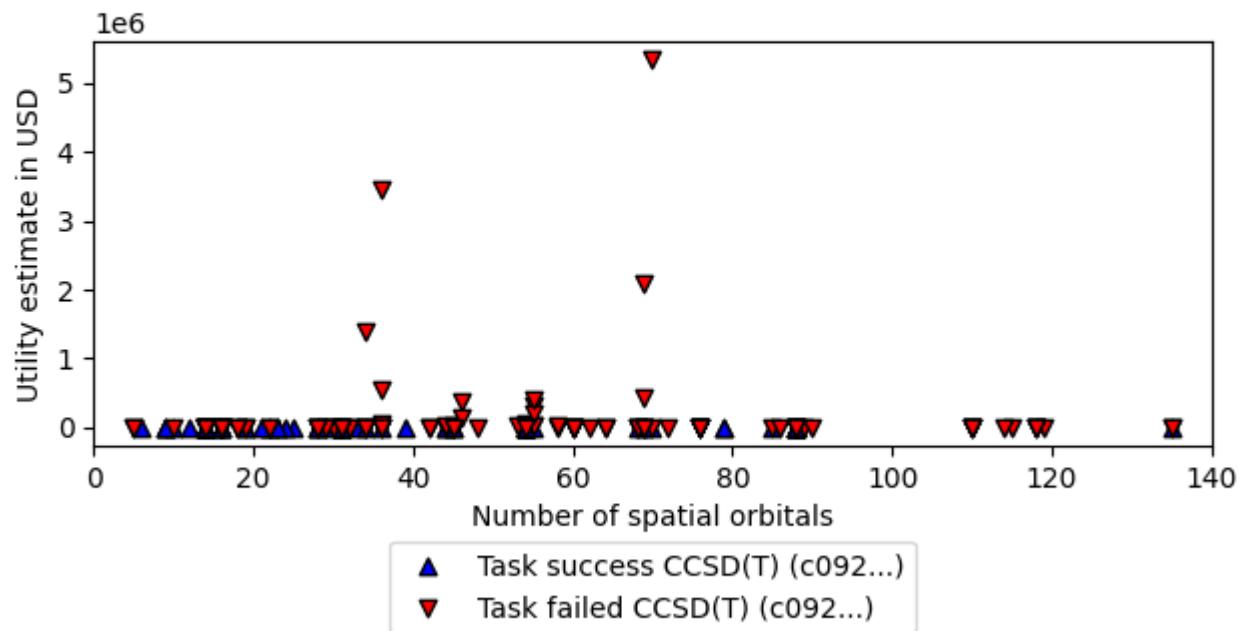
Run time for CCSD(T)/c092...



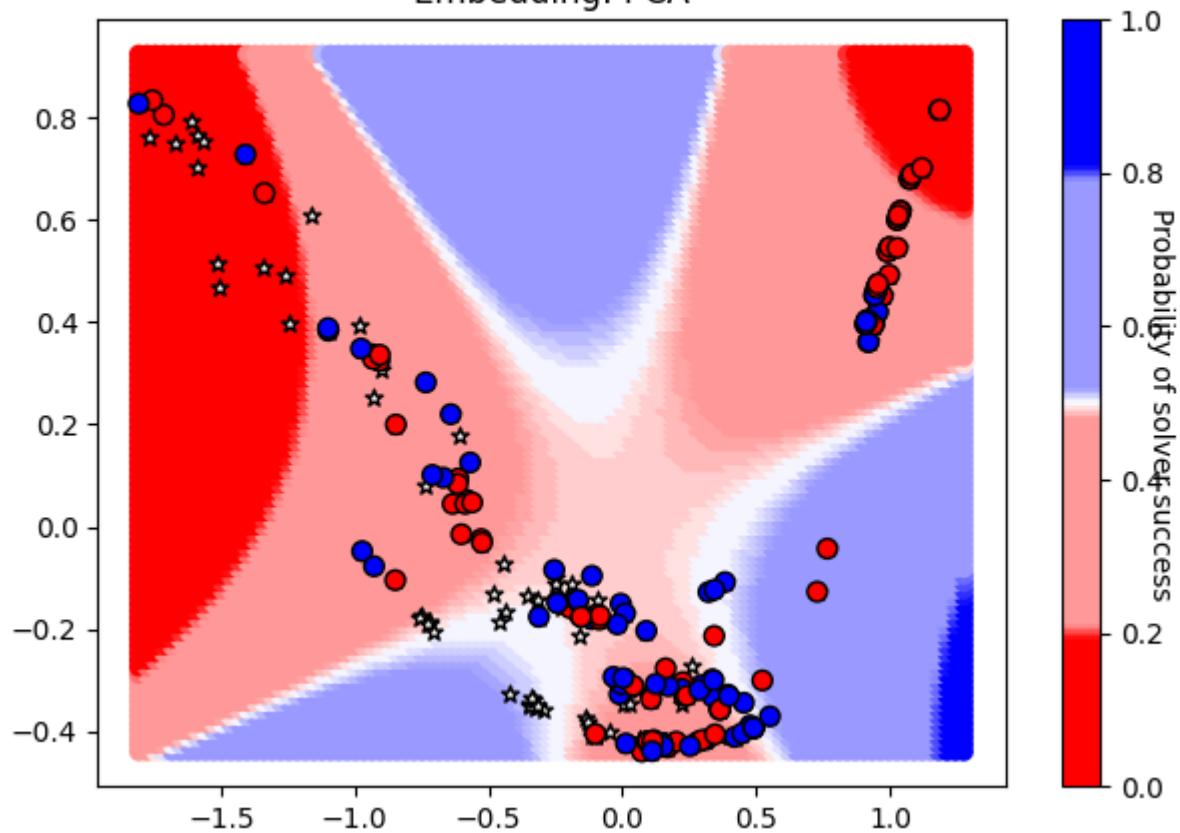
Note: plot only contains attempted tasks.

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

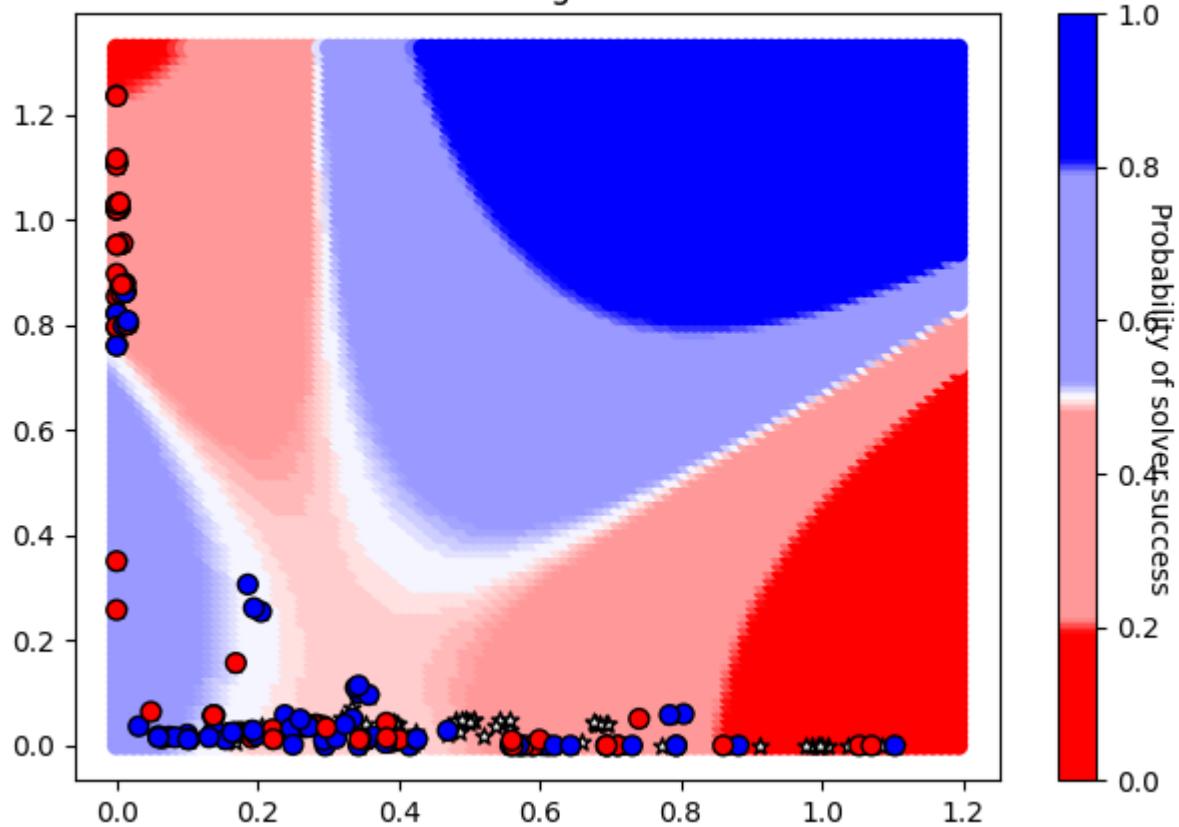
(captured: $\$1.8e+02/1.5e+07$, approximately $1.2e-03\%$)



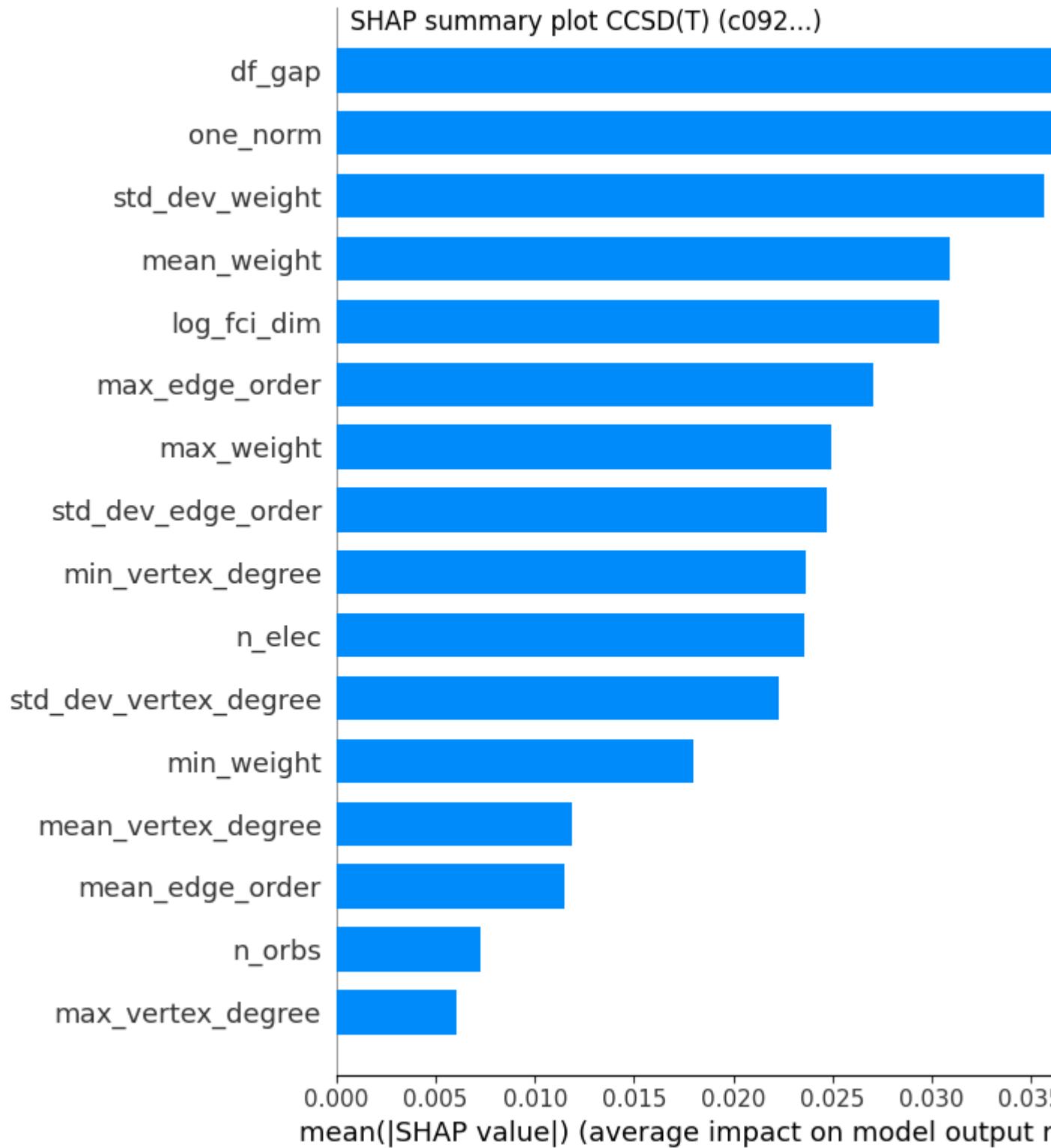
Solver CCSD(T) (c092...)
Embedding: PCA



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: e5bc538e-984d-47f7-b03d-af2d2656f900

creation_timestamp: 2025-02-24T20:41:03.349036+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

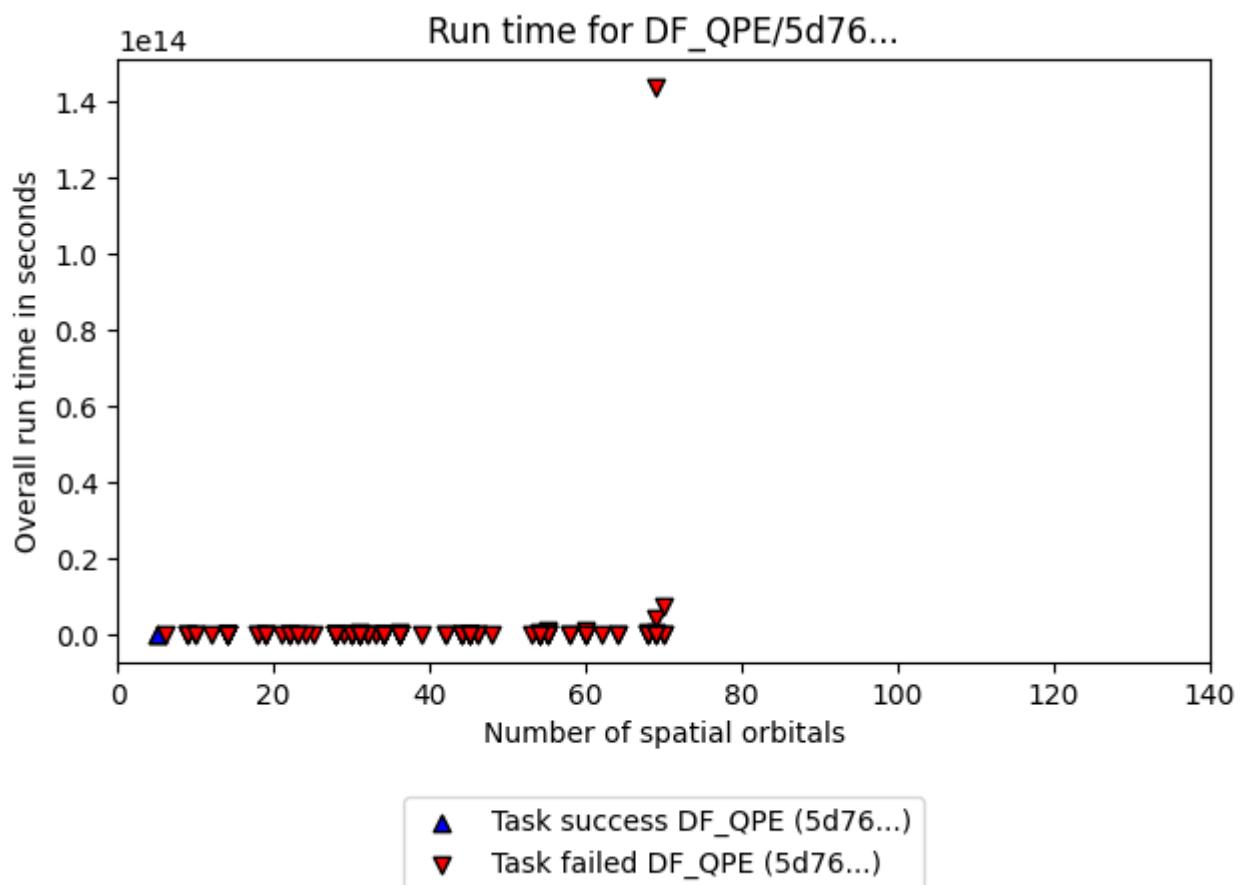
sum_of_run_time_of_attempted_tasks: 164517943847731.3

solvability_ratio: 0.0394

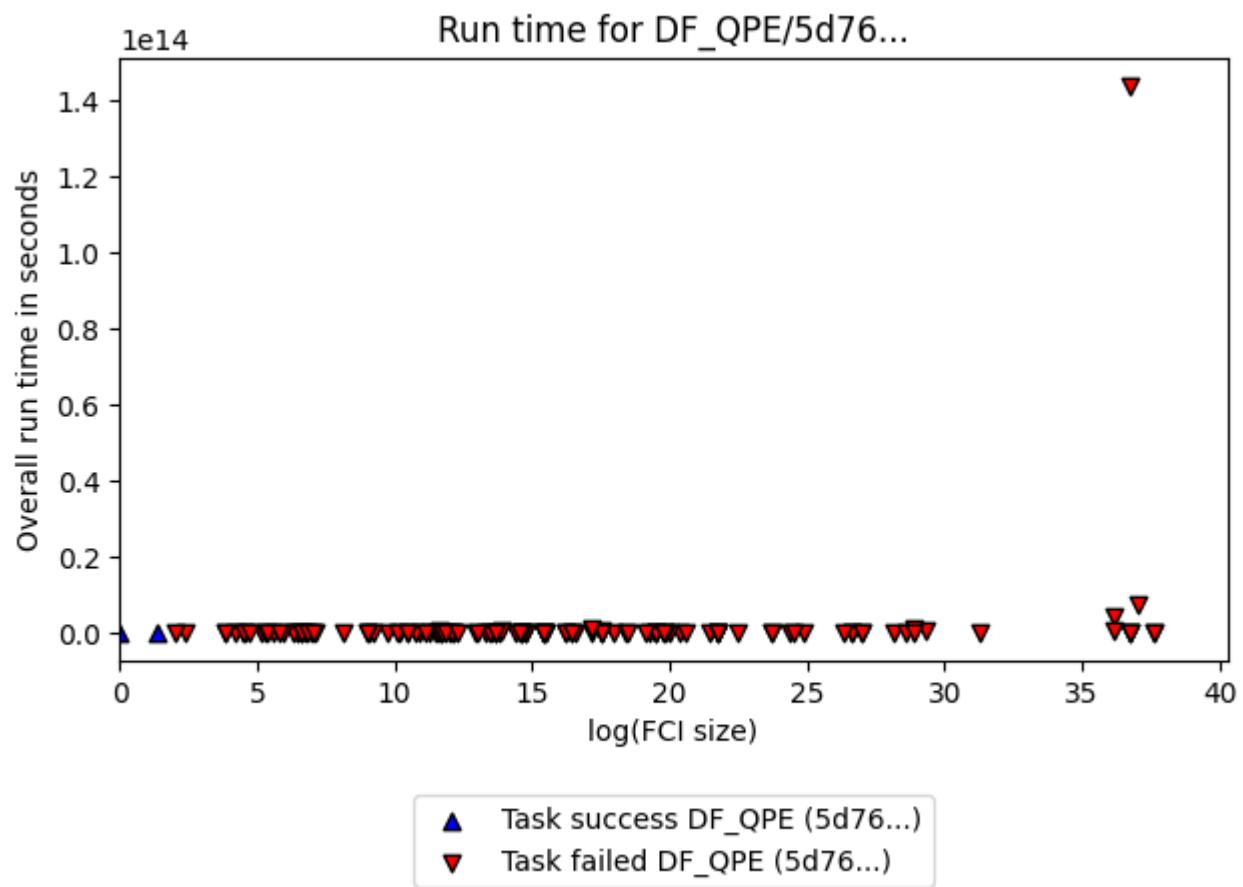
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



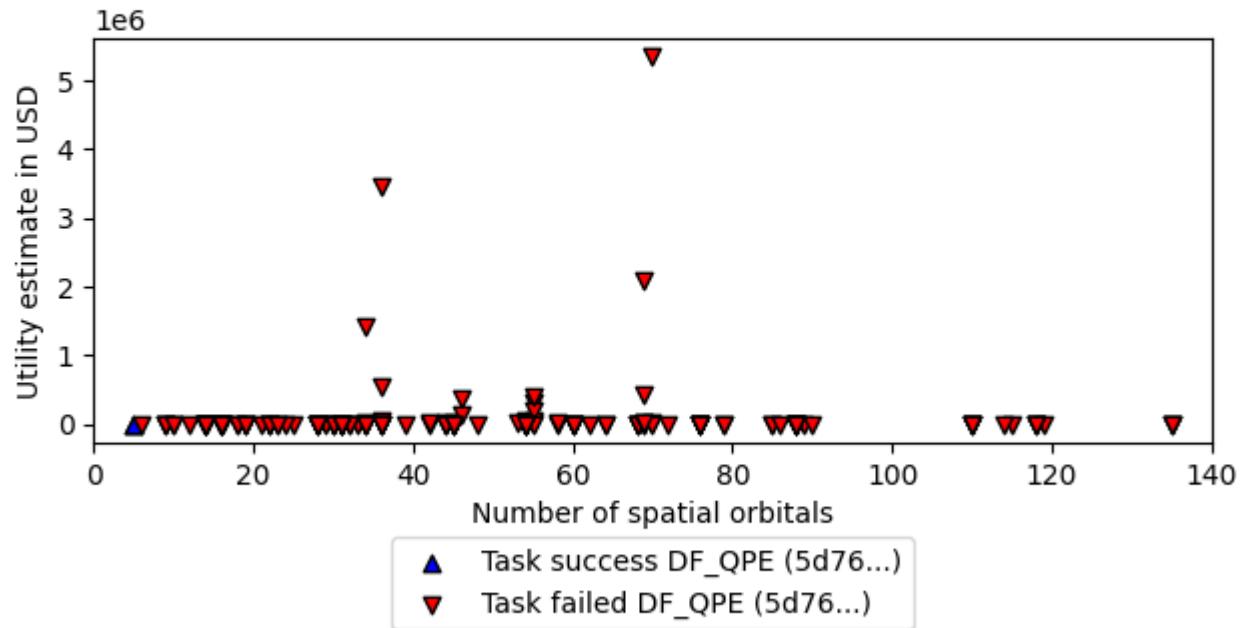
Note: plot only contains attempted tasks.



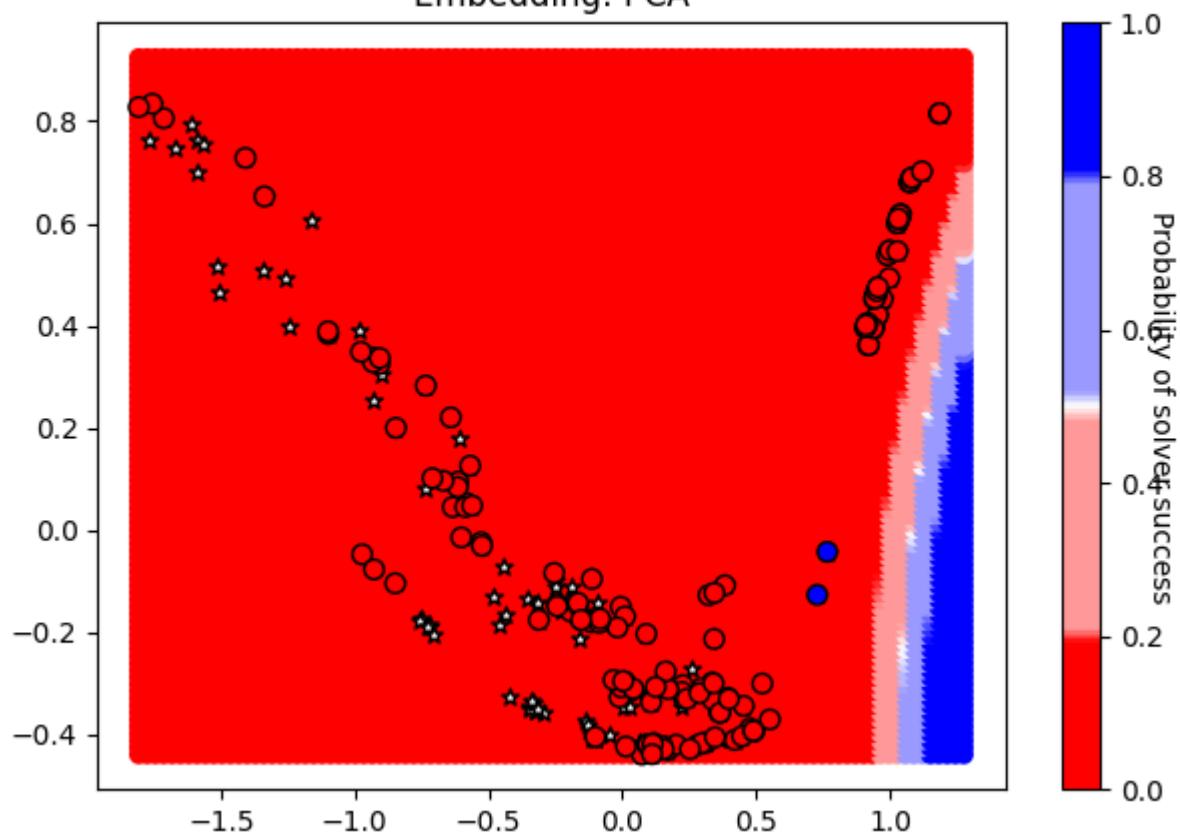
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5d76...

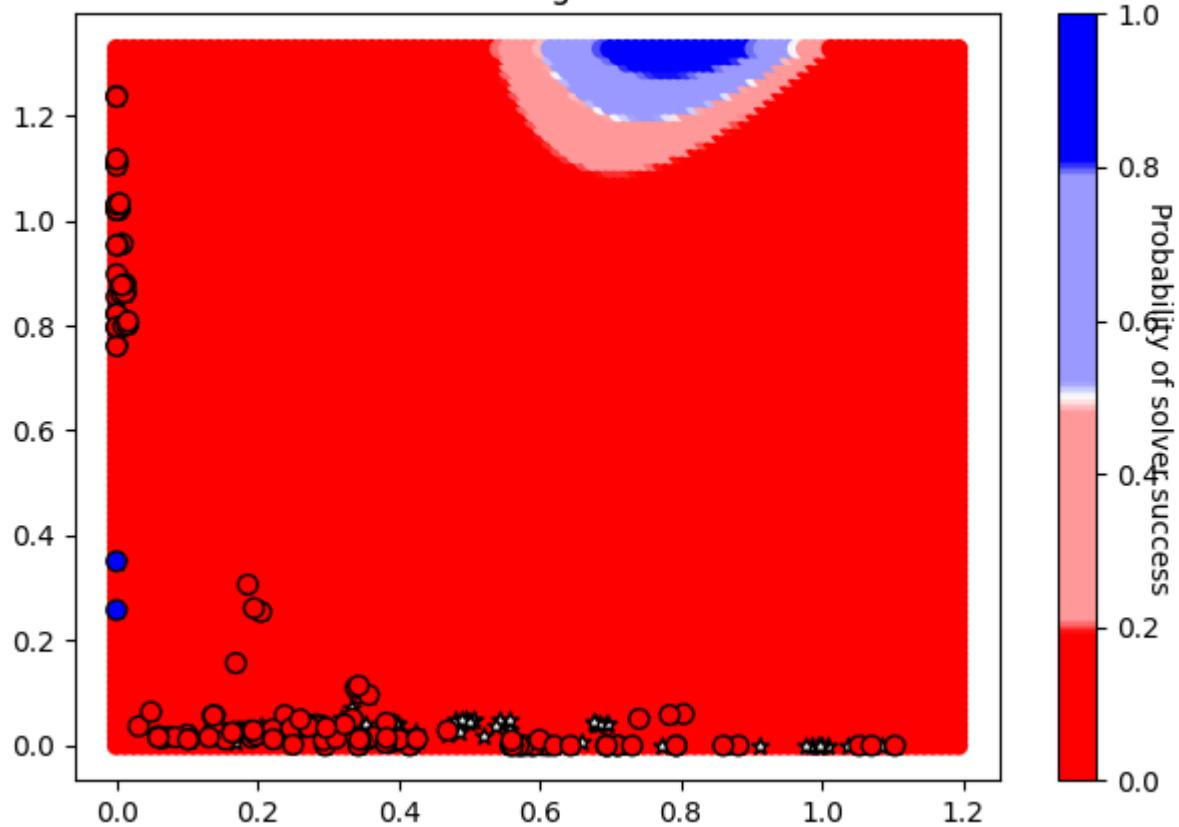
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



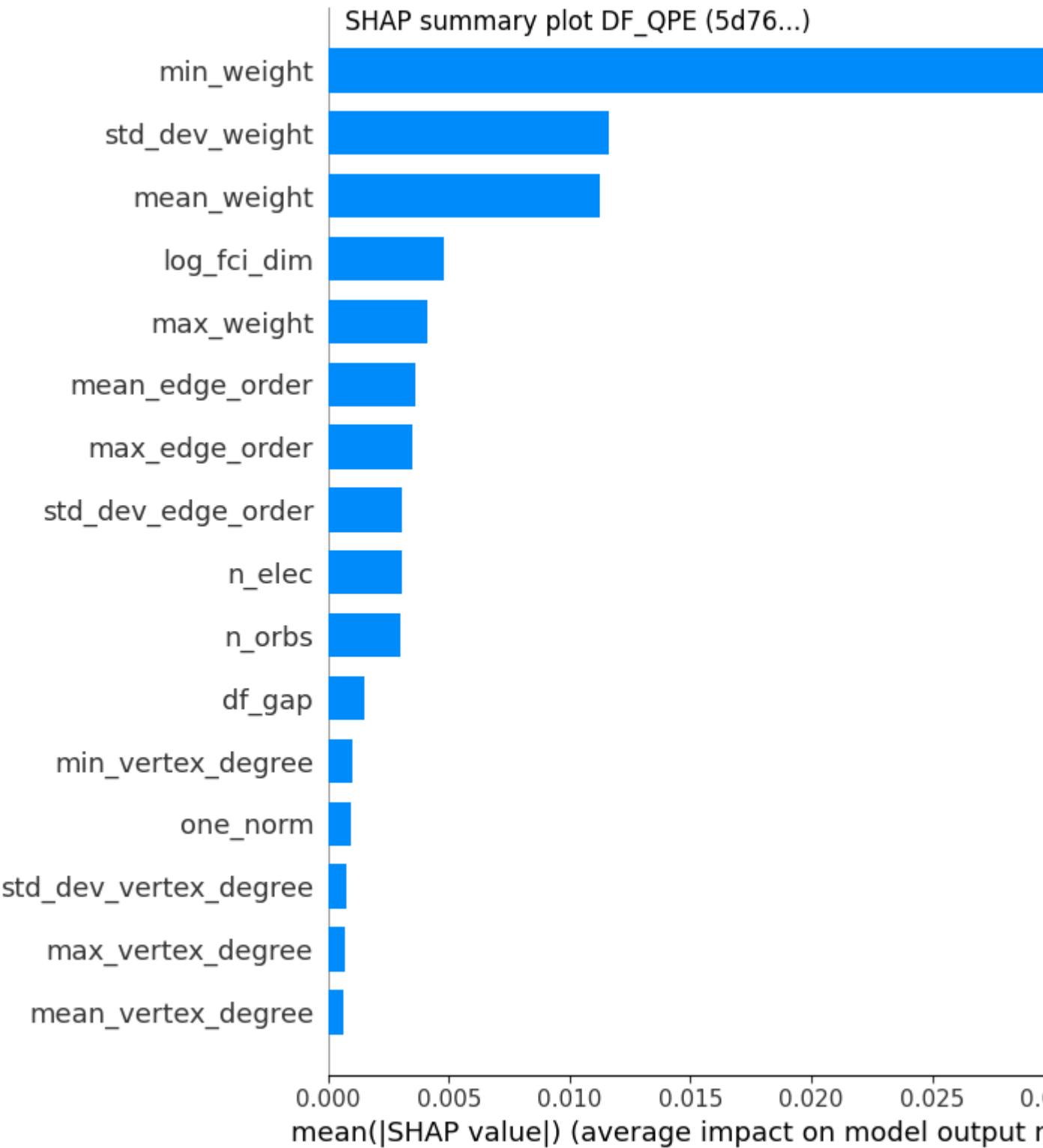
Solver DF_QPE (5d76...)
Embedding: PCA



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: d544e734-d678-4f16-863c-34b9d2084f40

creation_timestamp: 2025-02-24T20:41:03.349036+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

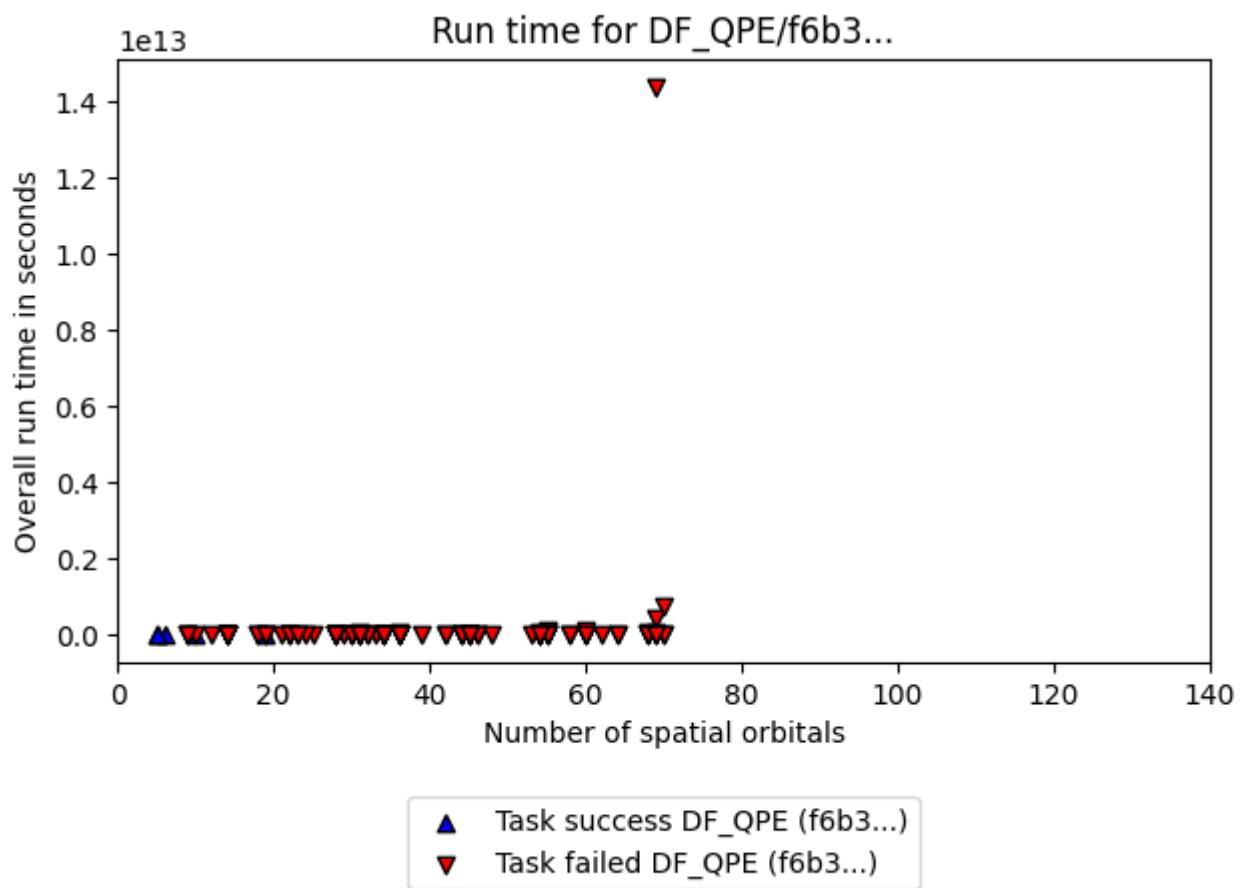
sum_of_run_time_of_attempted_tasks: 16451794516511.004

solvability_ratio: 0.013

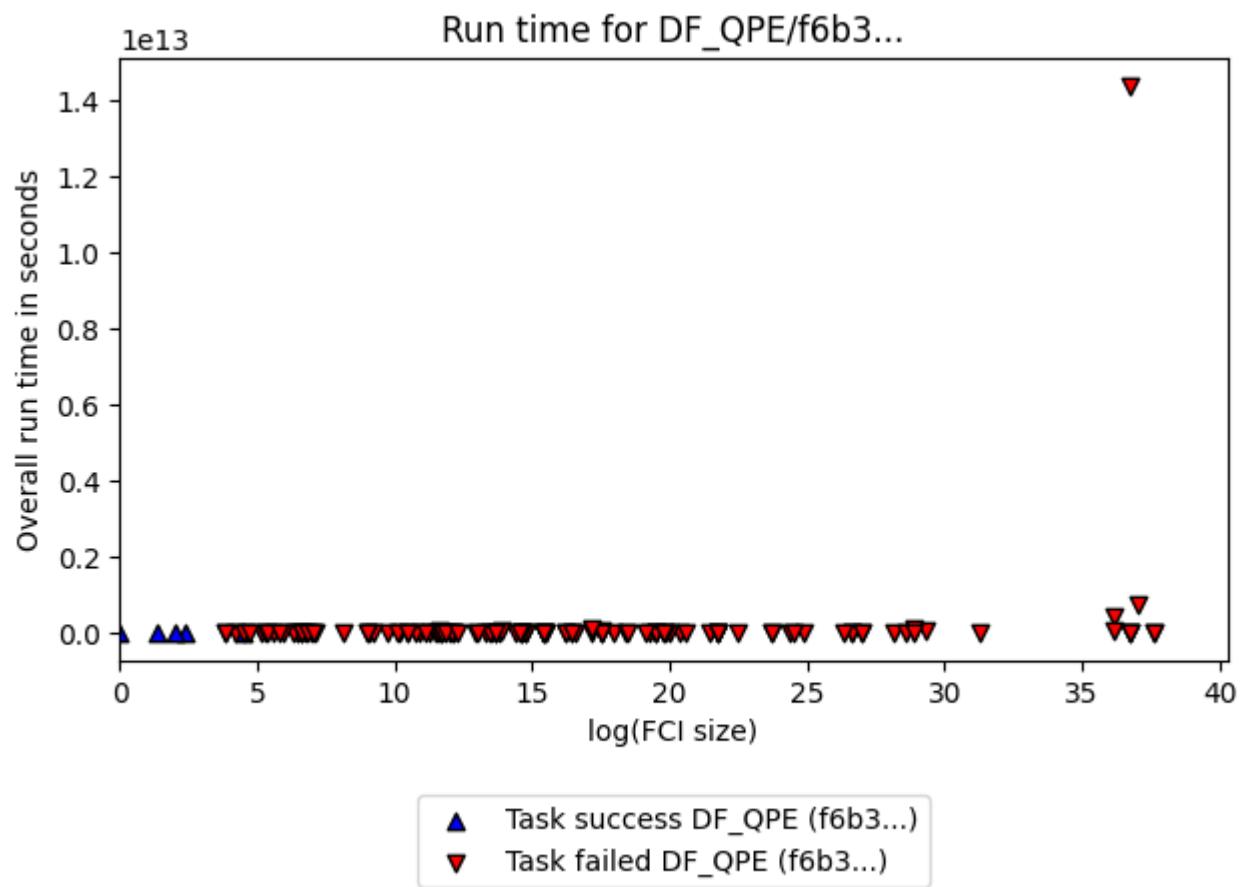
comment: solvability ratio based on PCA embedding.

f1_score: [0.9931972789115646, 0.8333333333333334]

ml_metrics_calculator_version: 1



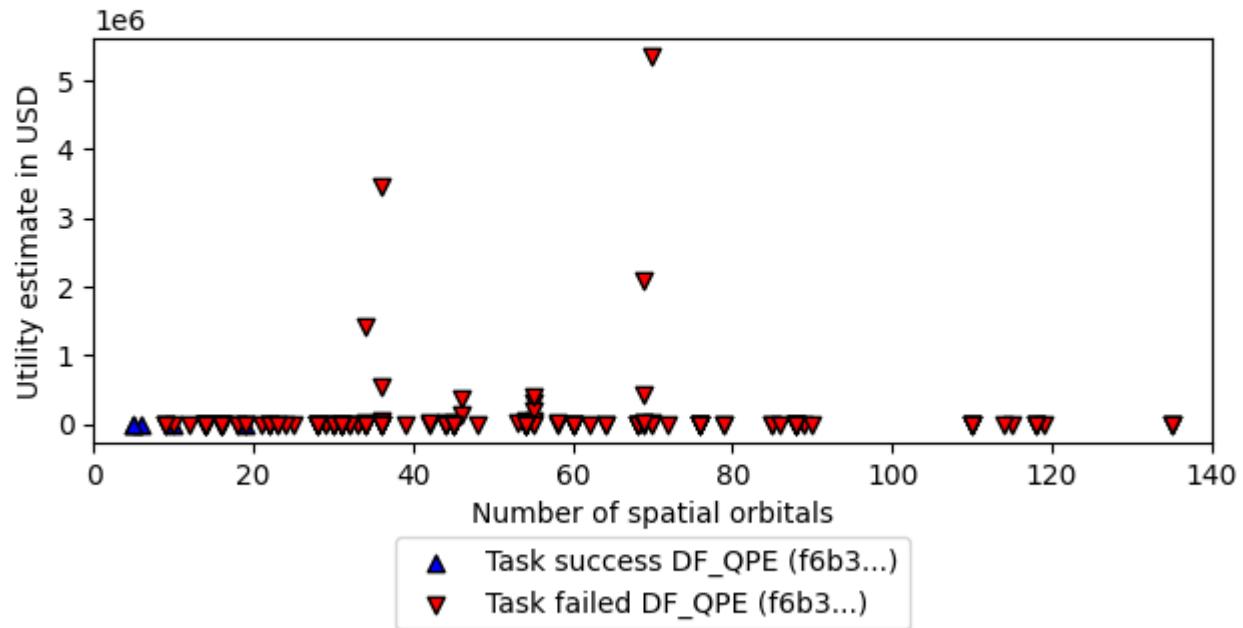
Note: plot only contains attempted tasks.



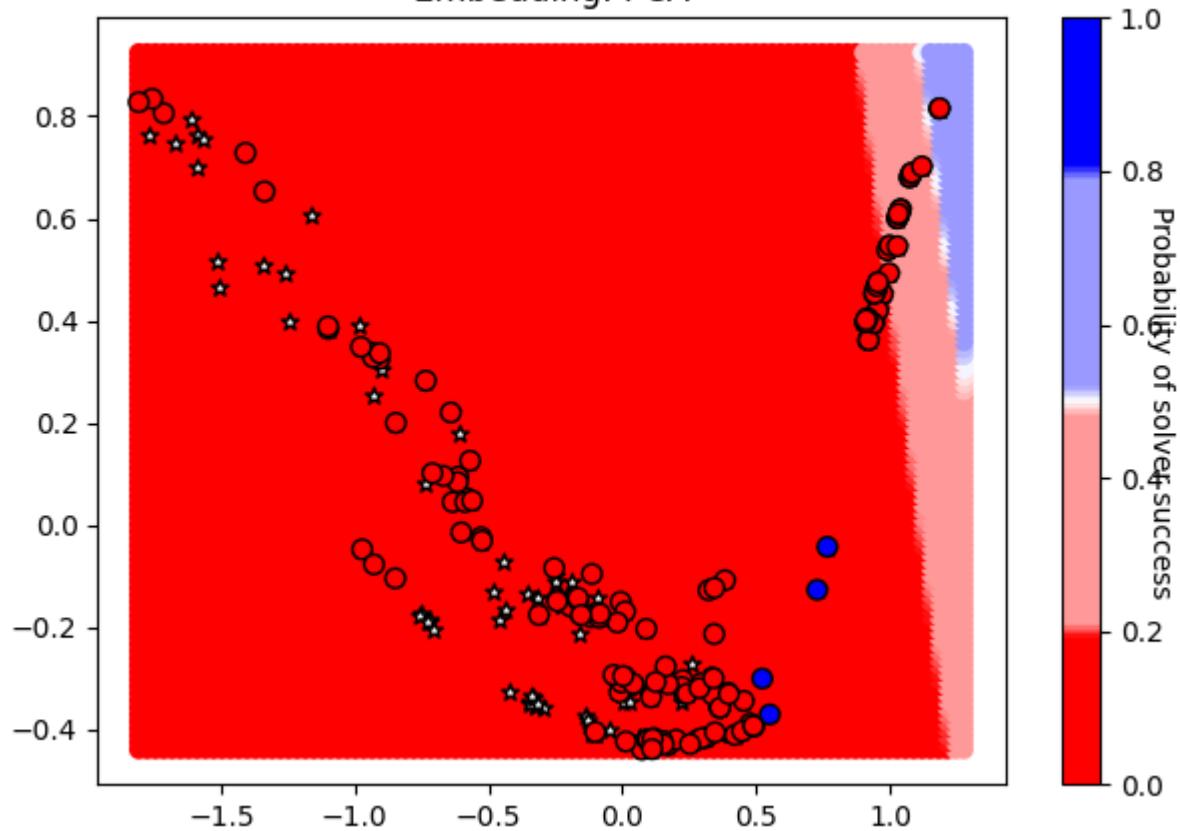
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/f6b3...

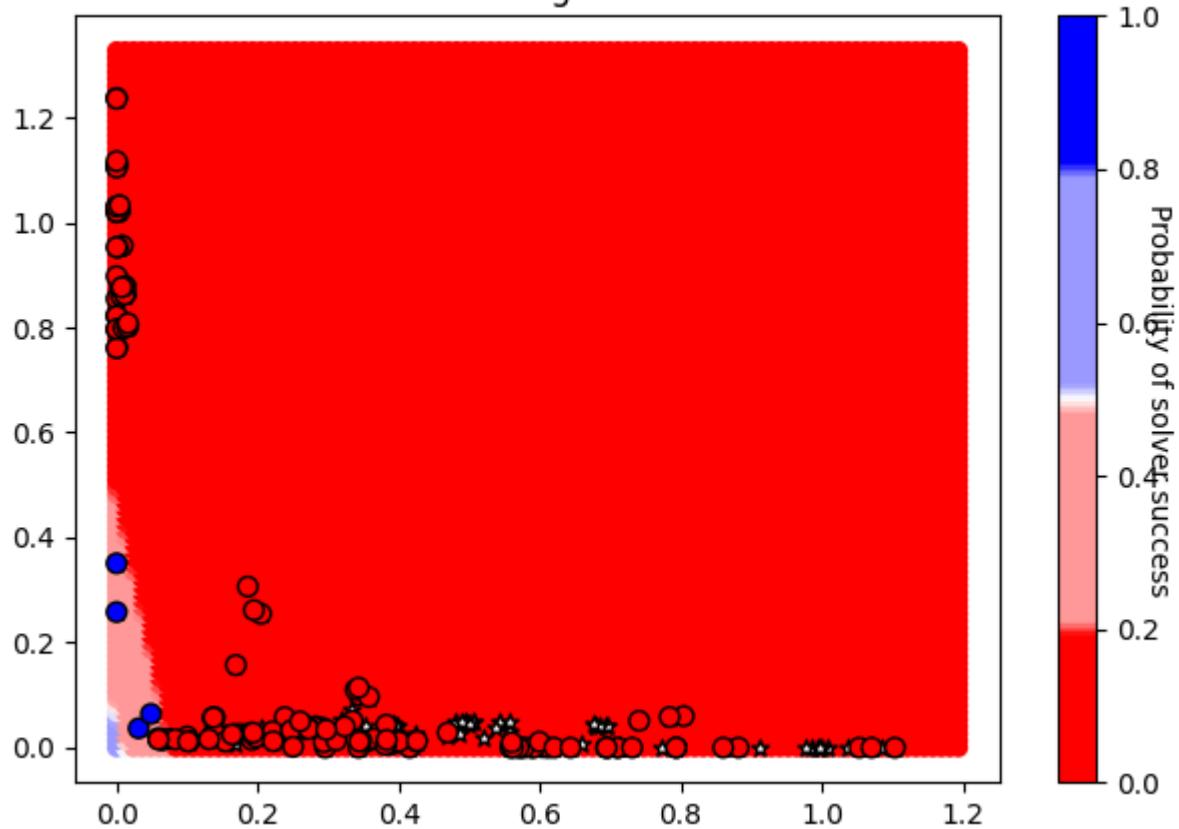
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



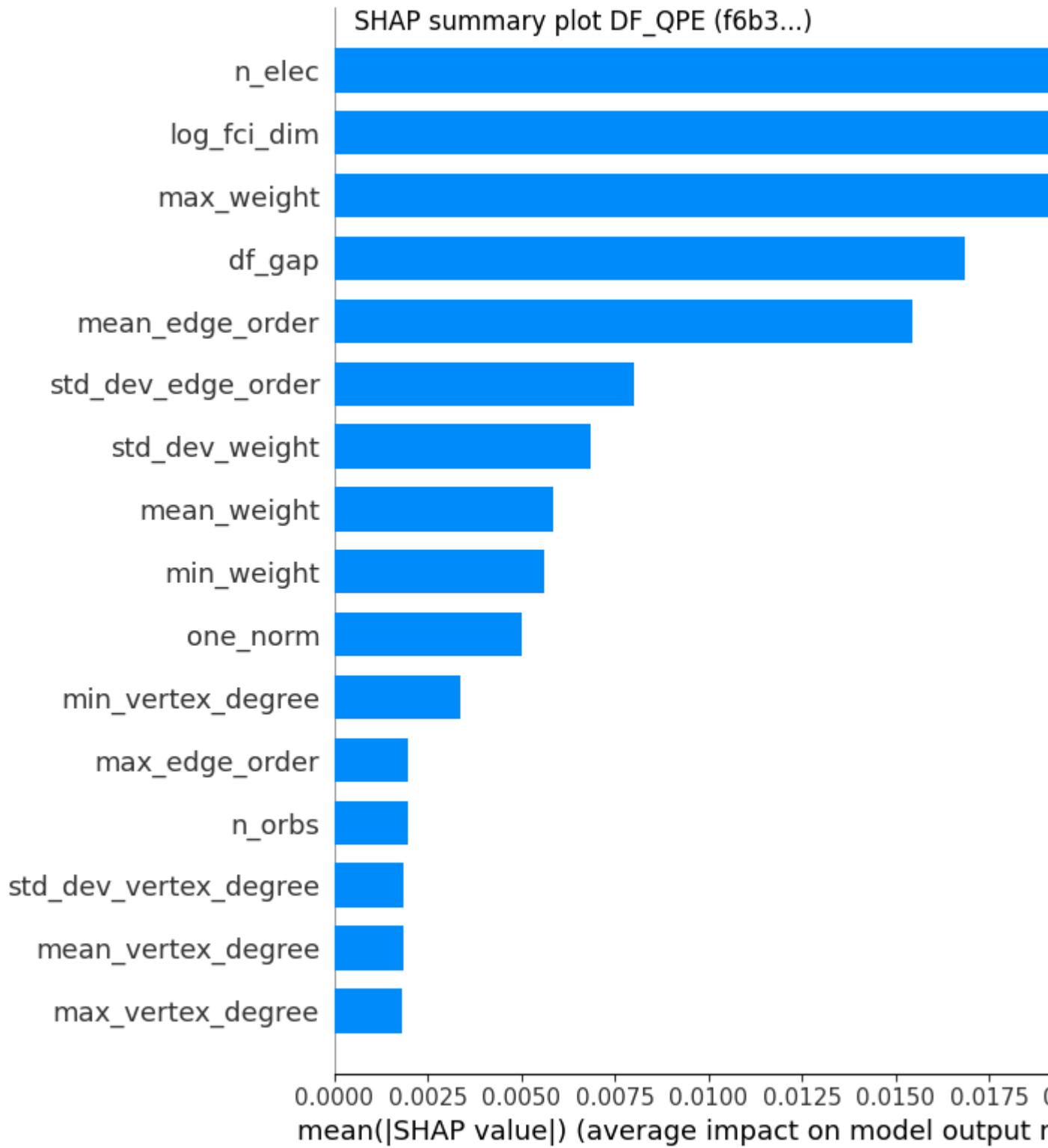
Solver DF_QPE (f6b3...)
Embedding: PCA



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: 9b81e277-8de8-4af2-8ceb-7fa1eb01caa9

creation_timestamp: 2025-02-24T20:41:03.349036+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

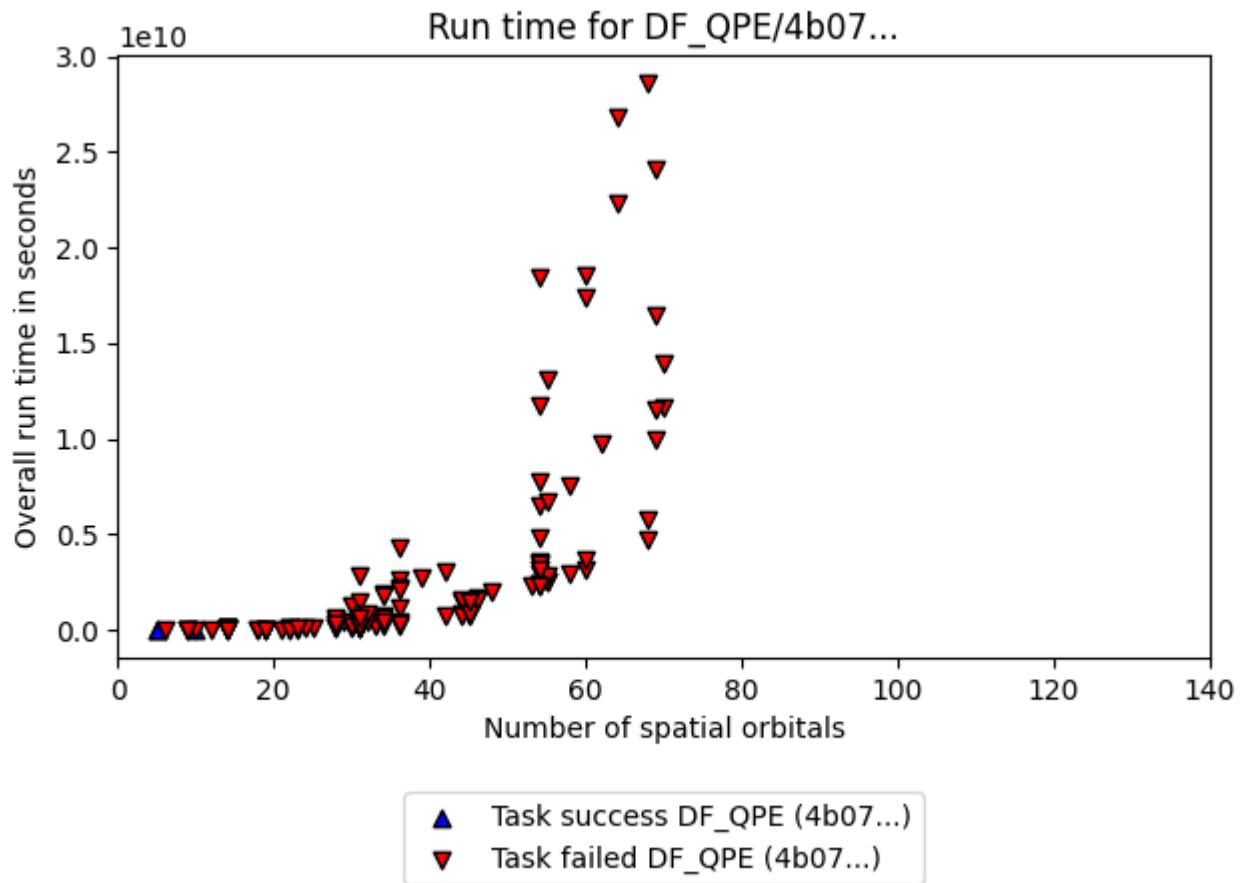
sum_of_run_time_of_attempted_tasks: 407899131893.85156

solvability_ratio: 0.0

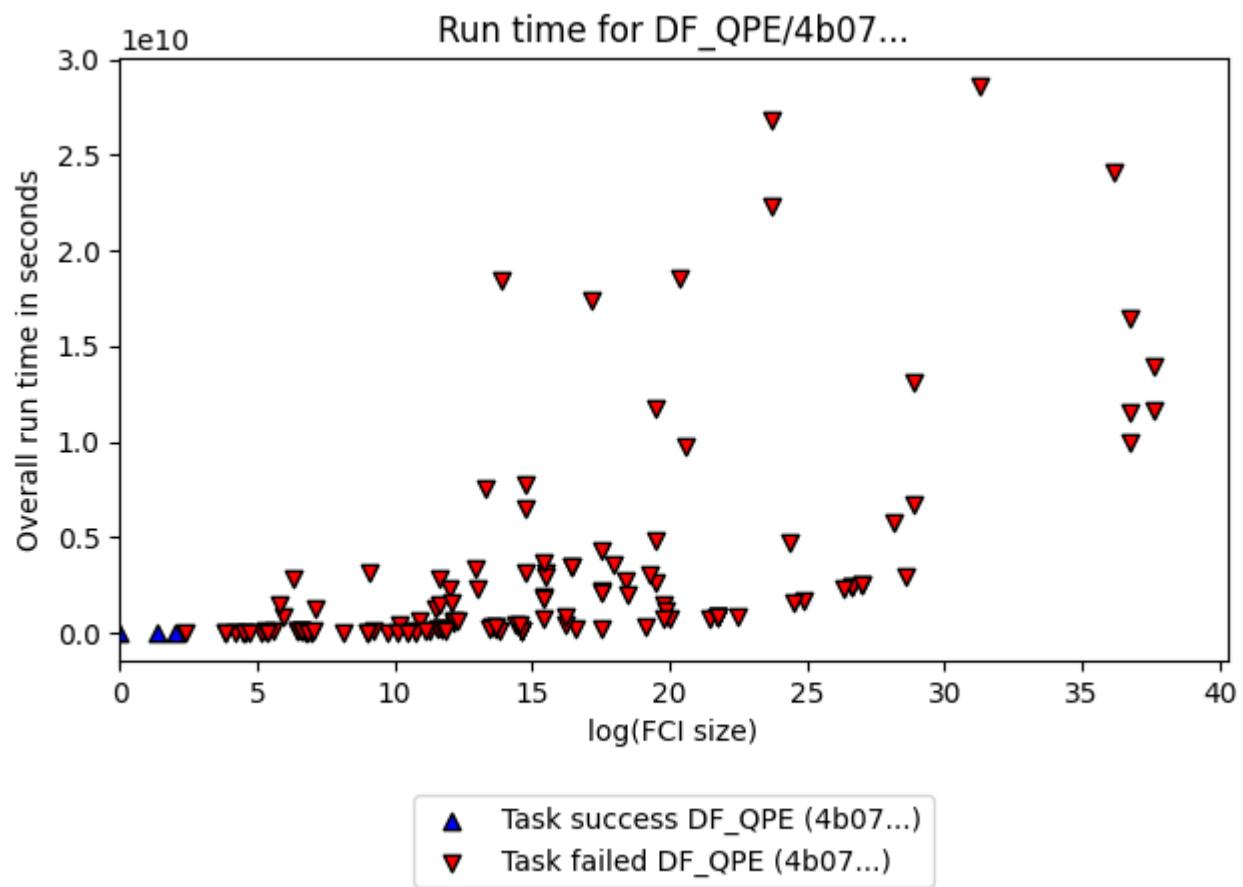
comment: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



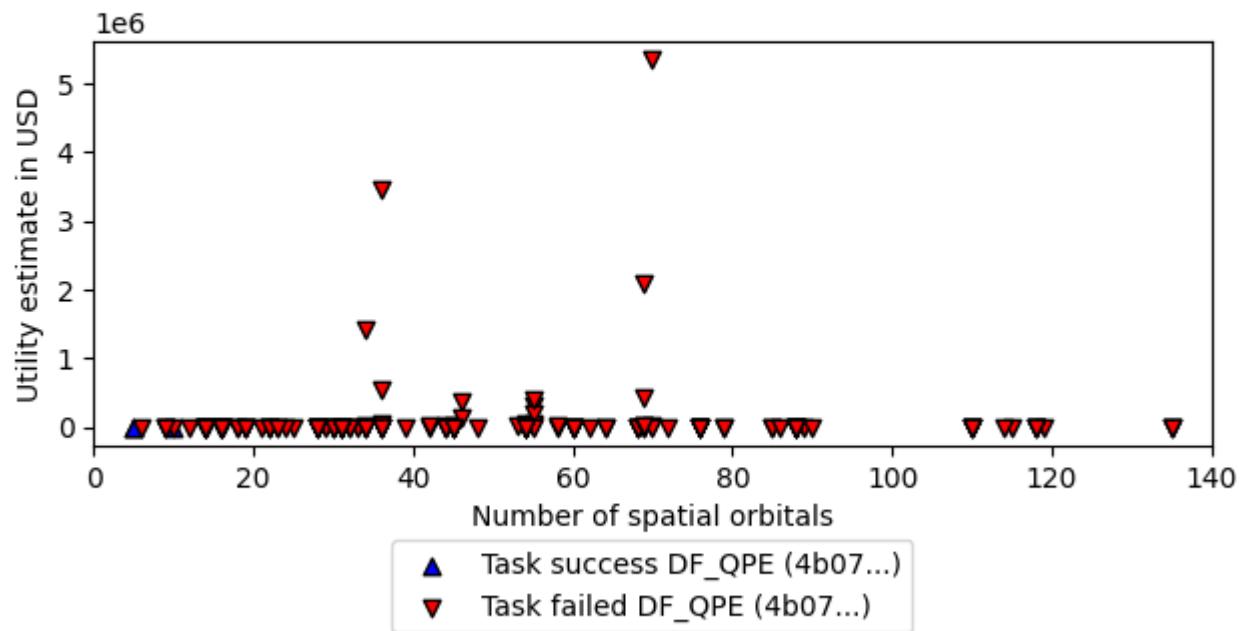
Note: plot only contains attempted tasks.



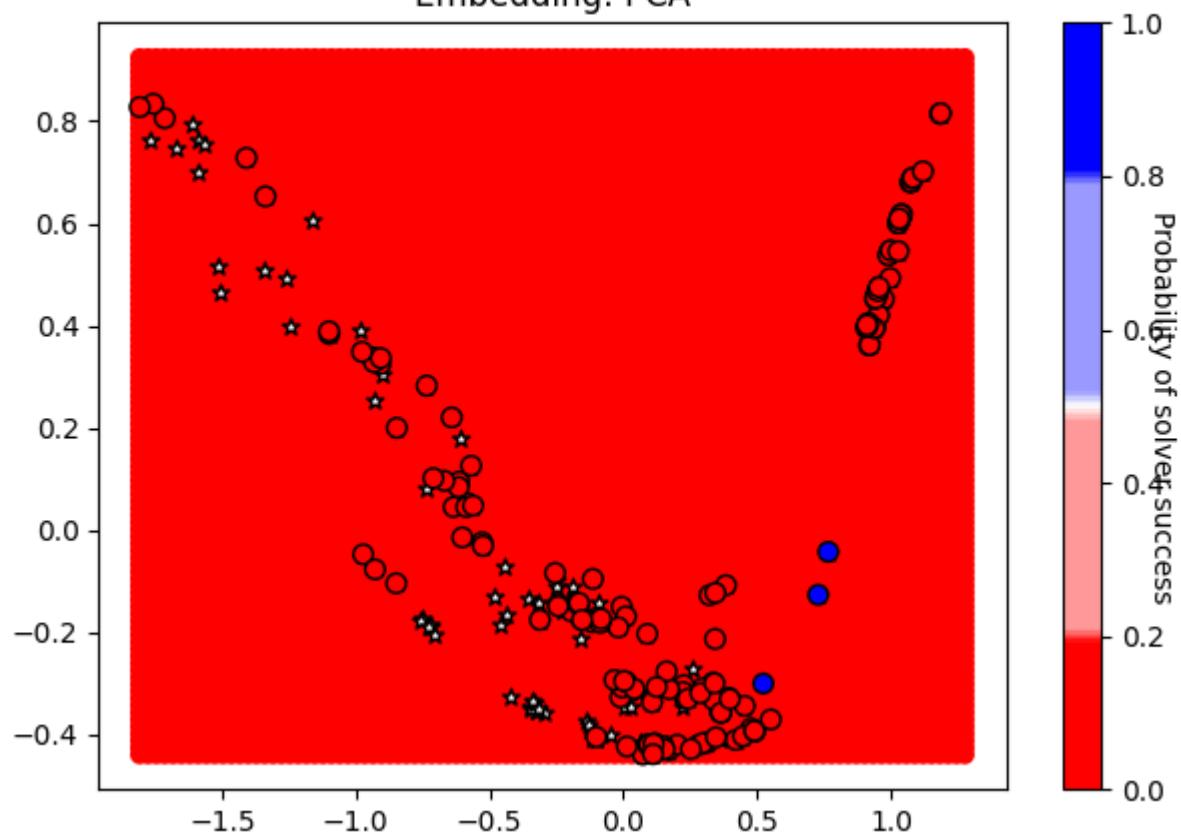
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/4b07...

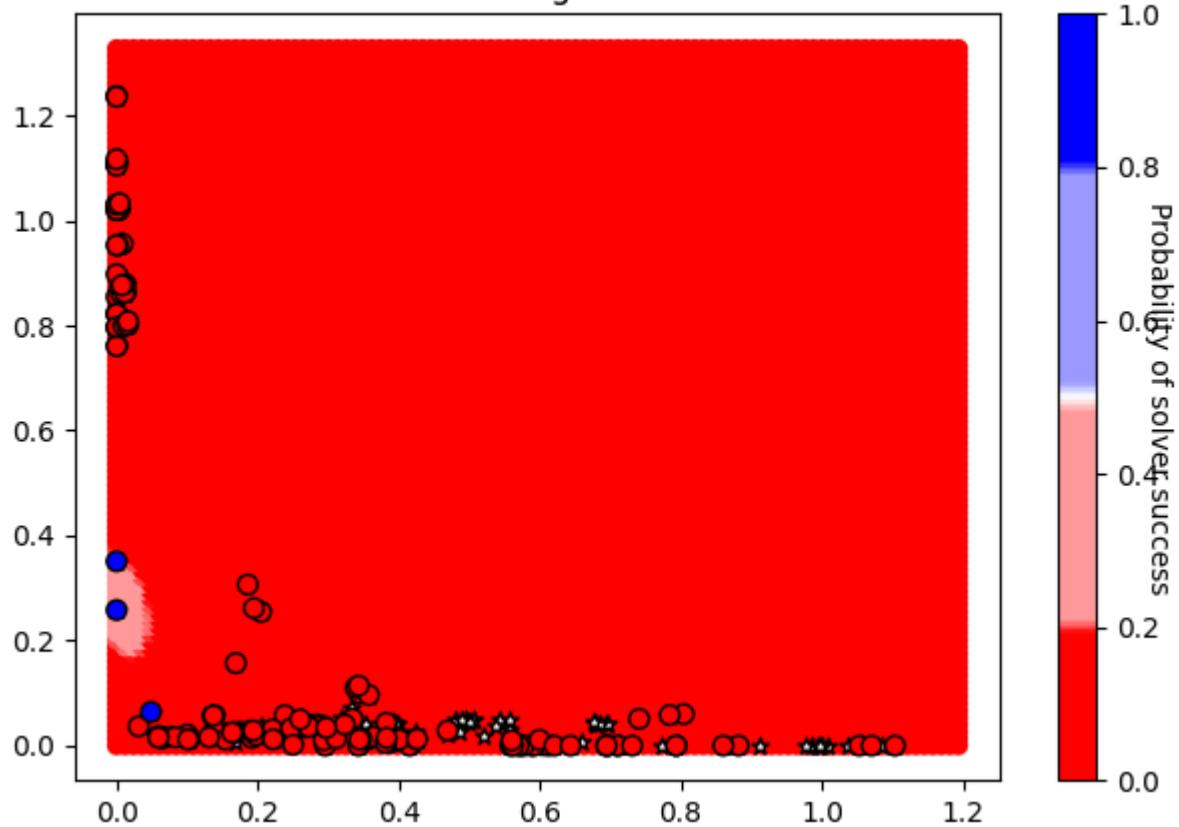
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



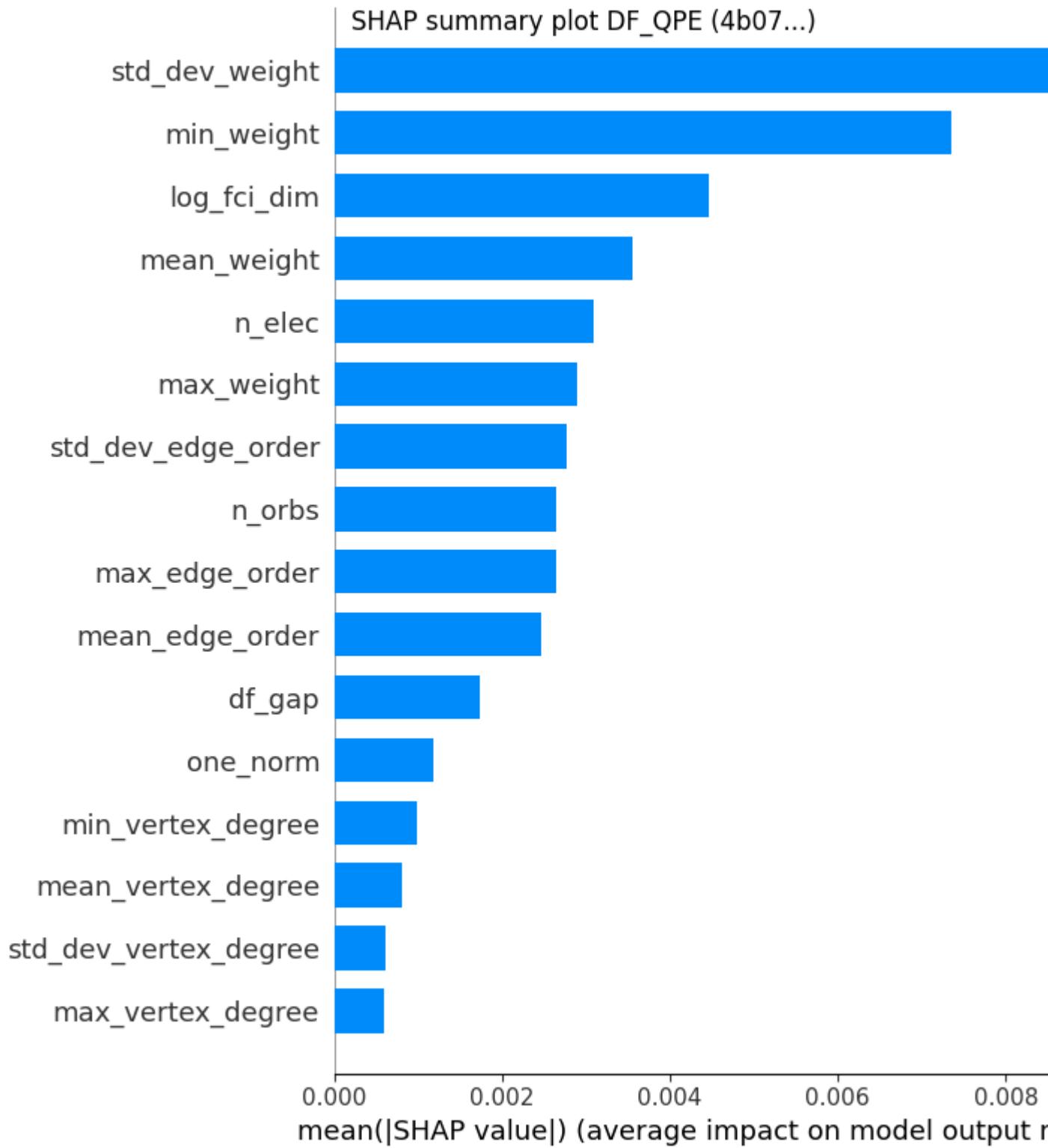
Solver DF_QPE (4b07...)
Embedding: PCA



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.

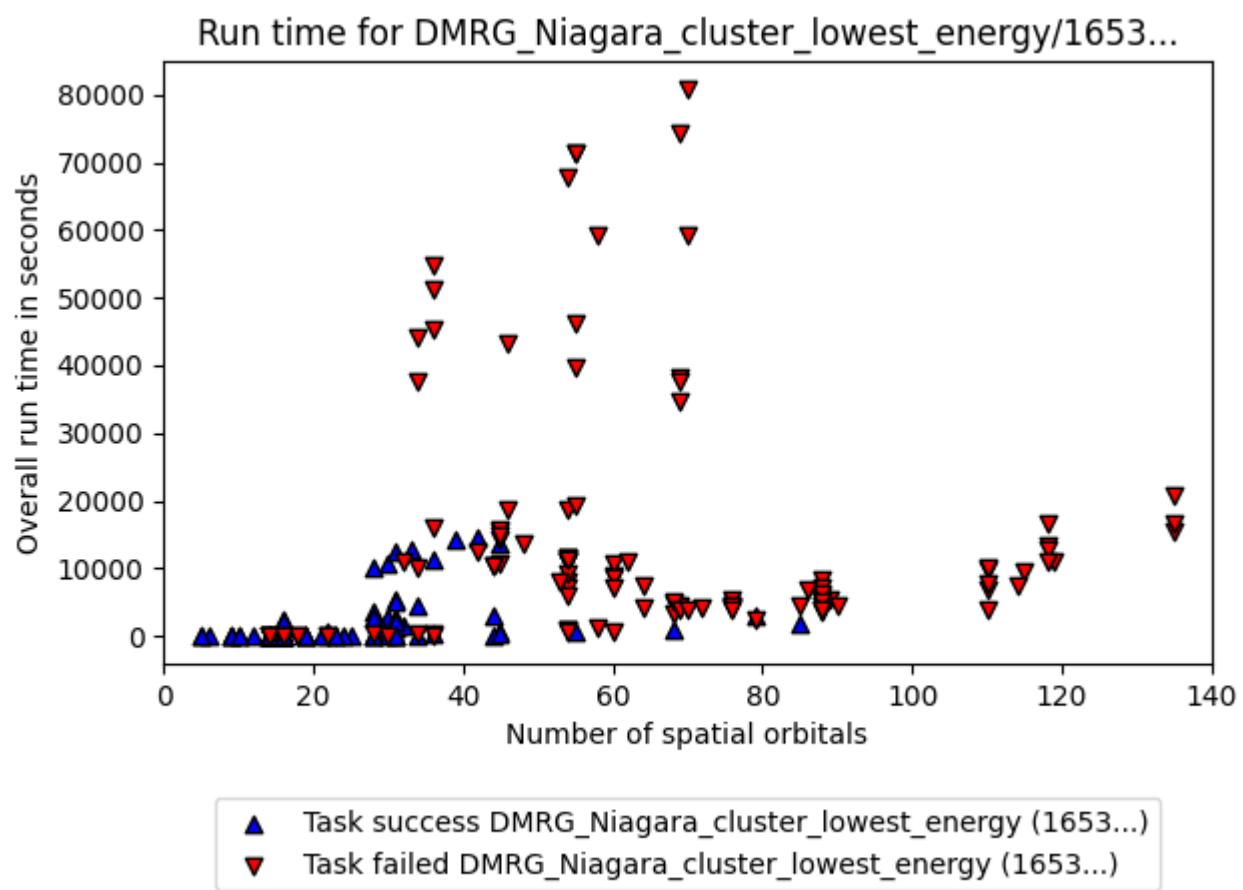


Solver DMRG_Niagara_cluster_lowest_energy, 16537433-9f4c-4eae-a65d-787dc3b35b59

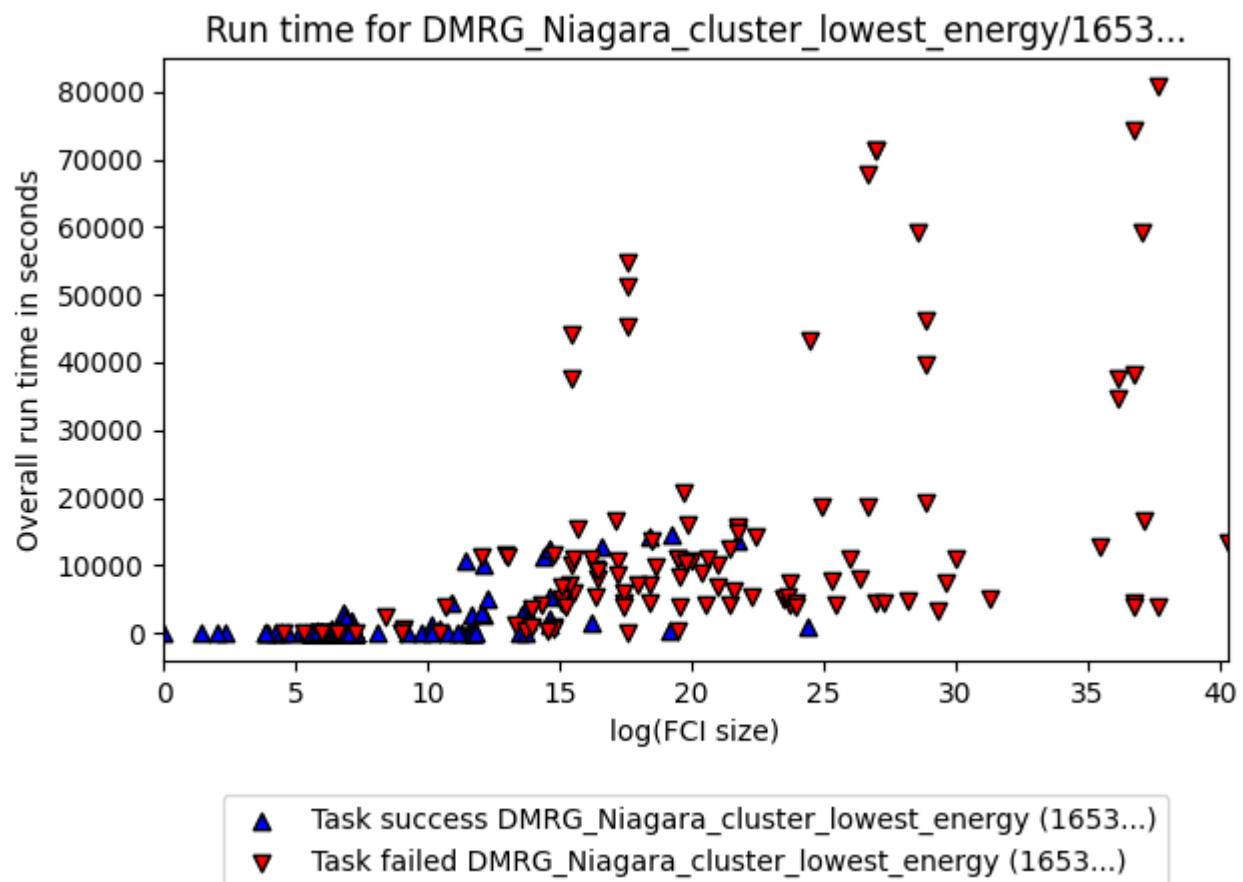
solver_uuid:16537433-9f4c-4eae-a65d-787dc3b35b59

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: 11a3a03a-fddc-439e-b11a-fc185adf19ff
creation_timestamp: 2025-02-24T20:41:03.349036+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



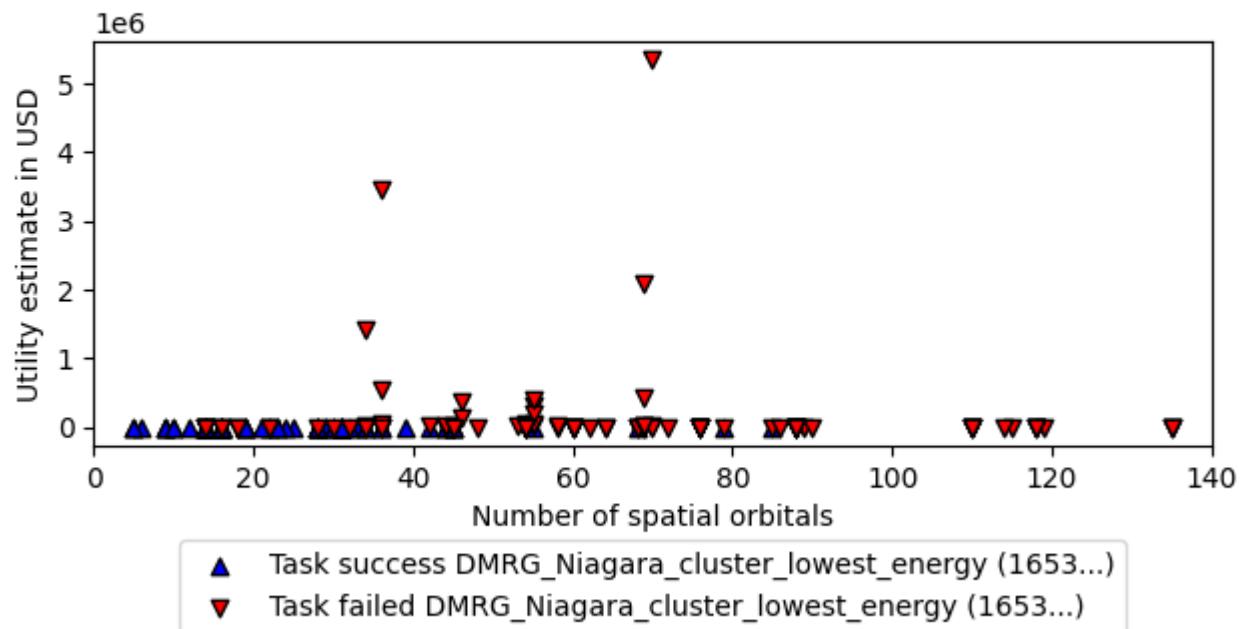
Note: plot only contains attempted tasks.



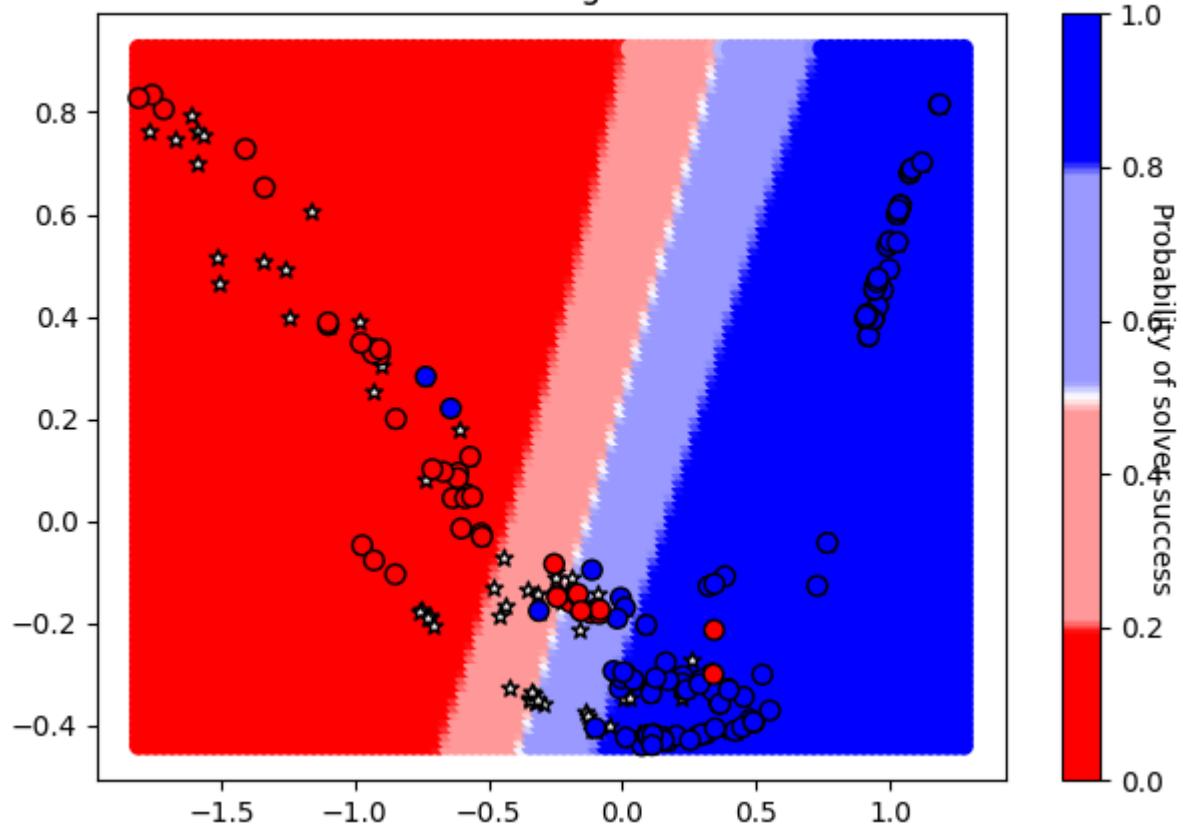
Note: plot only contains attempted tasks.

Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..

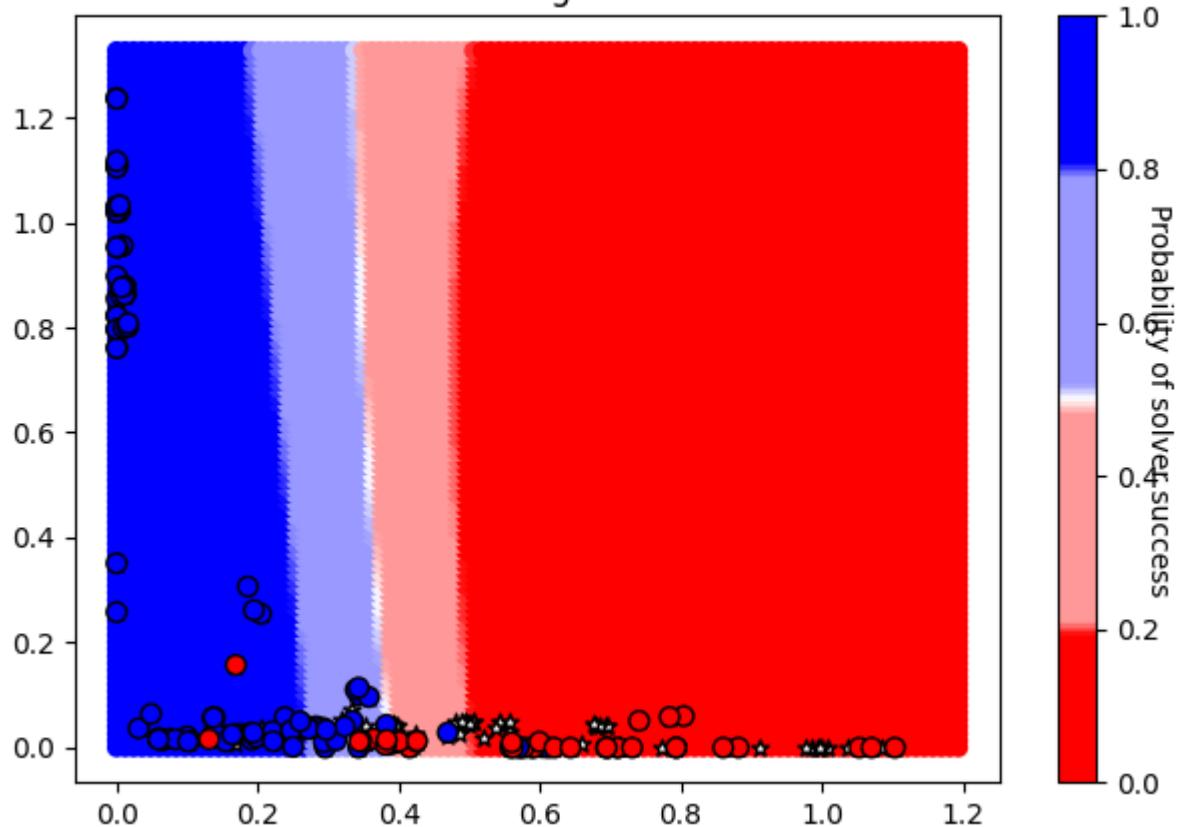
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



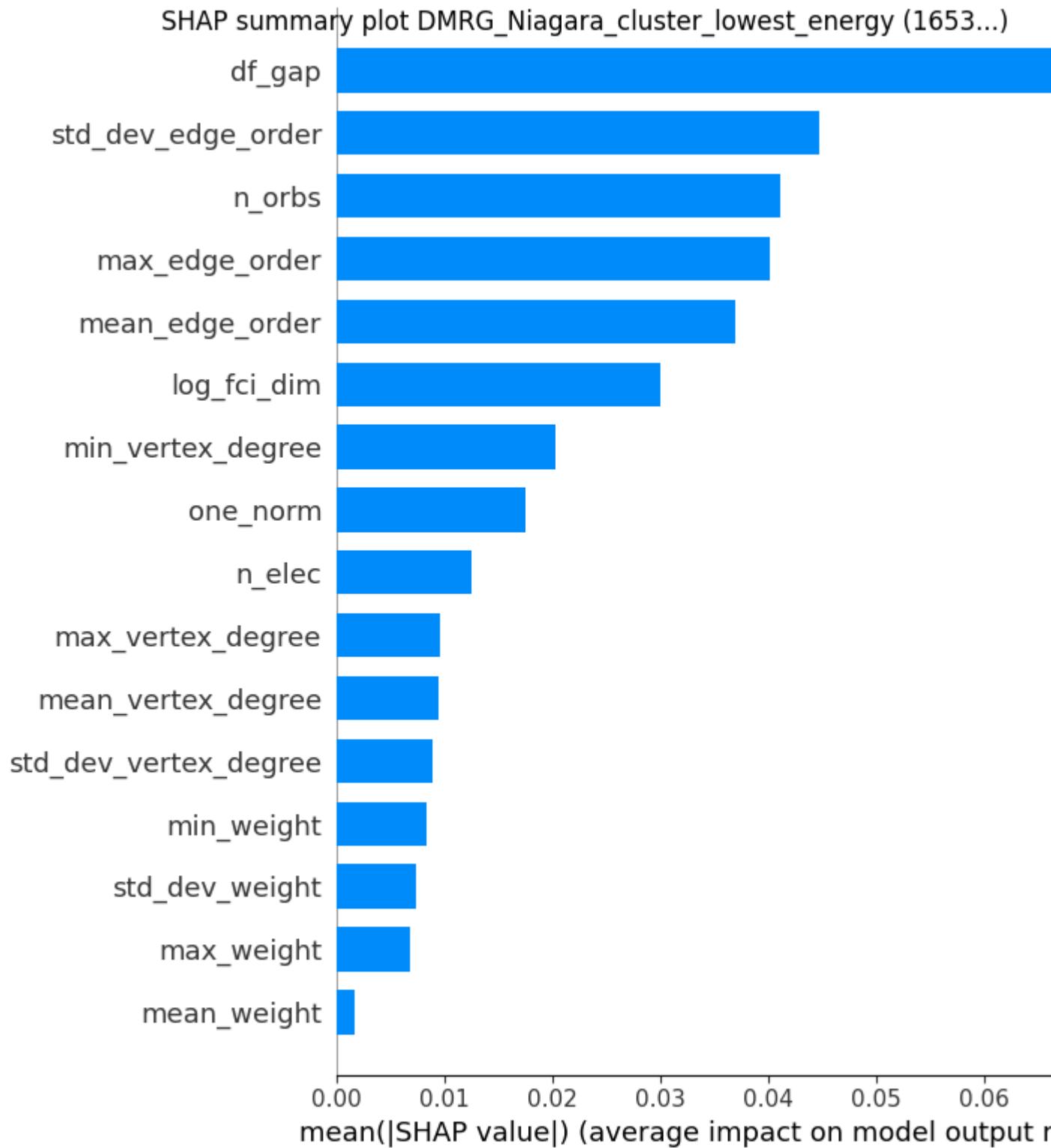
Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: PCA



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.



Solver DF_QPE, 6f385080-934b-4cbb-b813-39c2cb61349e

solver_uuid:6f385080-934b-4cbb-b813-39c2cb61349e

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, as implemented in BenchQ/OpenFermion. 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. Note that the target accuracy is 1 mHa, which is smaller than required by the problem instances.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', '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 that described in https://arxiv.org/abs/2011.03494, but with Litinski factories (Quantum 3, 205 (2019)).', 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.001, 'cycle_time_microseconds': 1}}

logical_resource_estimate_solution_uuid:0b647970-5b30-47f0-bbca-1a83704b9e06

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

performance_metrics_uuid: 7902fb49-8240-42c8-8ac3-93ee3a185fcd

creation_timestamp: 2025-02-24T20:41:03.349036+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 3

number_of_problem_instances_solved: 0

number_of_tasks: 228

number_of_tasks_attempted: 23

number_of_tasks_solved: 0

number_of_tasks_solved_within_run_time_limit: 0

number_of_tasks_solved_within_accuracy_threshold: 23

max_run_time_of_attempted_tasks: 441362513808.82544

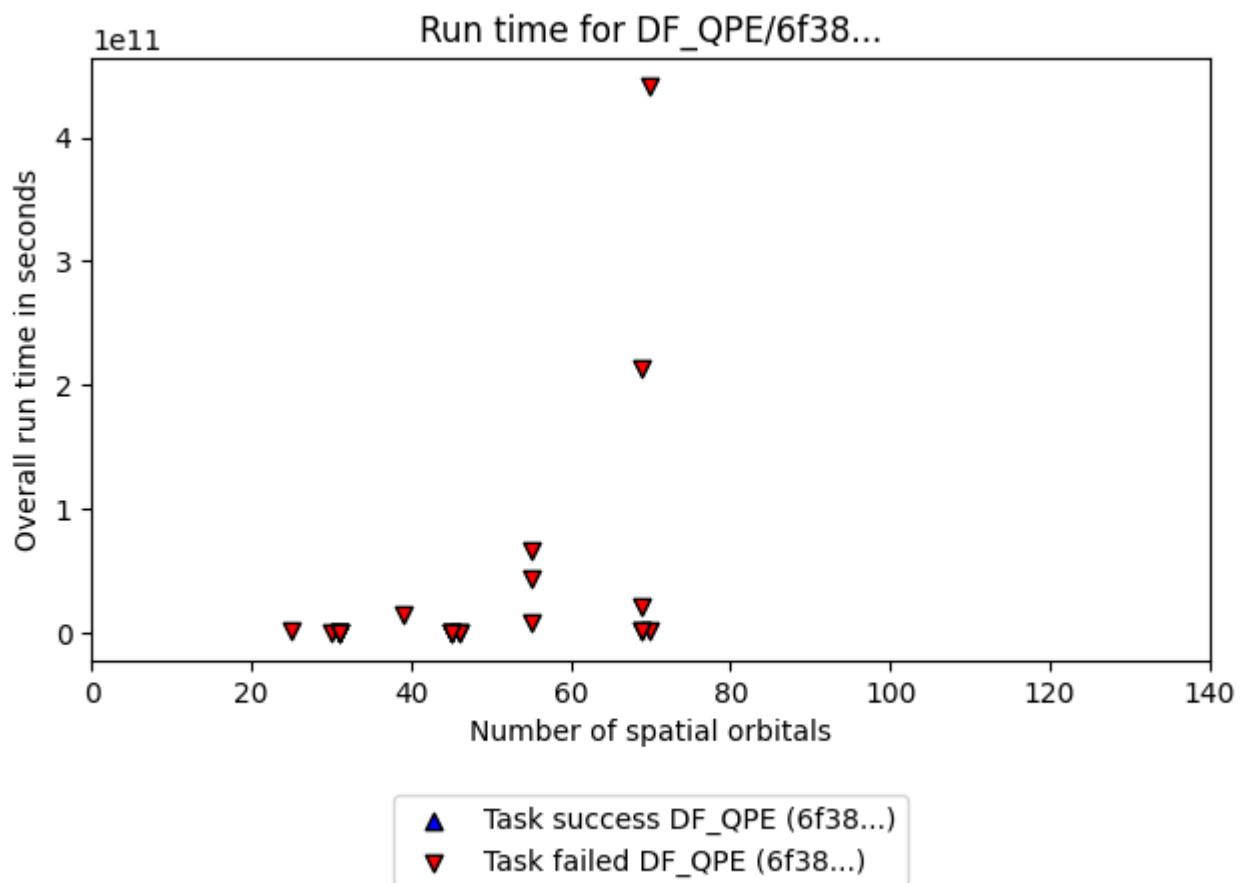
sum_of_run_time_of_attempted_tasks: 819346667619.2955

solvability_ratio: None

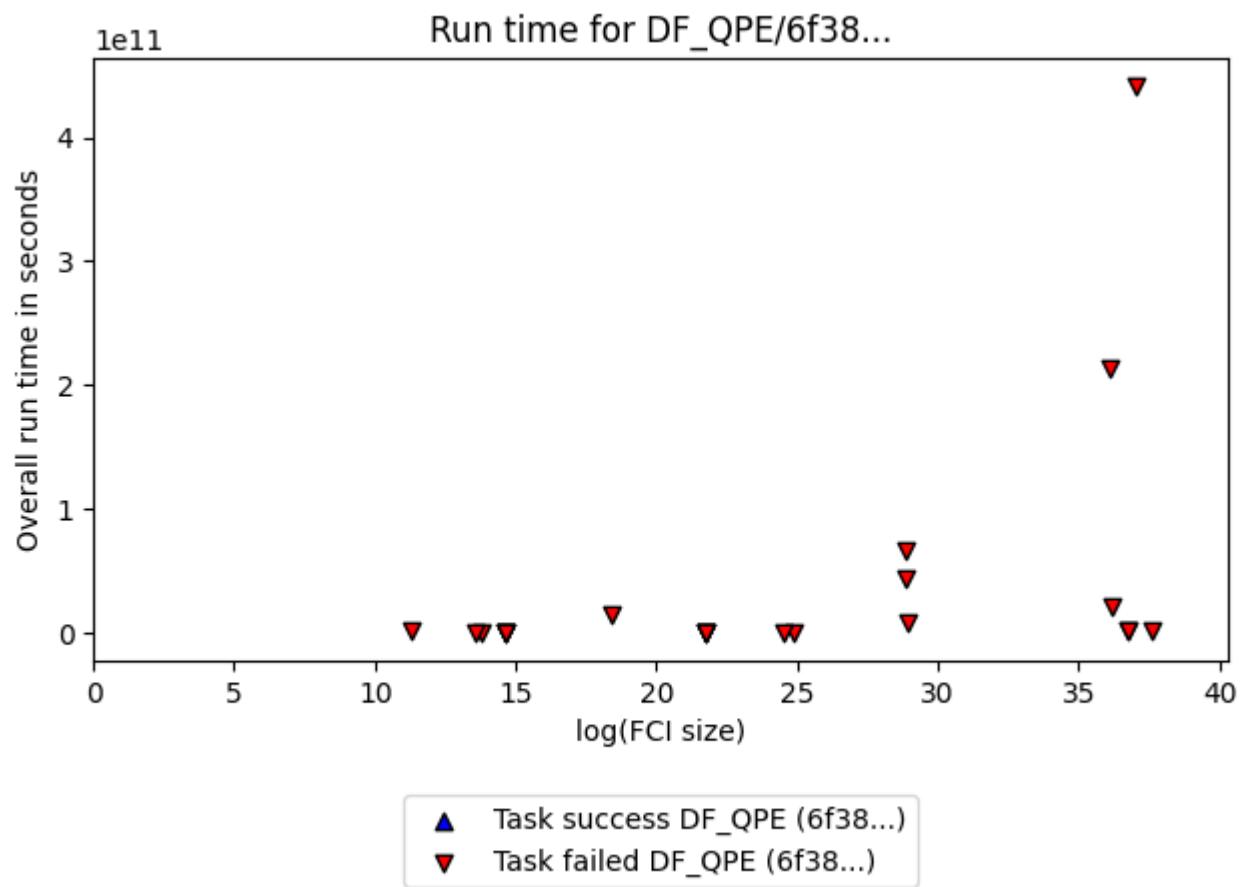
f1_score: None

ml_metrics_calculator_version: 1

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



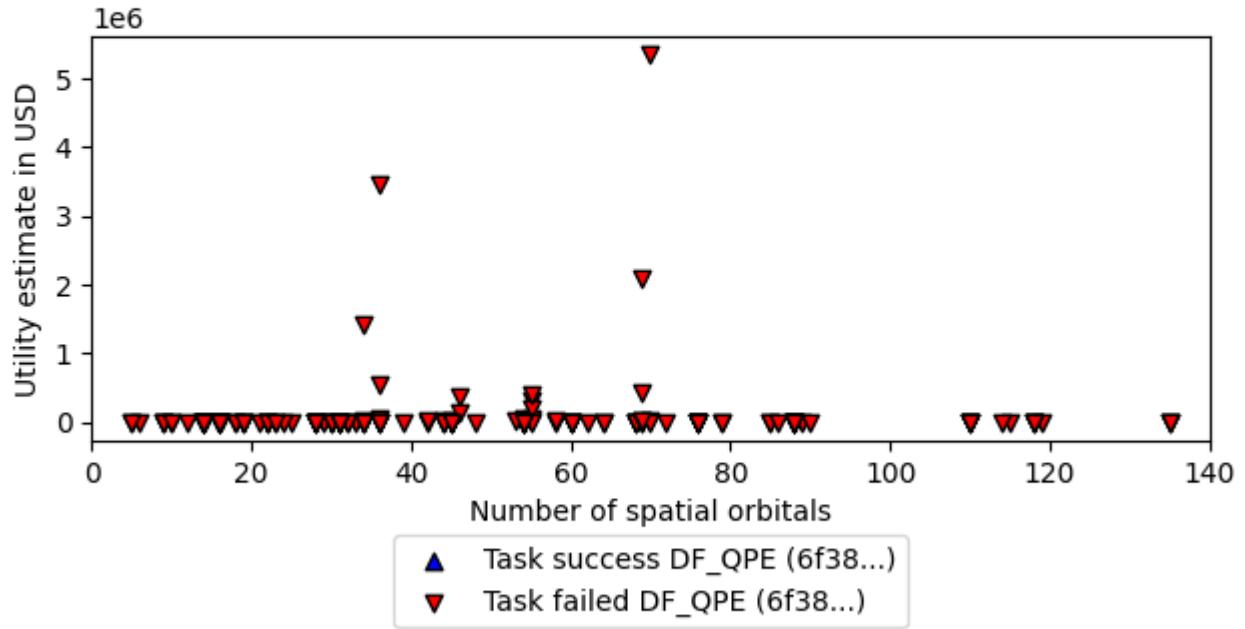
Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/6f38...

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



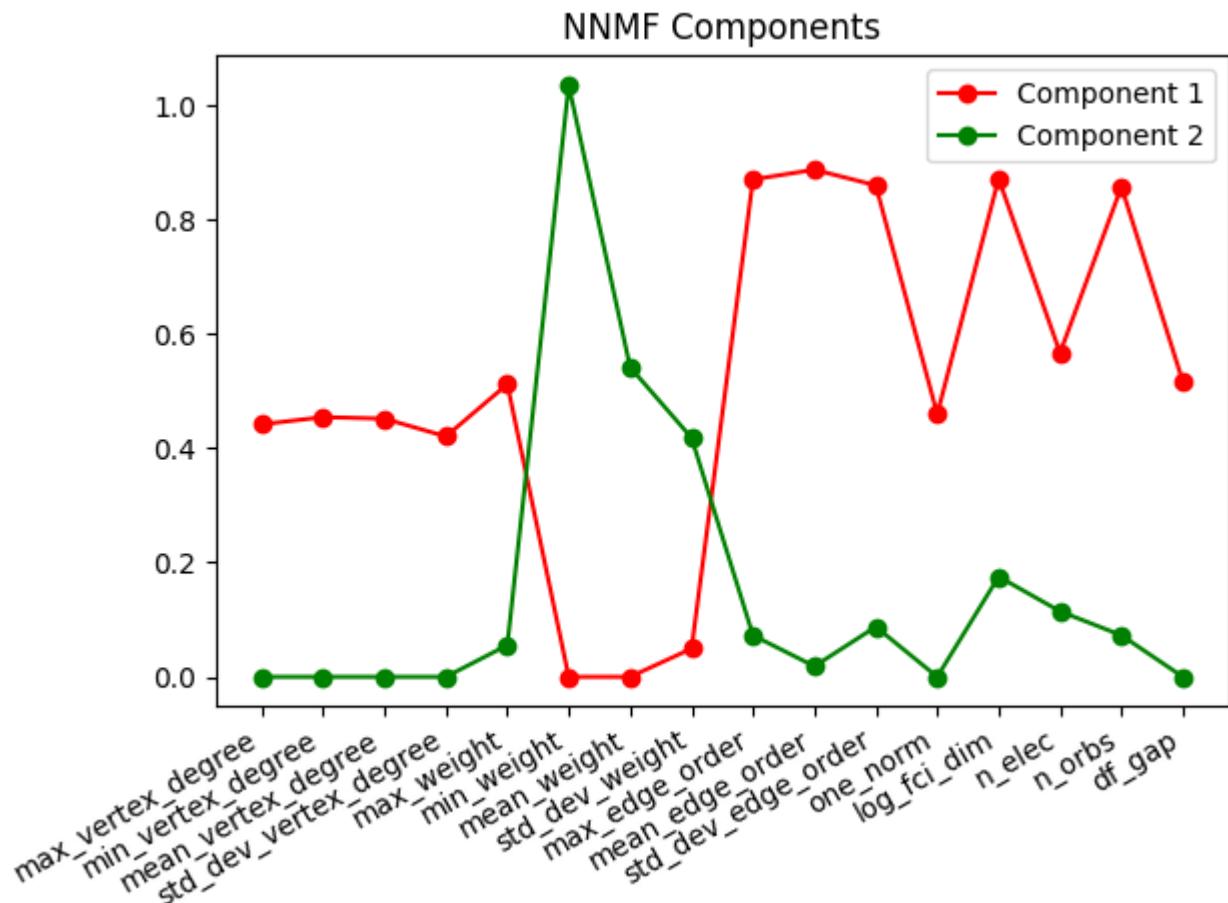
Solver PCA plot

Solver NNMF plot

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

SHAP summary plot

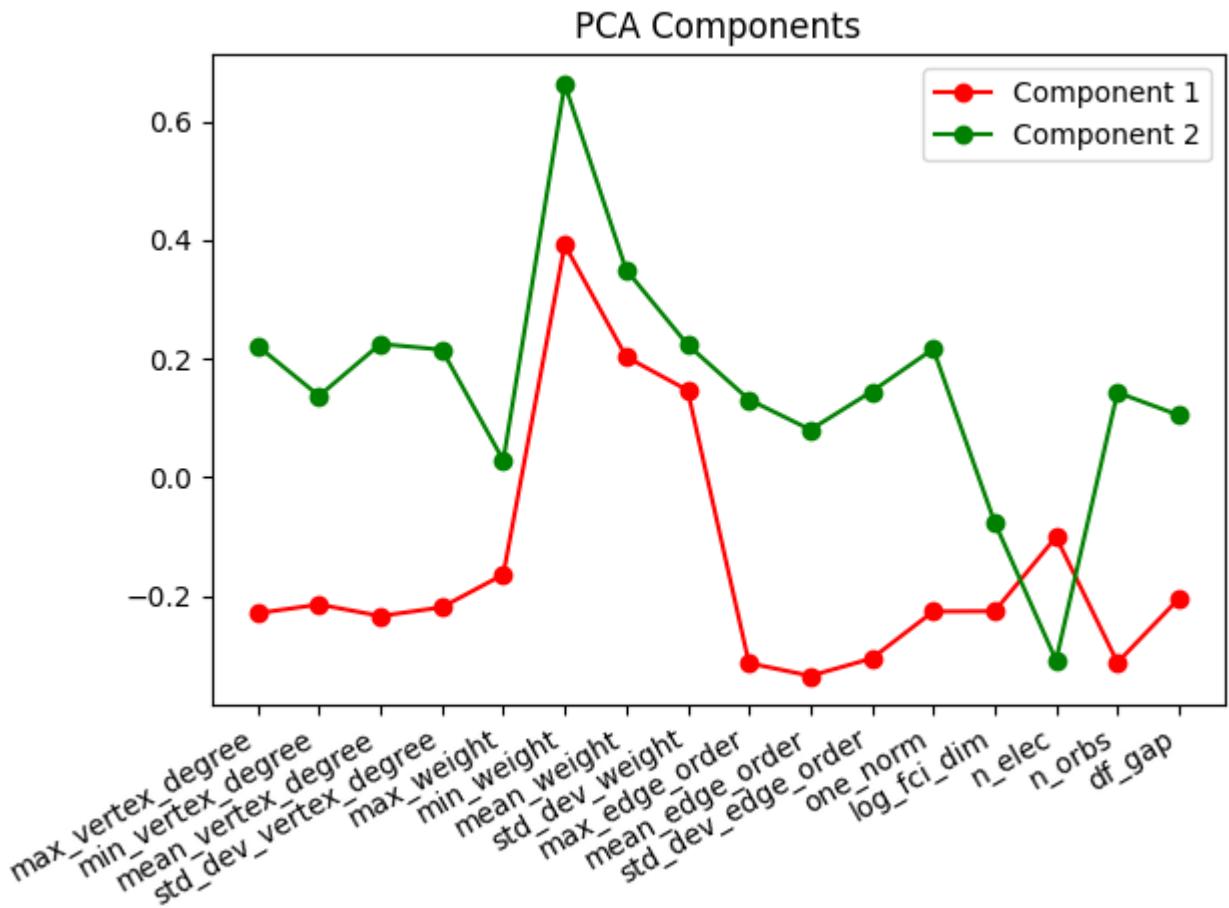
ML Feature Analysis



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.]

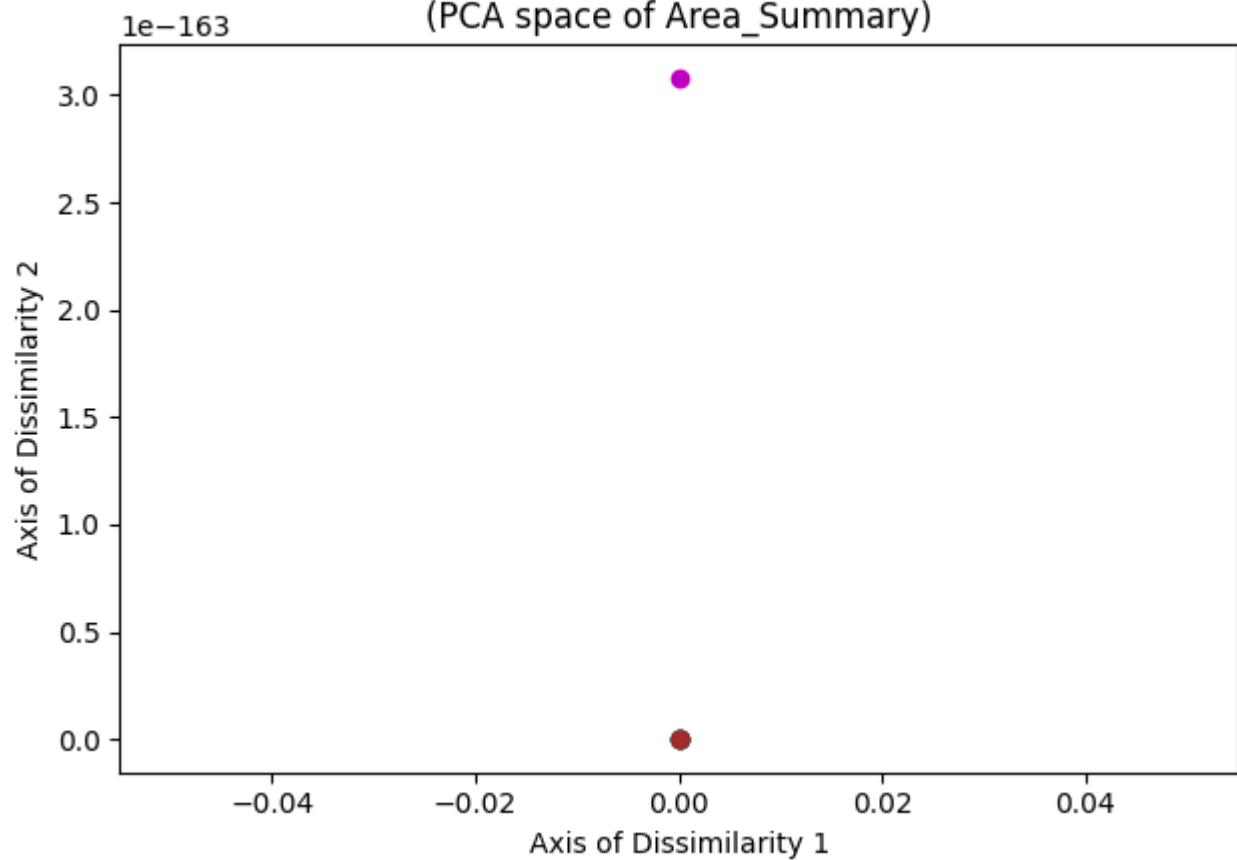


Features: ['max_vertex_degree', 'min_vertex_degree', 'mean_vertex_degree', 'std_dev_vertex_degree', 'max_weight', 'min_weight', 'mean_weight', 'std_dev_weight', 'max_edge_order', 'mean_edge_order', 'std_dev_edge_order', 'one_norm', 'log_fci_dim', 'n_elec', 'n_orbs', 'df_gap']

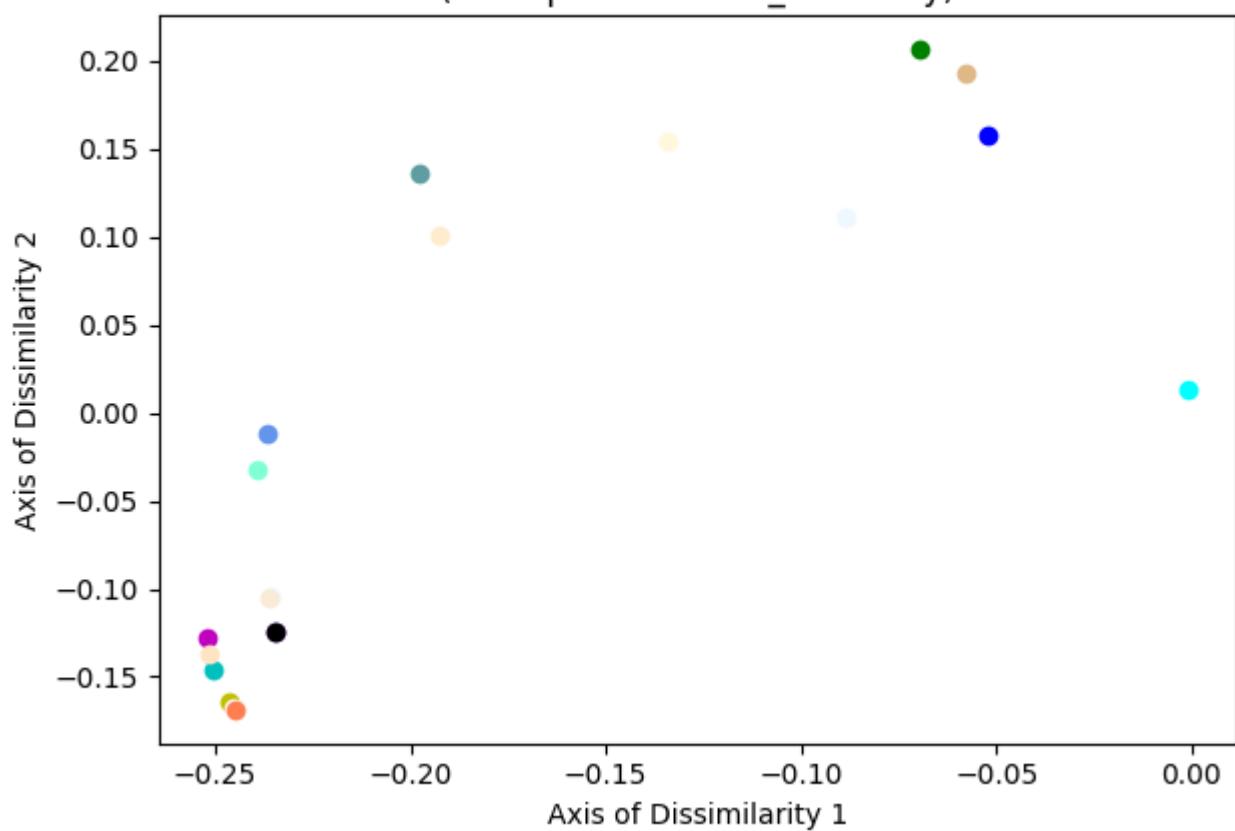
PCA Component 1: [-0.22922229 -0.21461603 -0.23398401 -0.21923522
 -0.16402432 0.39183587 0.20302013 0.14659357 -0.3134204 -0.33485059
 -0.30553226 -0.22630863 -0.2258685 -0.10070305 -0.31226268
 -0.20457232]

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]

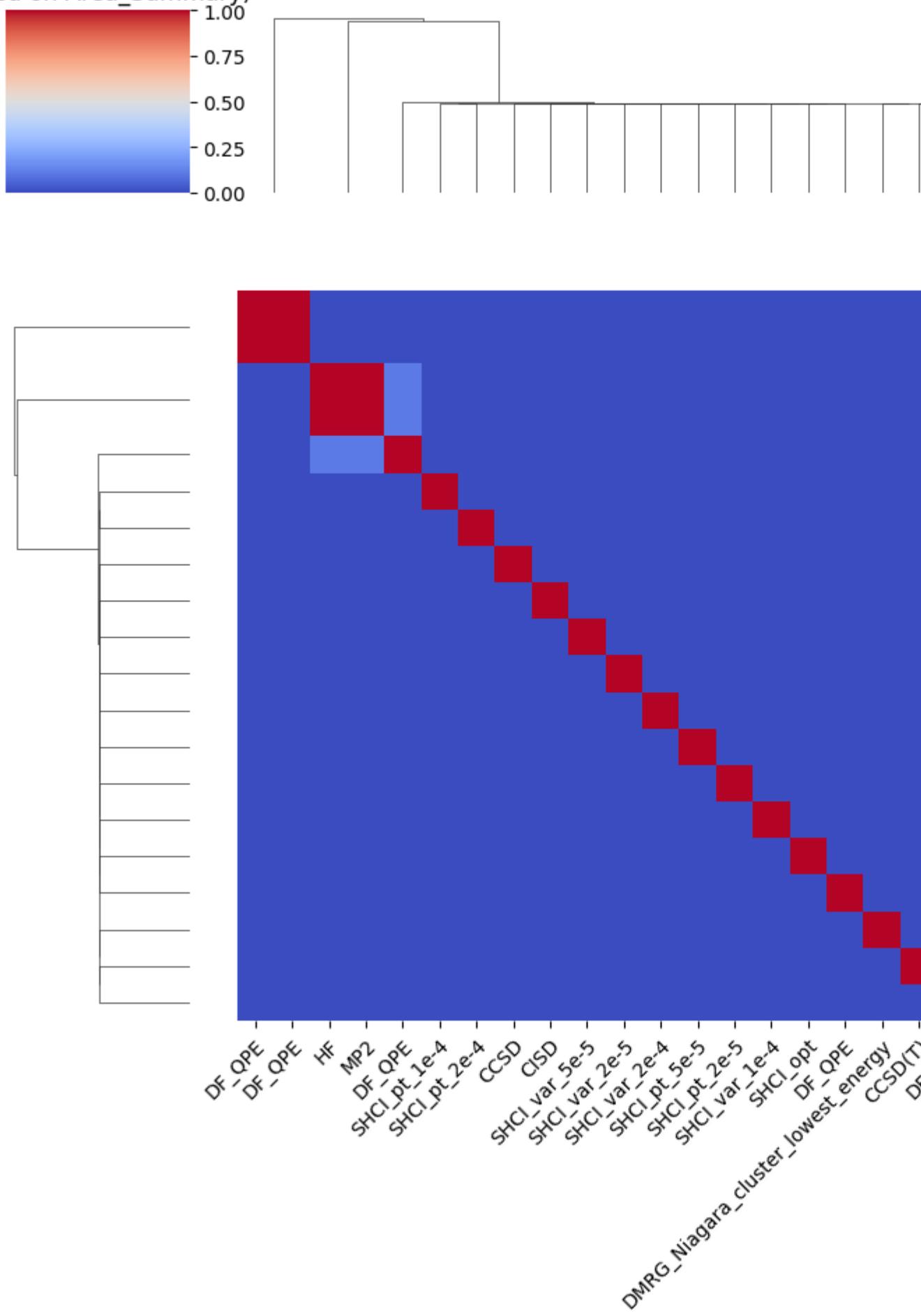
Solver points in PCA space
(PCA space of Area_Summary)



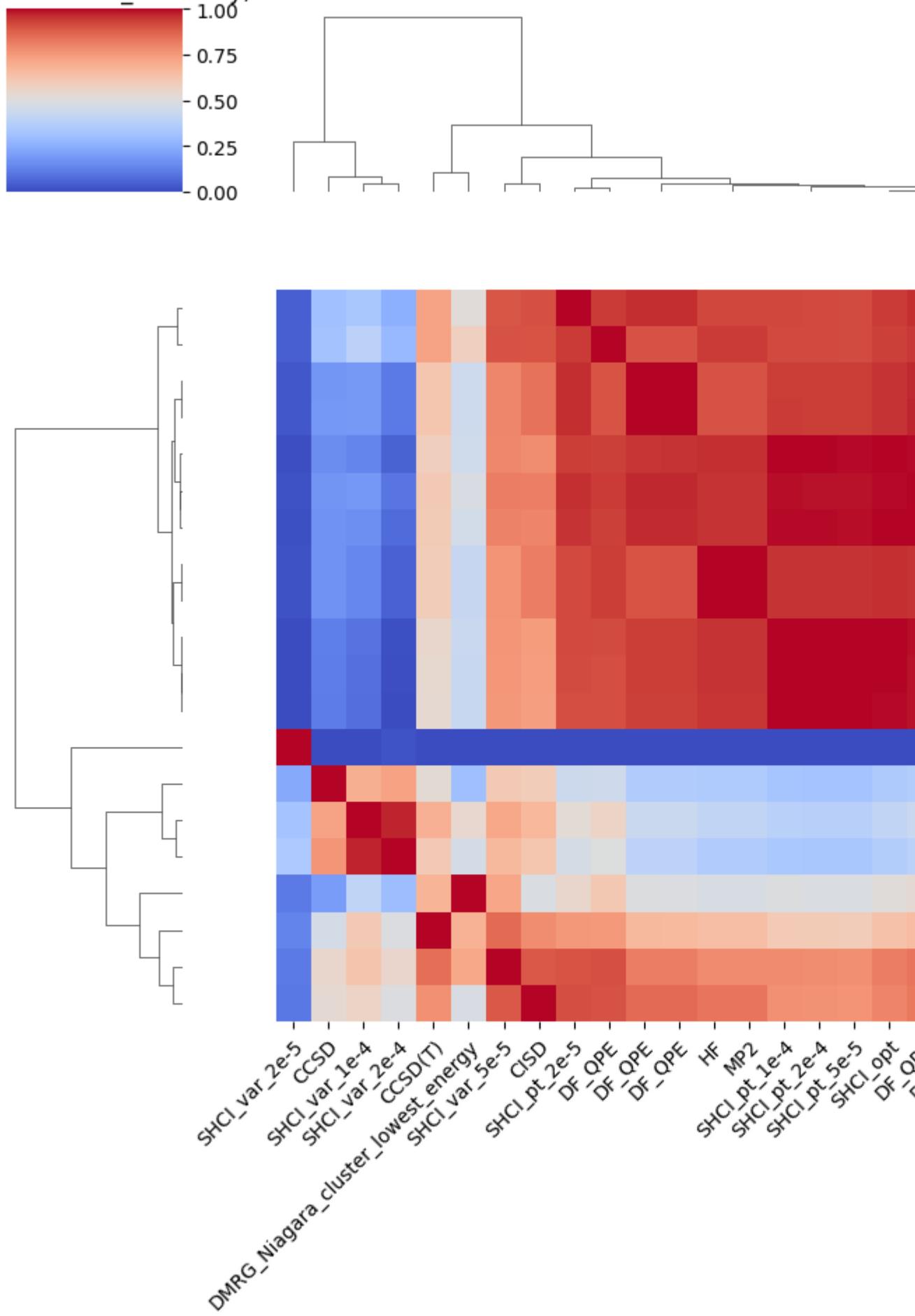
Solver points in PCA space
(PCA space of SHAP_summary)

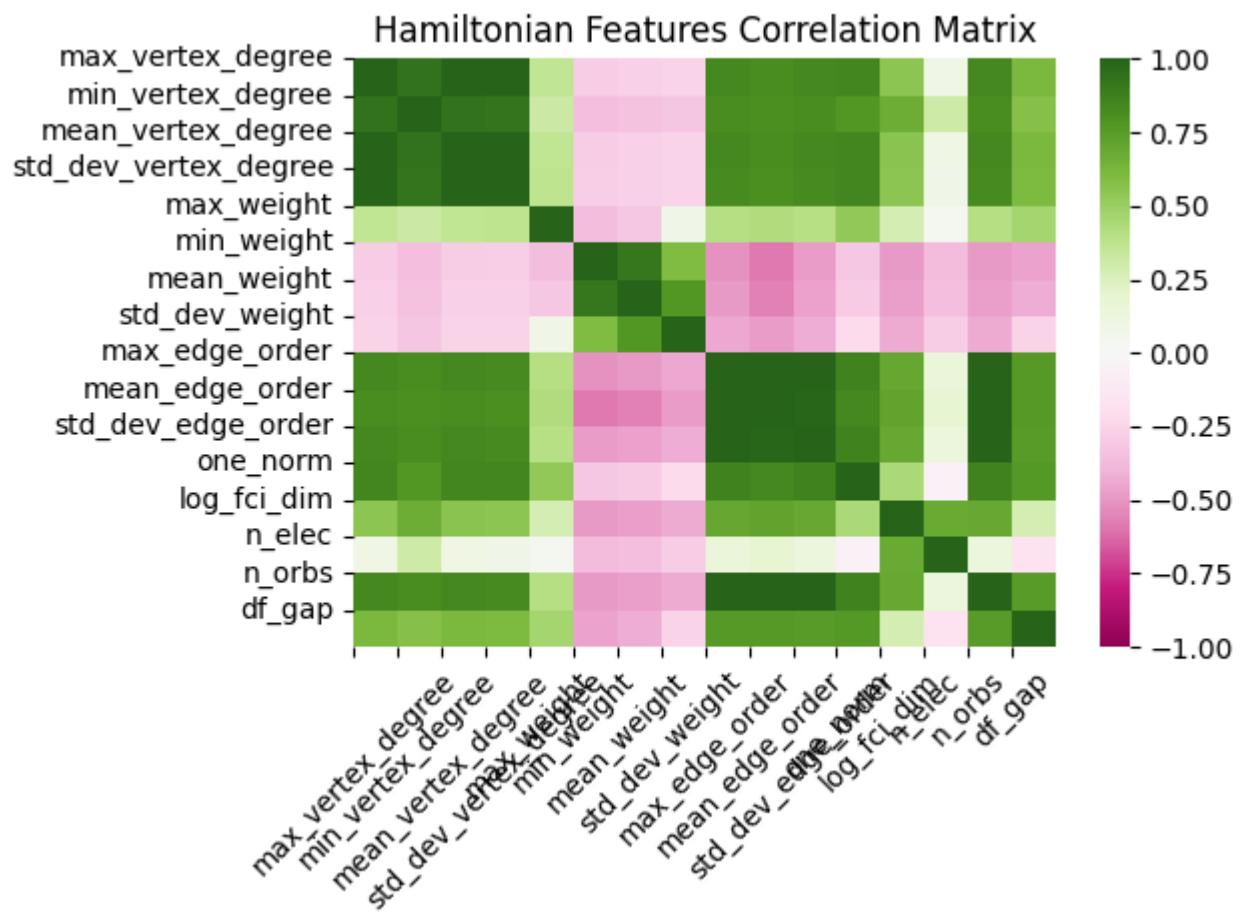


Solver similarity matrix
(based on Area_Summary)

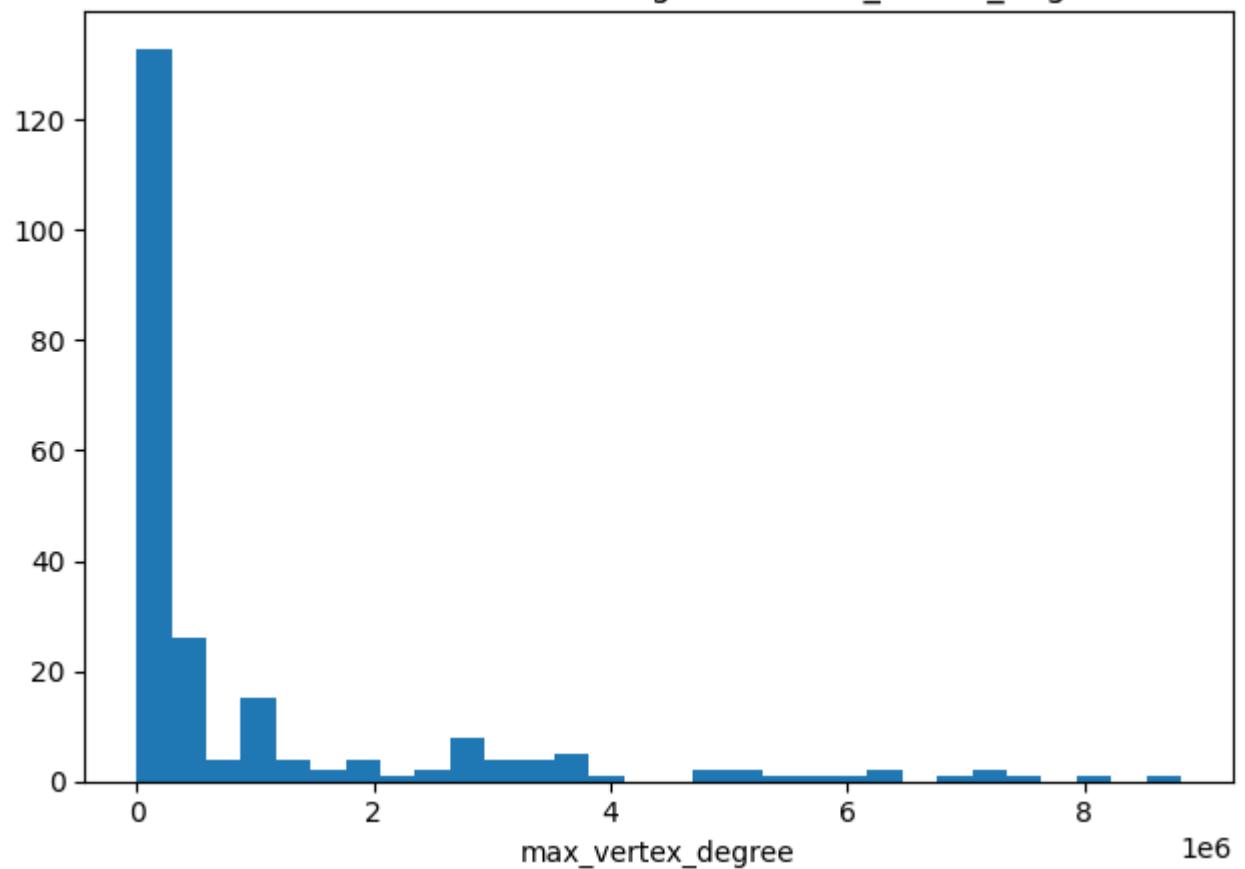


Solver similarity matrix
(based on SHAP_summary)

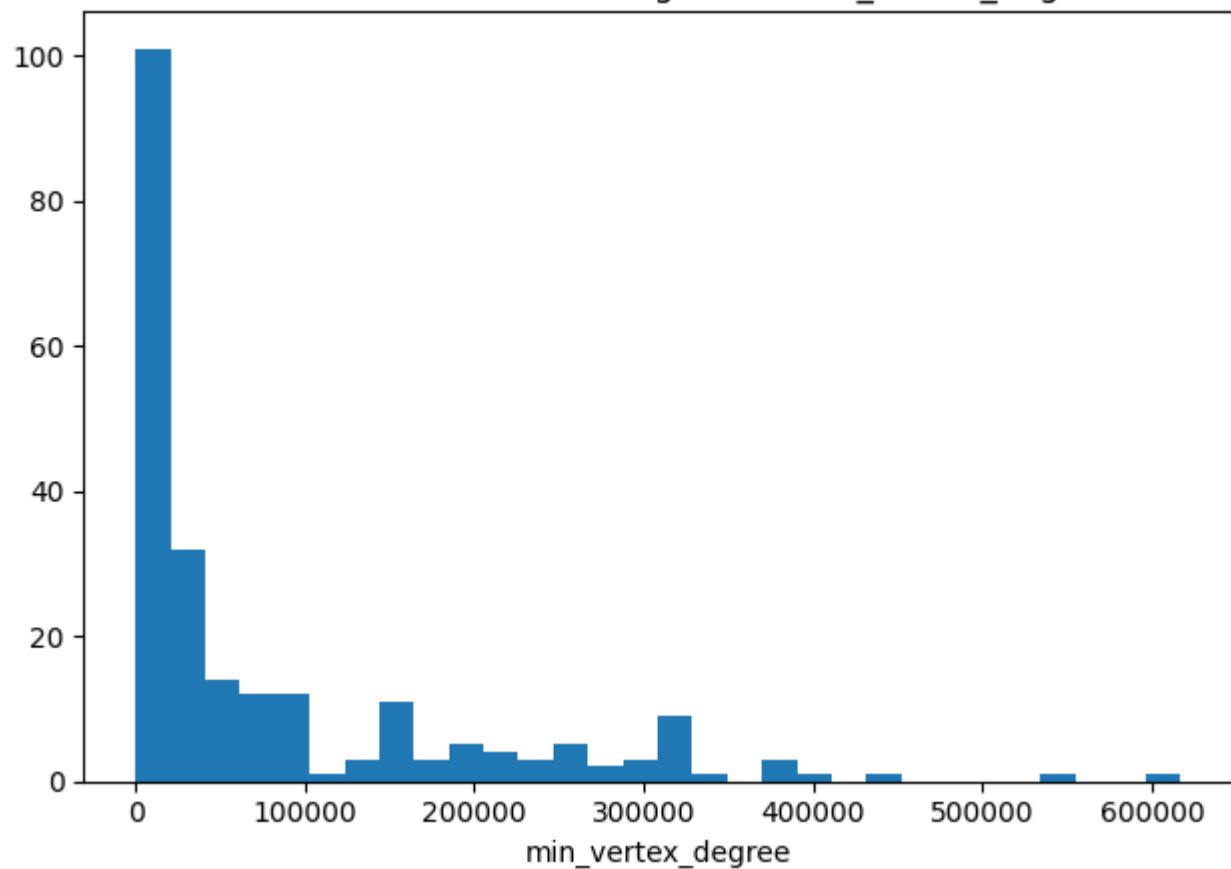




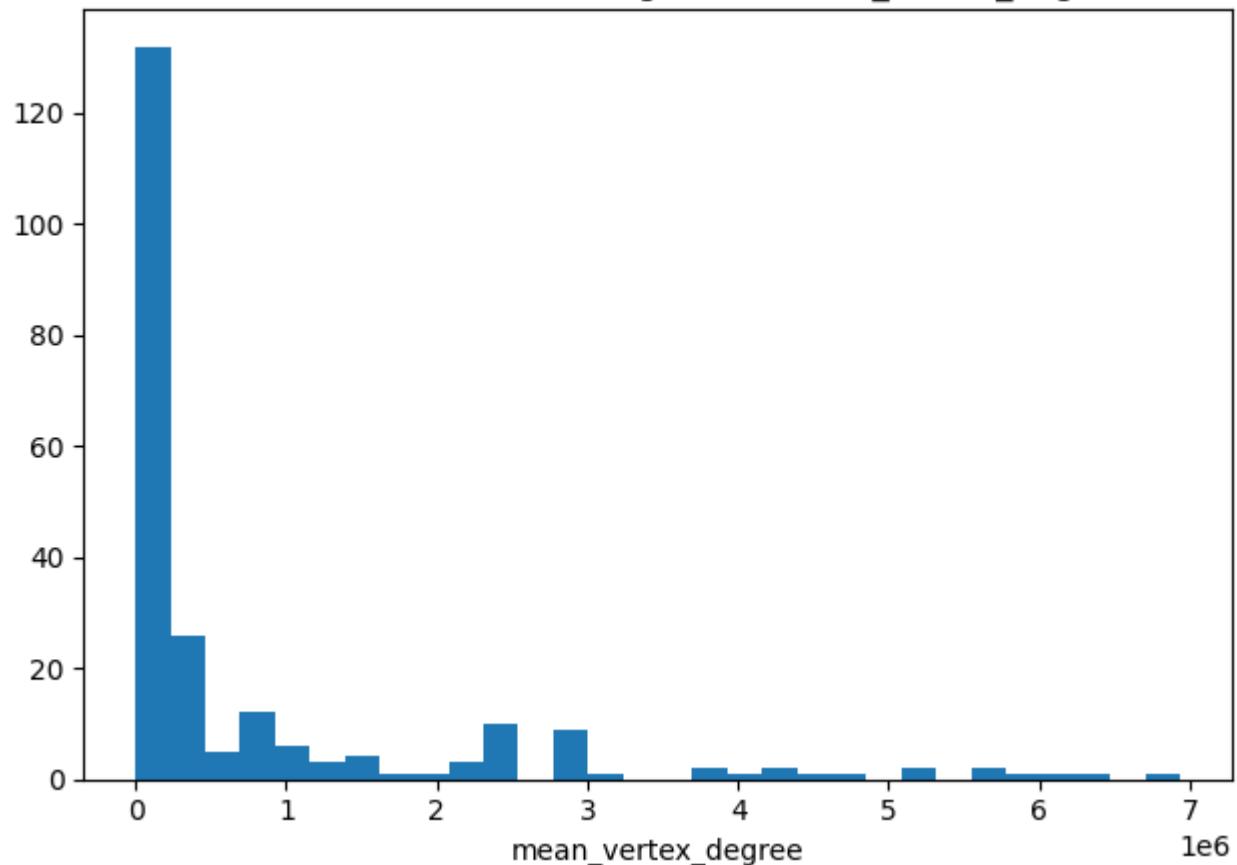
Hamiltonian features: histogram of max_vertex_degree



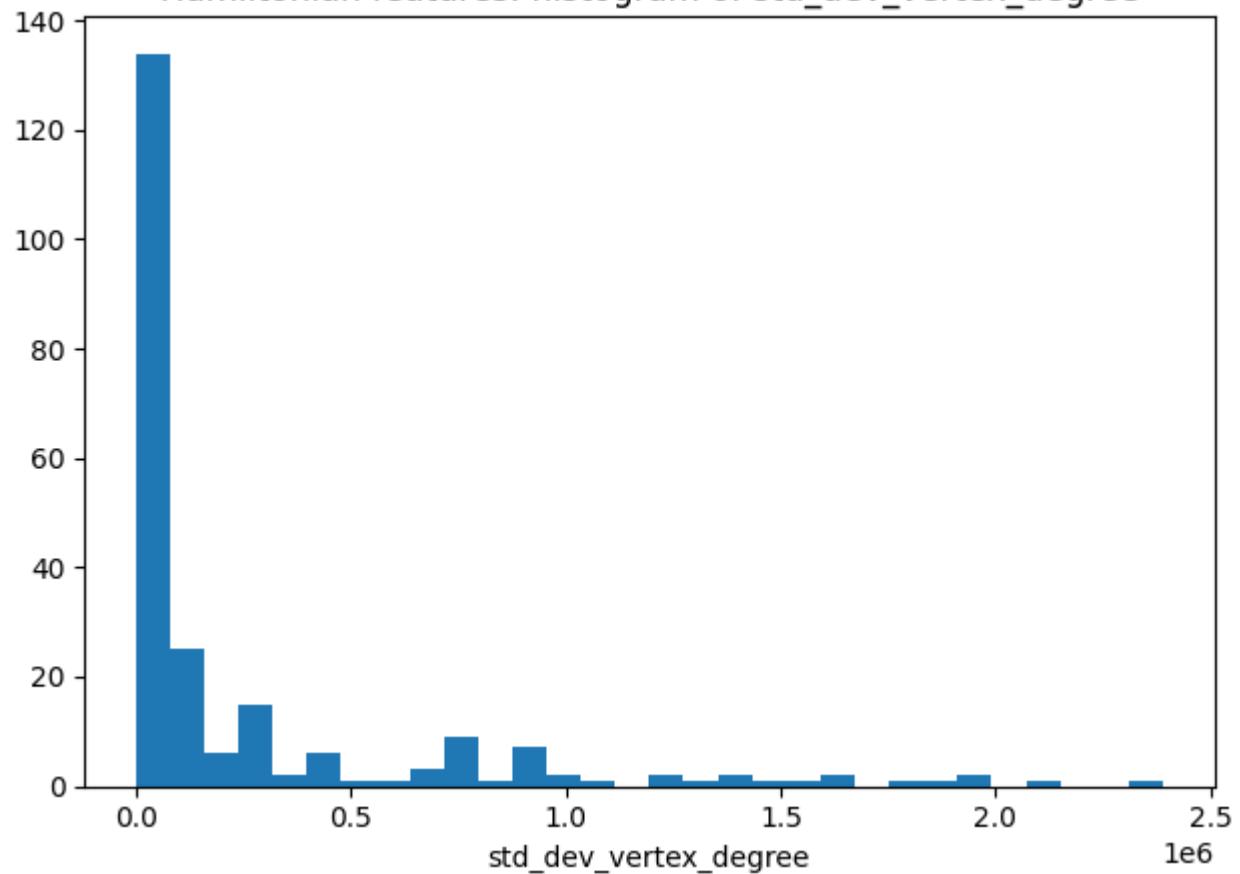
Hamiltonian features: histogram of min_vertex_degree



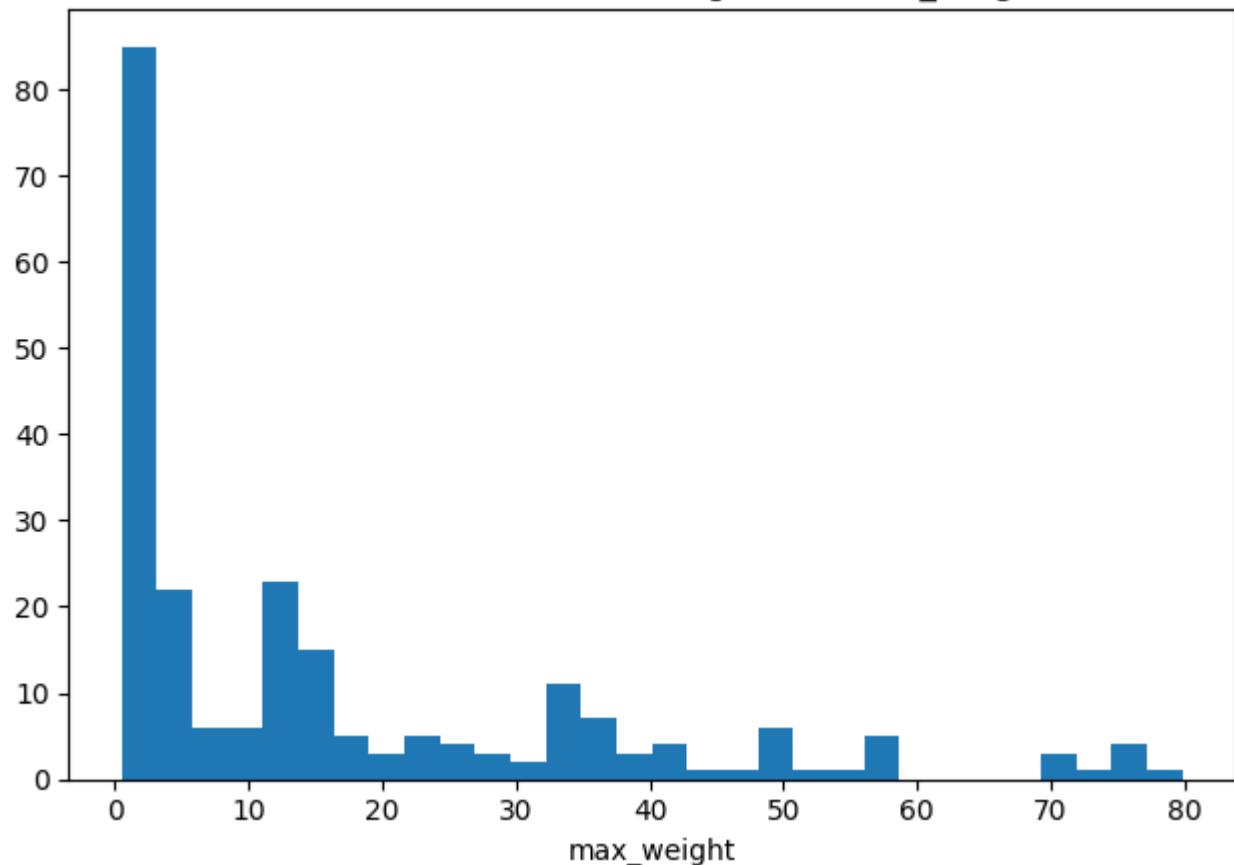
Hamiltonian features: histogram of mean_vertex_degree



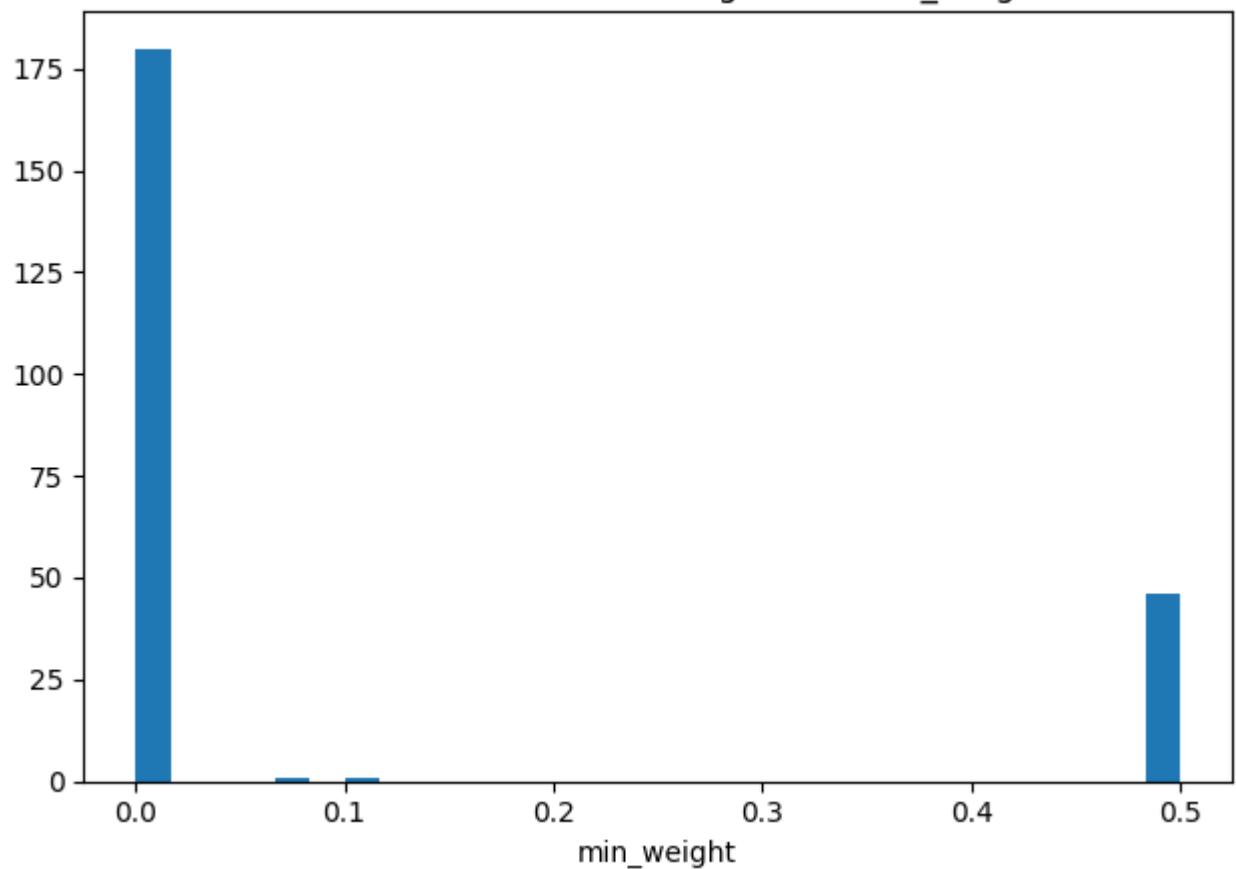
Hamiltonian features: histogram of std_dev_vertex_degree



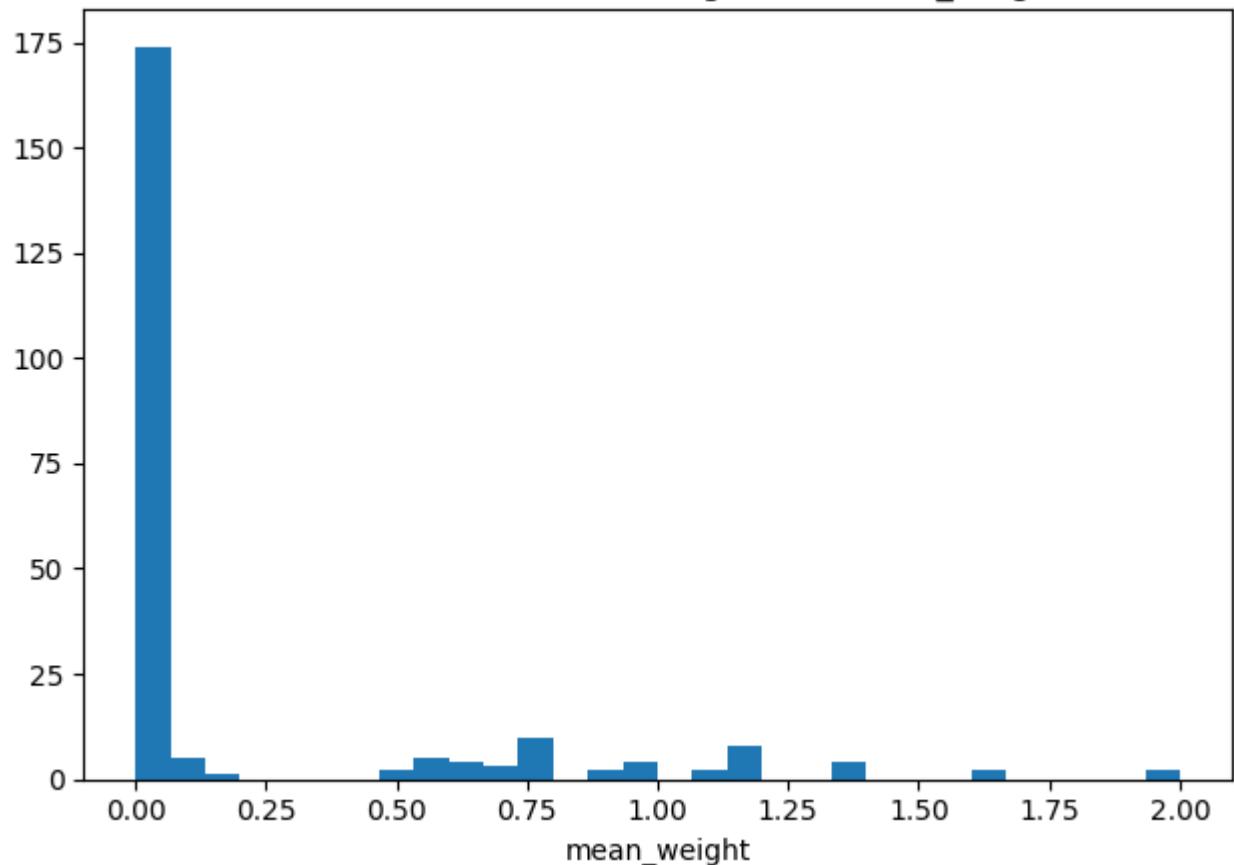
Hamiltonian features: histogram of max_weight



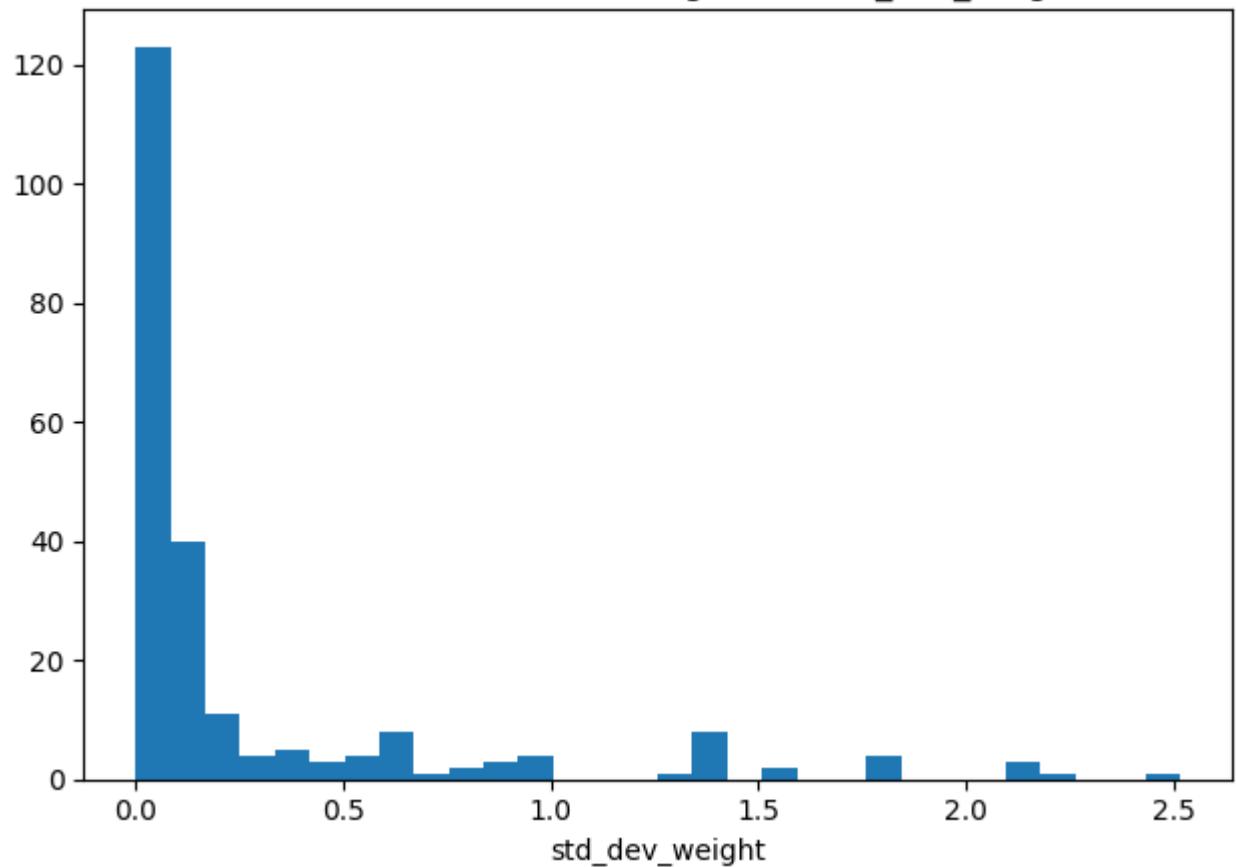
Hamiltonian features: histogram of min_weight



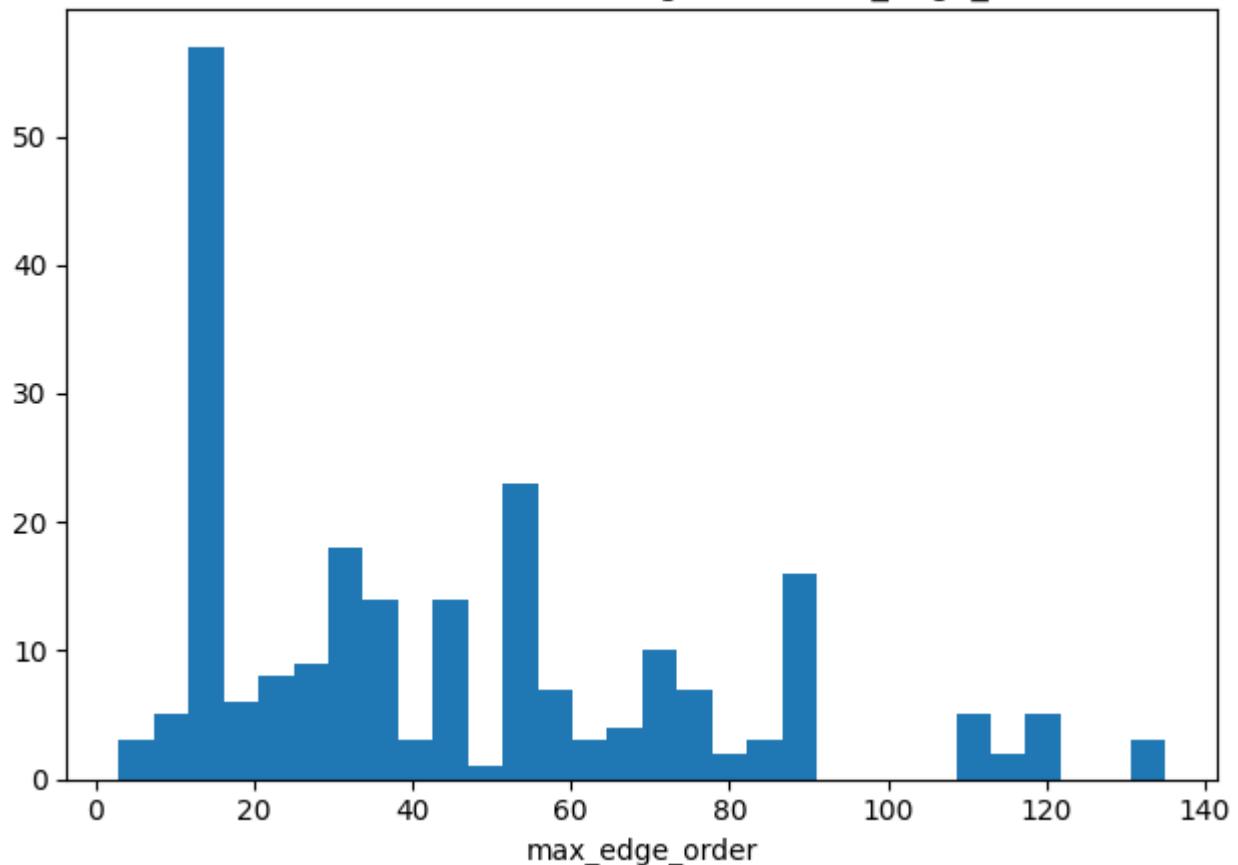
Hamiltonian features: histogram of mean_weight



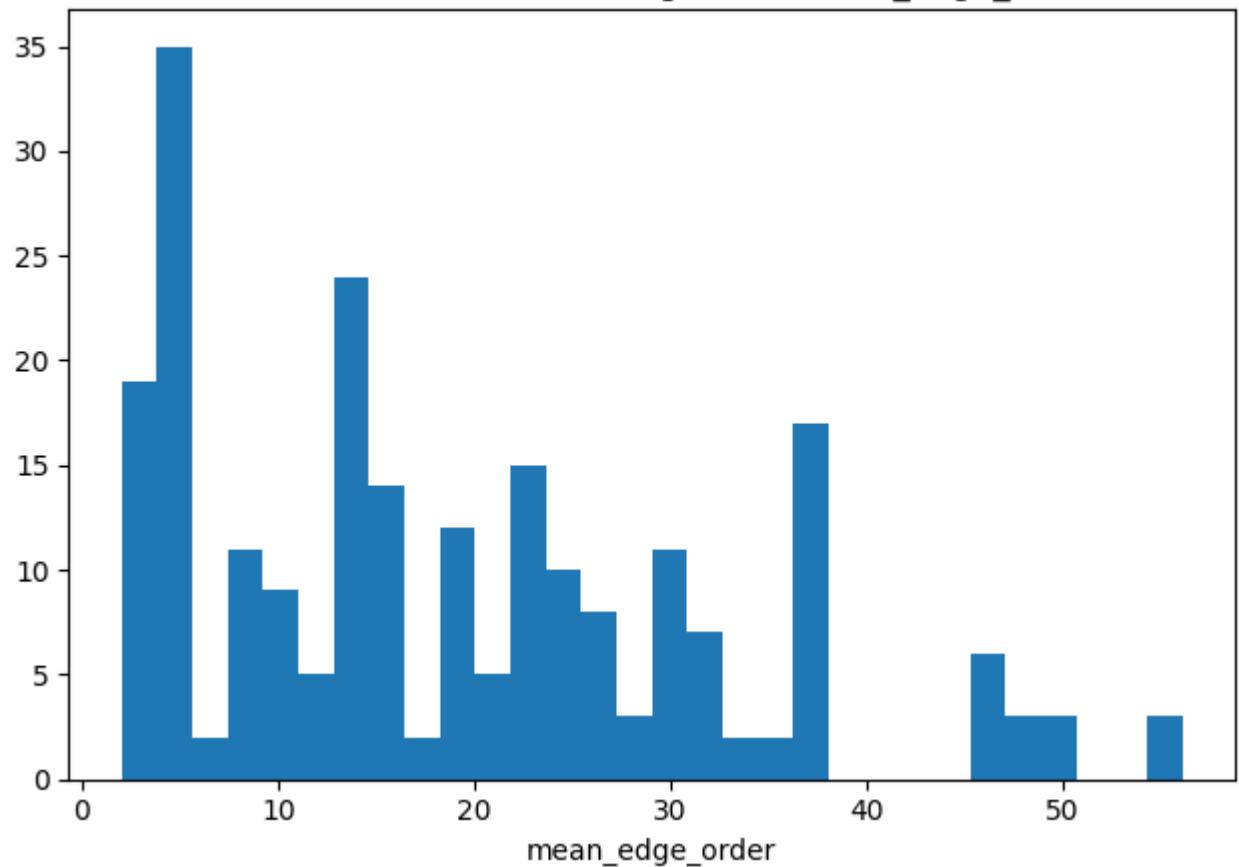
Hamiltonian features: histogram of std_dev_weight



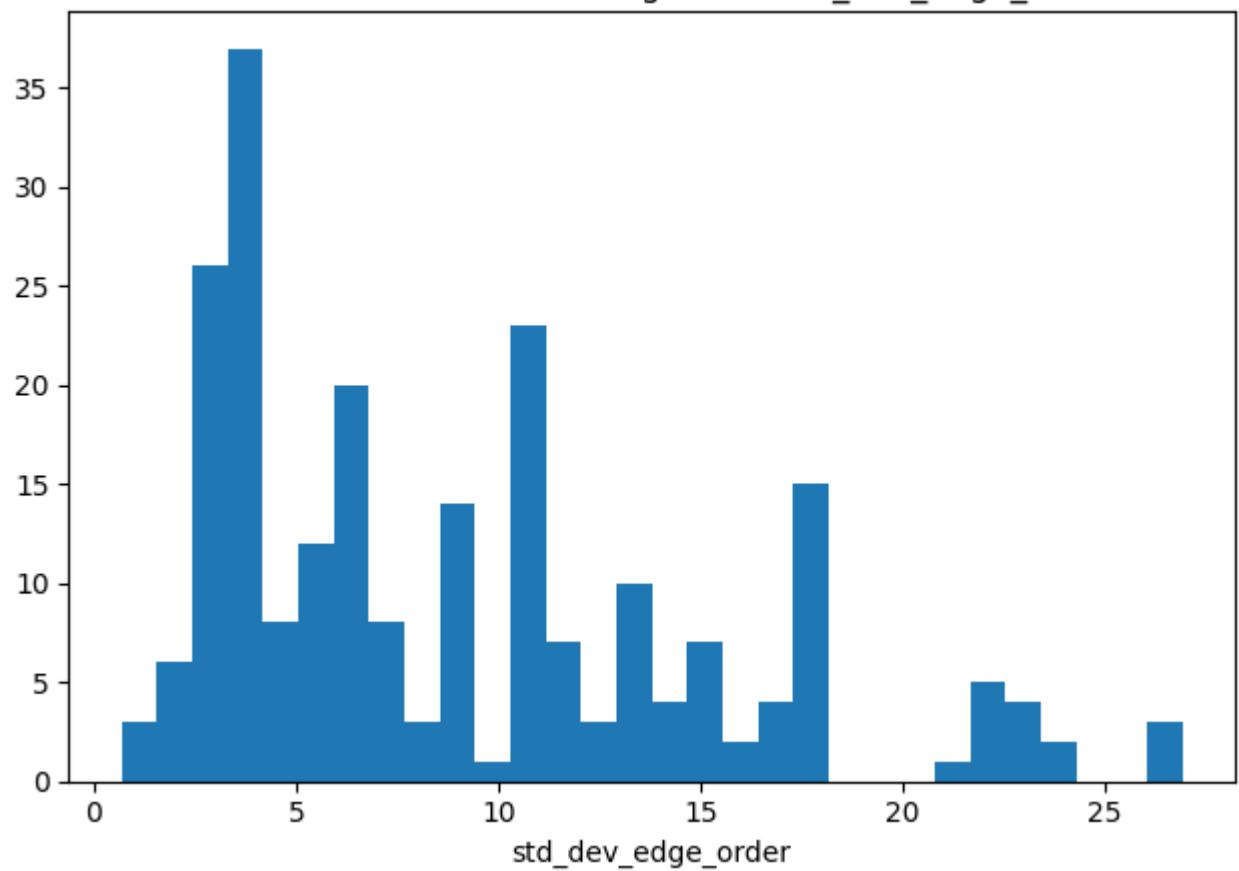
Hamiltonian features: histogram of max_edge_order



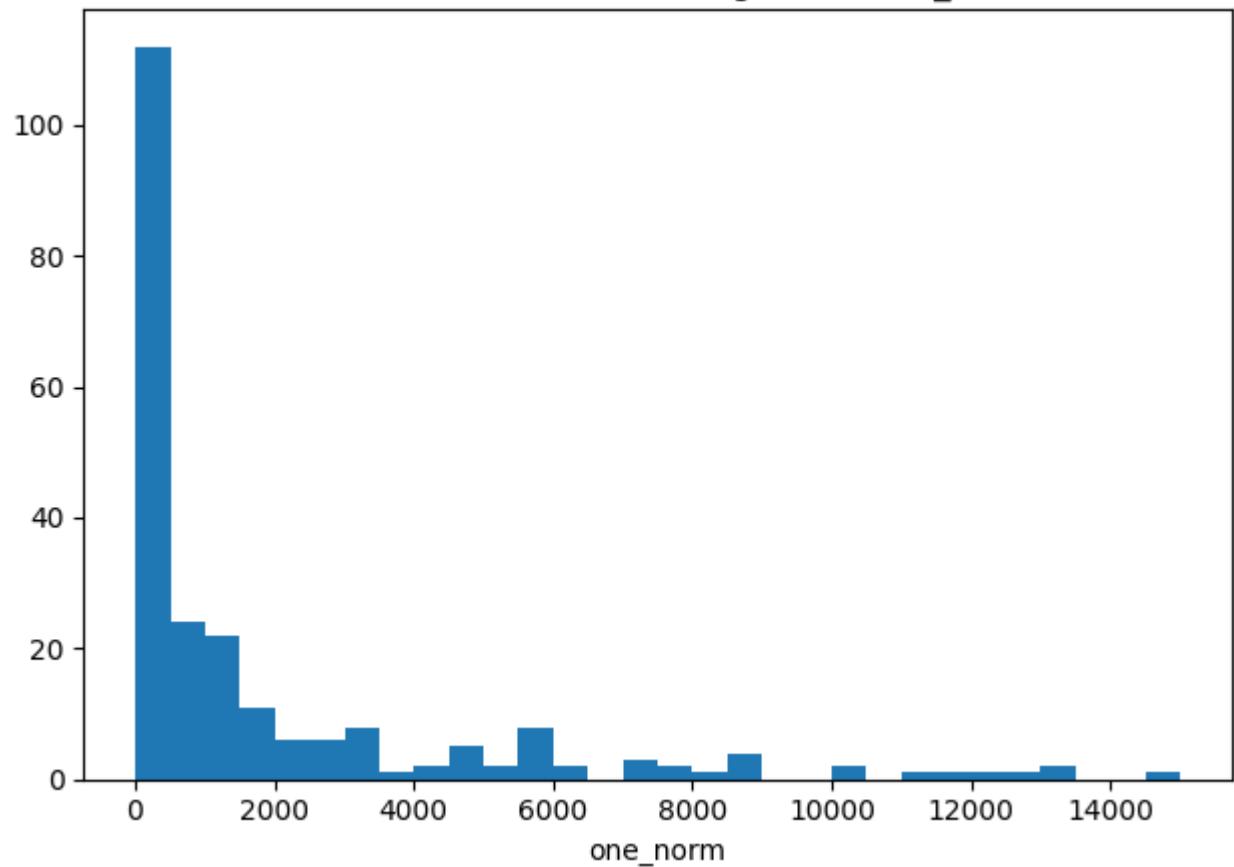
Hamiltonian features: histogram of mean_edge_order



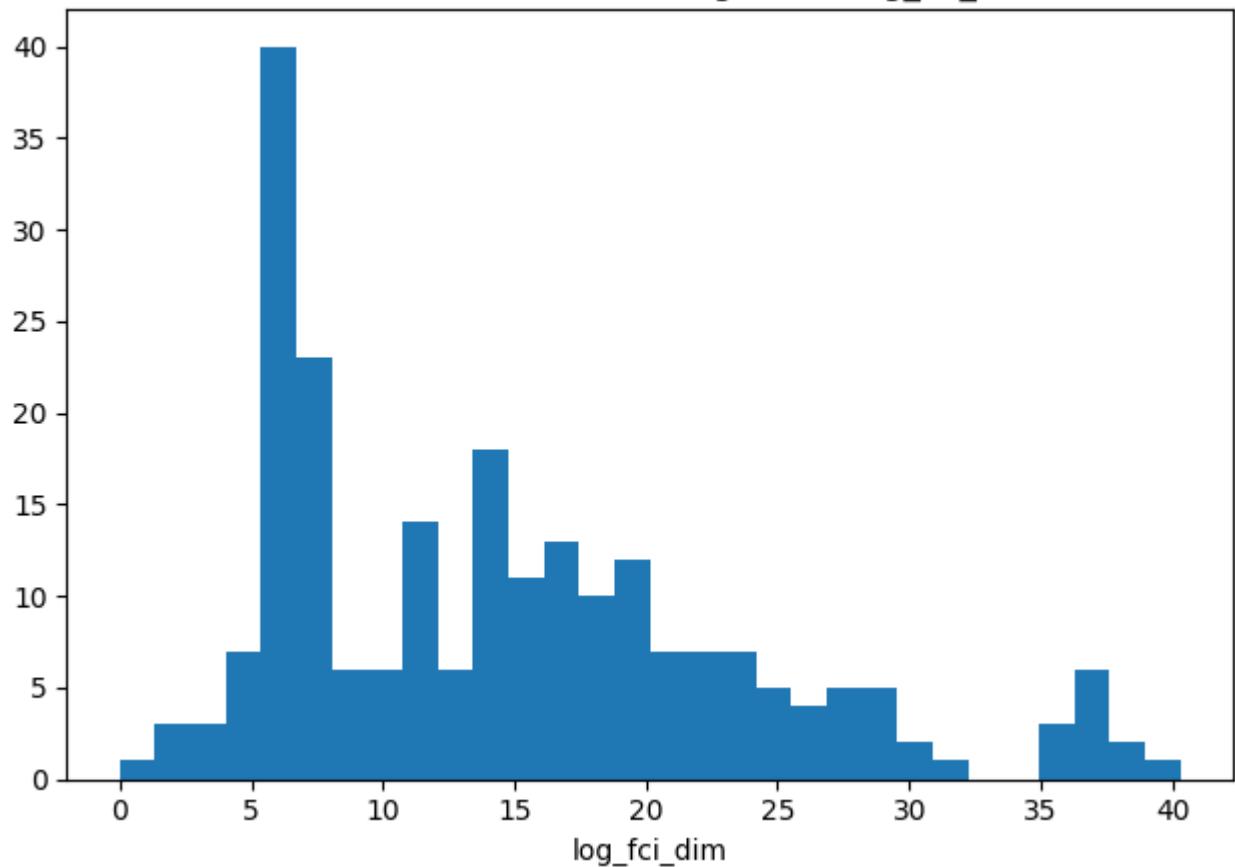
Hamiltonian features: histogram of std_dev_edge_order



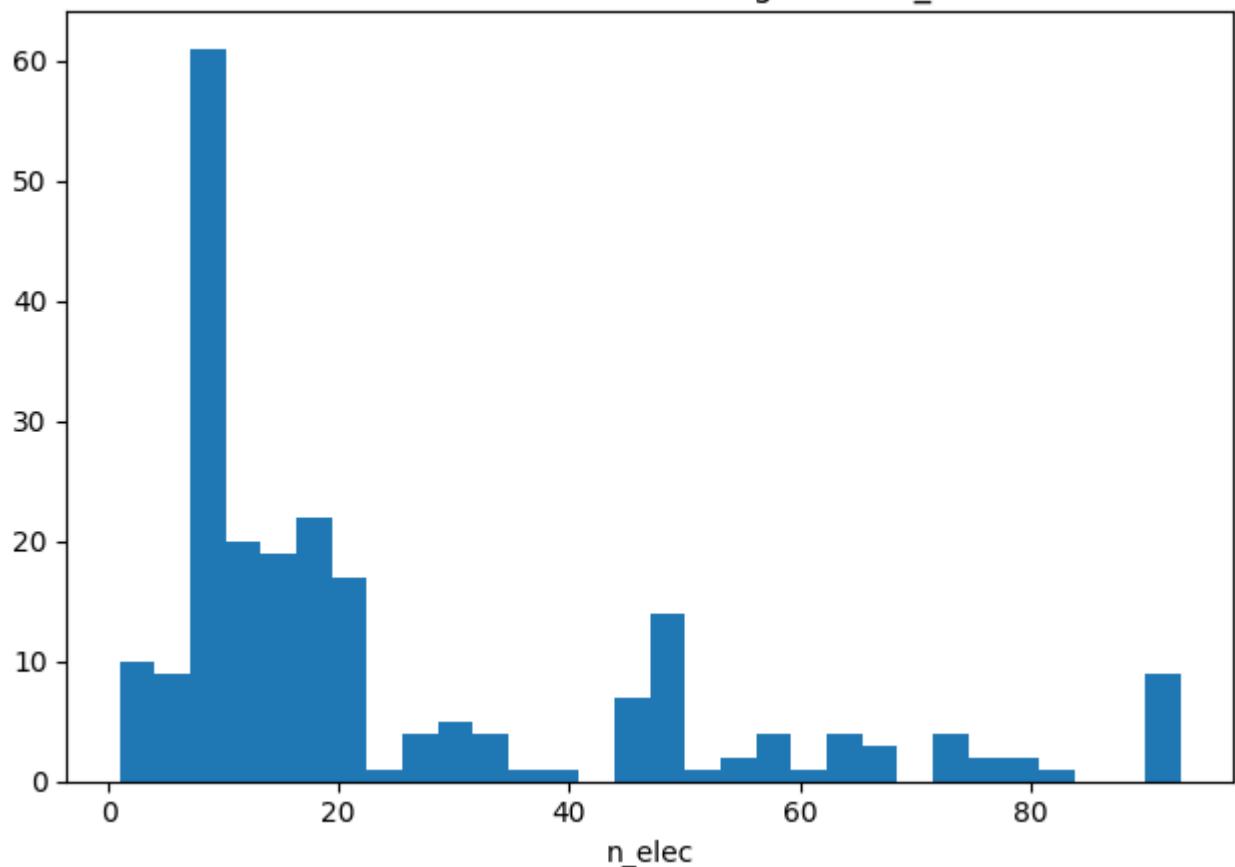
Hamiltonian features: histogram of one_norm



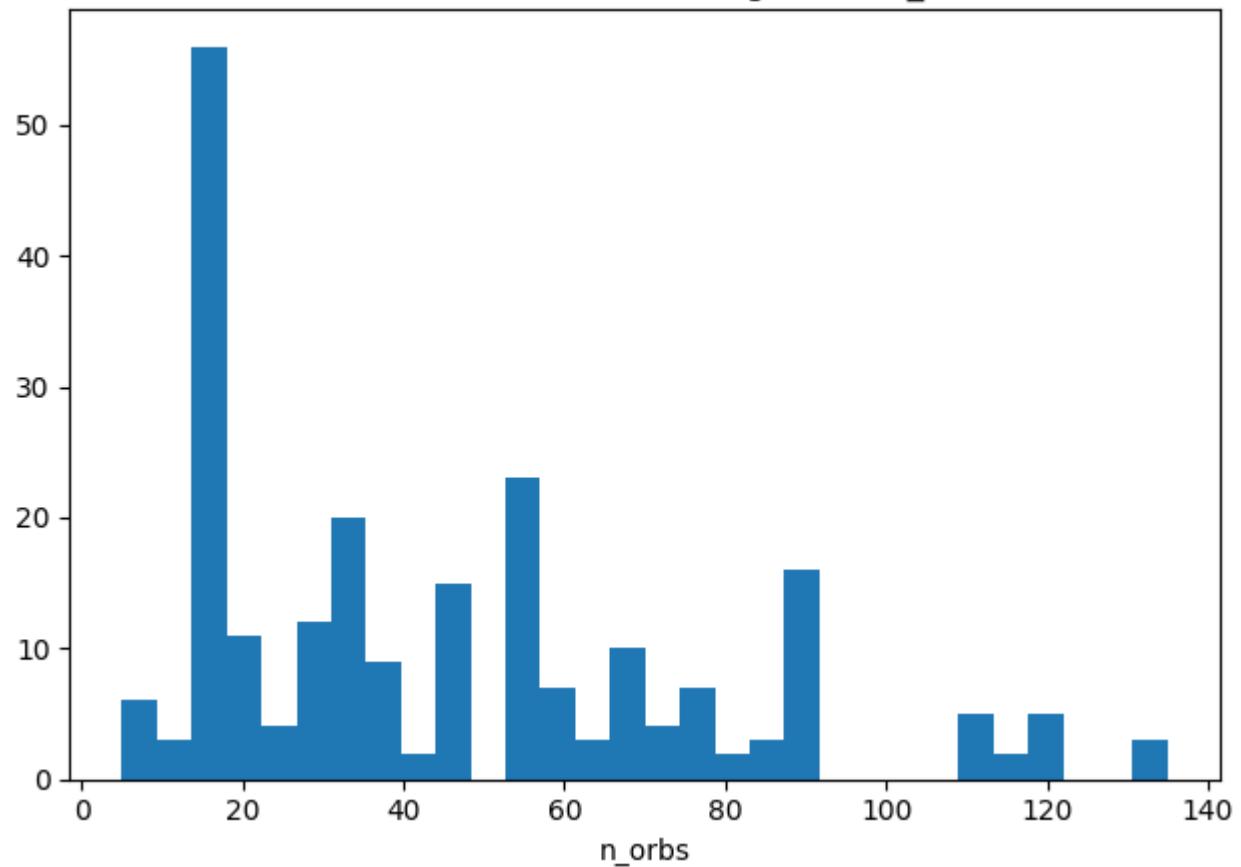
Hamiltonian features: histogram of log_fci_dim



Hamiltonian features: histogram of n_elec



Hamiltonian features: histogram of n_orbs



Hamiltonian features: histogram of df_gap

