

GSEE Benchmark Standard Report

Report based on data from 2025-06-12T20:42:55.603395+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Thu Jun 12 14:47:27 2025

Input data: GSEE-
`HC_utility_estimates_all_instances_task_uuids_v2.csv`, last modified
Thu Jun 12 14:47:27 2025

Latest creation time for a `problem_instance.json` file: Thu Jun 12 14:47:26 2025

Latest creation time for a `solution.json` file: Thu Jun 12 16:36:35 2025

Problem Instance Summary Statistics

number of `problem_instances`: 68.

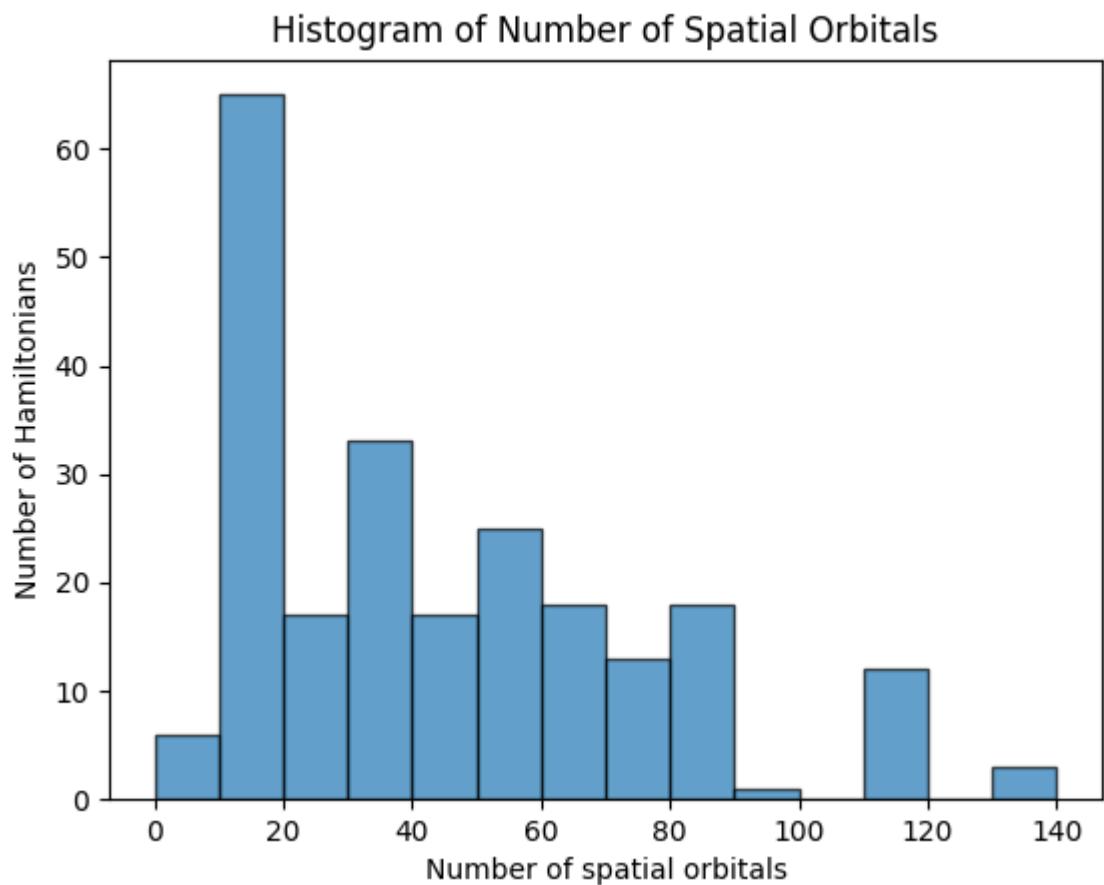
`problem_instance.json` with the most tasks: 30 (`hubbard_square/614c4444-a31a-4348-b24d-01040208651c`)

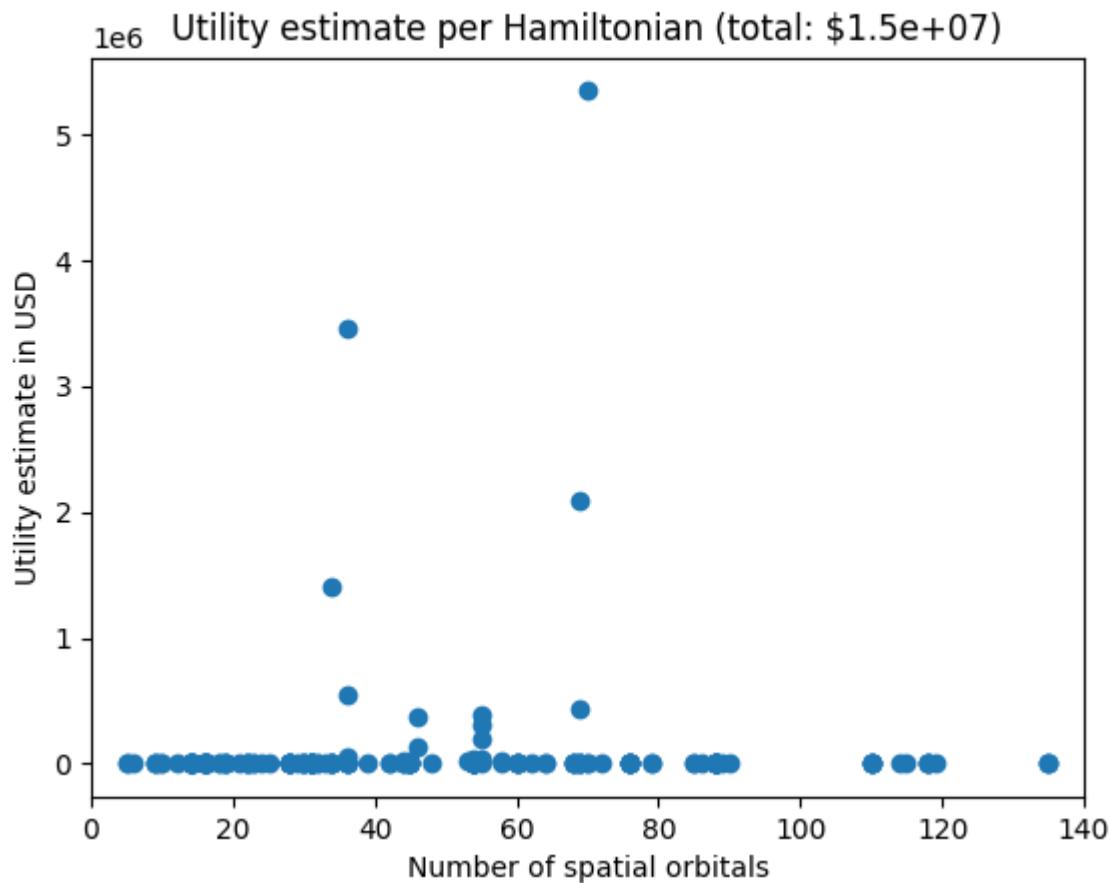
number of Hamiltonians (i.e., tasks) we have features calculated for: 228

minimum number of orbitals: 5

median number of orbitals: 36.0

maximum number of orbitals: 135





Solver Summary Statistics

number of unique participating solvers: 23

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

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

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

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

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

Solver: CCSD(T)/c09217e6-d0f7-4b0f-81c4-79210b7ac878, ML Solvability Ratio: {'PCA': 0.2847, 'NNMF': 0.092}, F1 Score: [0.96855346 0.96598639]

Solver: CCSD/0a29e54f-bef9-4d19-bafa-d94b1c4b37aa, ML Solvability Ratio: {'PCA': 0.011, 'NNMF': 0.0418}, F1 Score: [0.98795181 0.94736842]

Solver: CISD/418f060e-496b-4024-8d2d-9b1f8791e76d, ML Solvability Ratio: {'PCA': 0.0233, 'NNMF': 0.0051}, F1 Score: [0.98069498 0.89361702]

Solver: HF/5f5e617a-19c2-4d82-bebc-b2d6b3dc012, ML Solvability Ratio: {'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0. 0.0754717]

Solver: MP2/b420358b-5def-41e6-8c5d-b9d93b6aec02, ML Solvability Ratio: {'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0. 0.0754717]

Solver: SHCI_opt/2dde727e-a881-44fa-aabf-bba6248e4baf, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.83333333 0.99319728]

Solver: SHCI_pt_1e-4/4ed500f1-0650-41e3-af00-e4d0359394b4, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.71428571 0.97122302]

Solver: SHCI_pt_2e-4/ad964781-302e-4728-a26d-39918e0a6cdb, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 0.9868}, F1 Score: [0.89361702 0.98069498]

Solver: SHCI_pt_2e-5/c71b90bd-3250-4c0c-b4e7-fc9878f141f6, ML Solvability Ratio: {'PCA': 0.9317, 'NNMF': 0.5441}, F1 Score: [0.76470588 0.97058824]

Solver: SHCI_pt_5e-5/d626506c-7aae-4ad6-802a-b29af5f2bb93, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.9375 0.99270073]

Solver: SHCI_var_1e-4/7e730dfb-57ee-480b-a8a1-4b73f5f07c54, ML Solvability Ratio: {'PCA': 0.6562, 'NNMF': 0.7836}, F1 Score: [0.98387097 0.98901099]

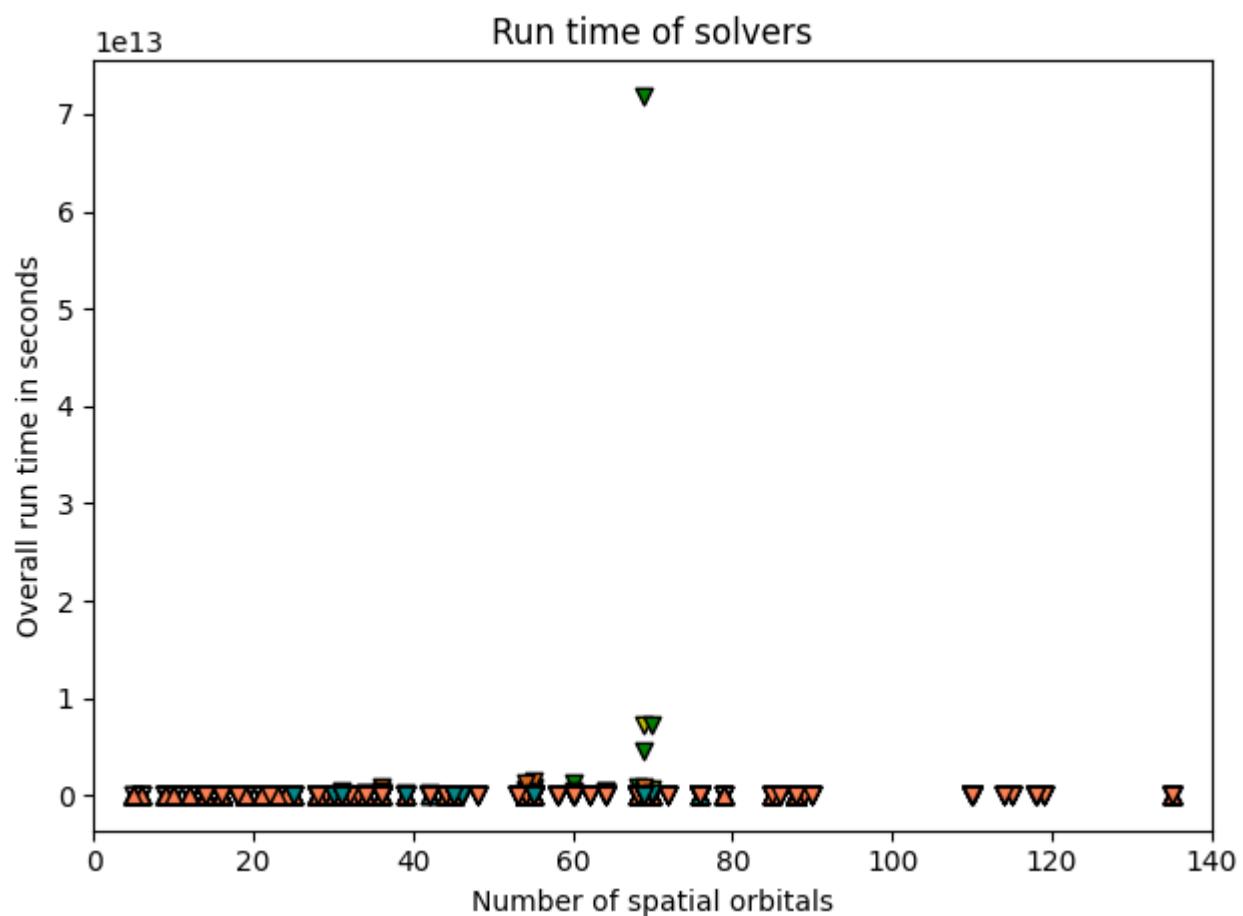
Solver: SHCI_var_2e-4/0db183e3-a86d-491b-9125-599556e37c7a, ML Solvability Ratio: {'PCA': 0.8125, 'NNMF': 0.8487}, F1 Score: [0.99280576 0.99401198]

Solver: SHCI_var_2e-5/86bfe50c-9342-4d54-bb68-abc8abd95688, ML Solvability Ratio: {'PCA': 0.6486, 'NNMF': 0.4057}, F1 Score: [0.88 0.9765625]

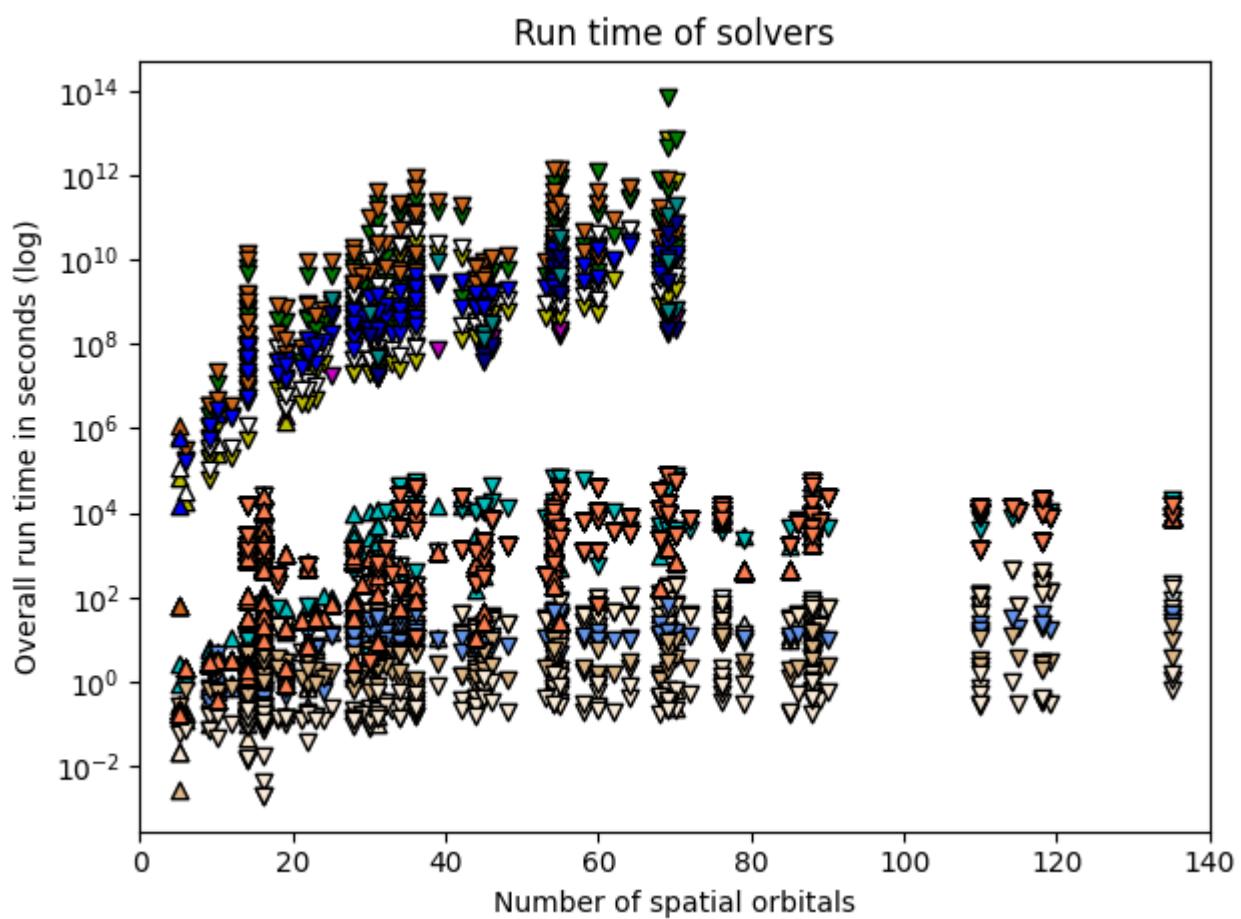
Solver: SHCI_var_5e-5/01949b95-c427-4693-9134-01f47f688c09, ML Solvability Ratio: {'PCA': 0.8749, 'NNMF': 0.391}, F1 Score: [0.83950617 0.94222222]

Solver: THC_BLISS_QPE_1mHa/b8ed03bd-9c3e-4d07-80af-8f77f0e7c2ac,
Model could not be calculated.

Solver: THC_QPE_1mHa/18c187af-3e5b-4e6c-87fd-73c26fd48a60, Model
could not be calculated.

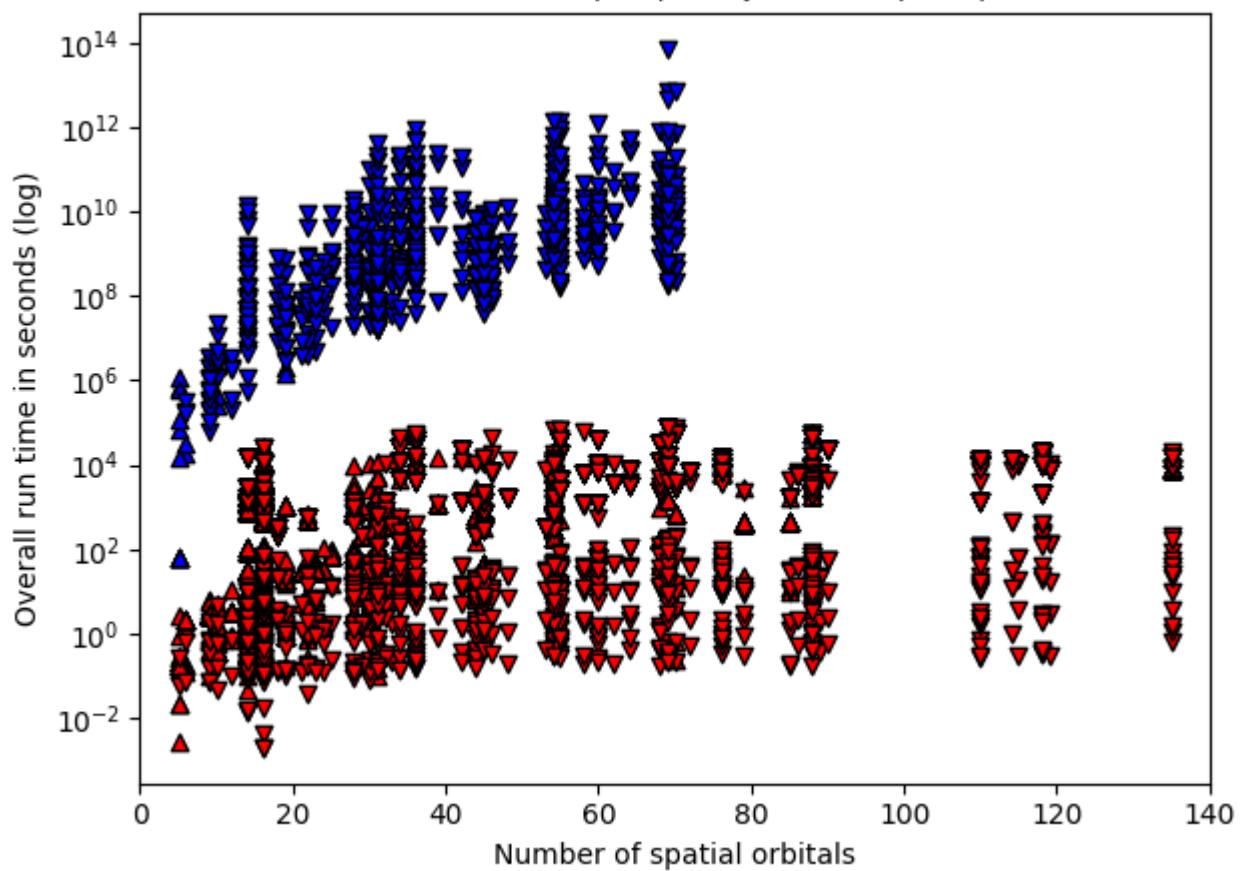


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

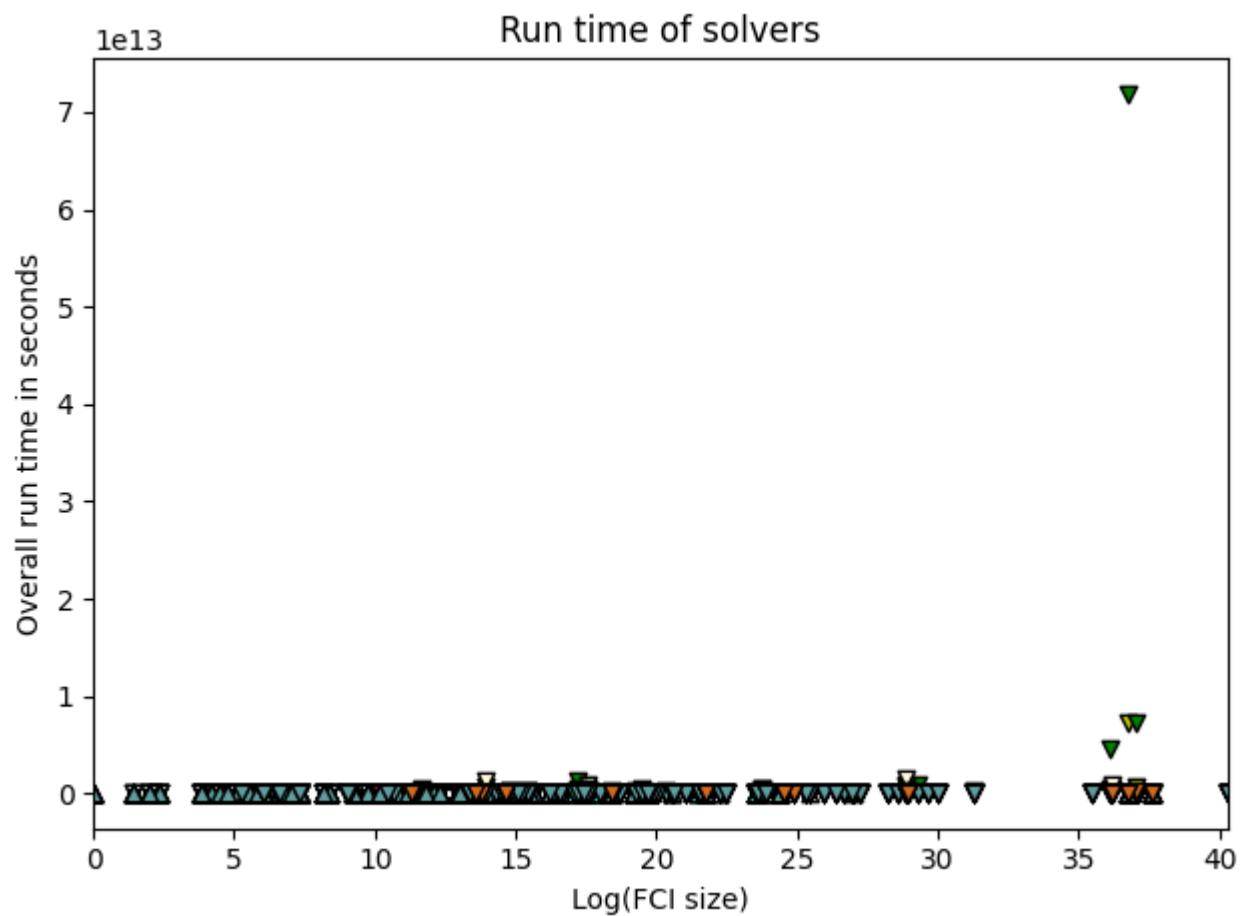


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

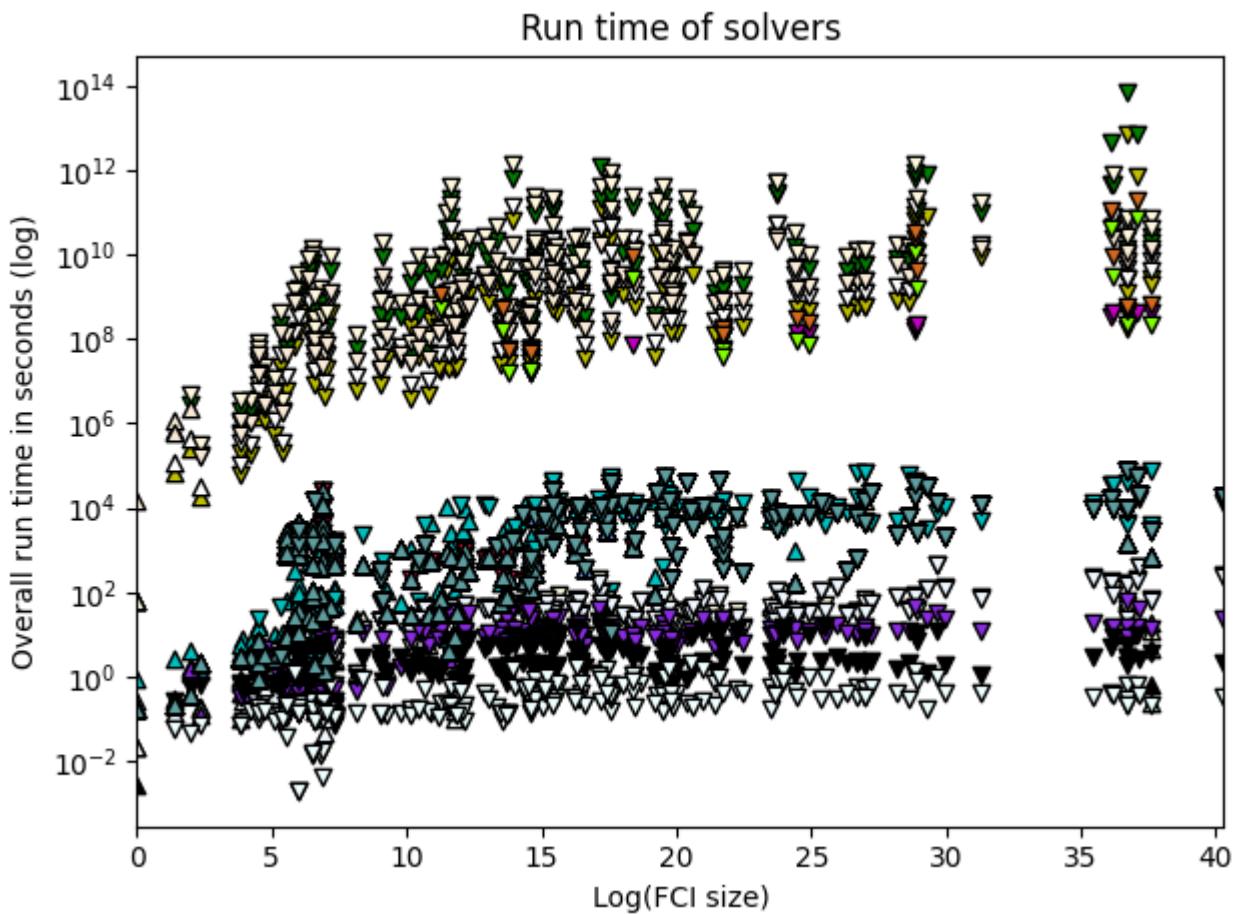
Run time of Classical (red) vs Quantum (blue) solvers



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



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

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}

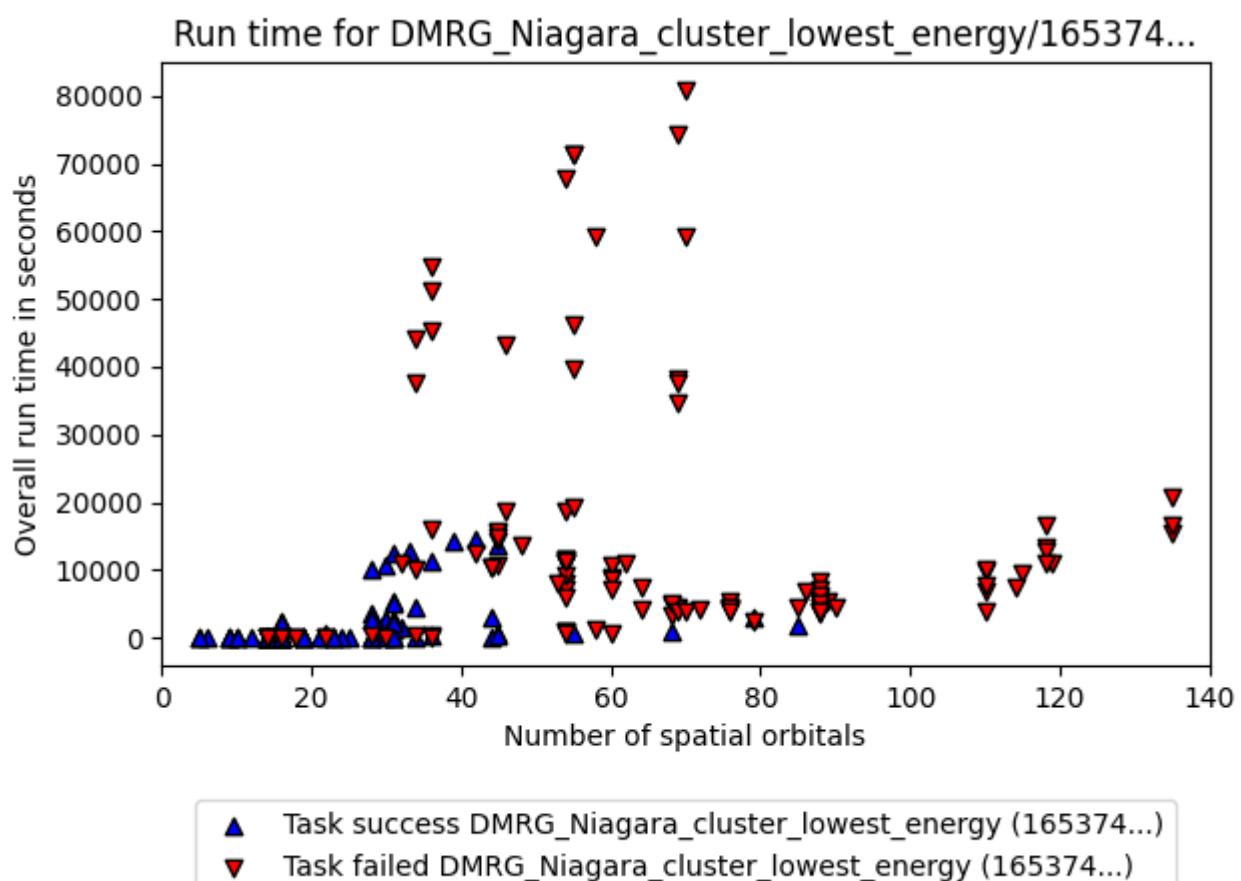
algorithm_details:DMRG with the lowest variational energy obtained so far.

software_details:Block2 v0.5.3rc16 with dmrghandler, commit version d603fdc6409fc194a416aa3a519362d5d91790d9 or later.

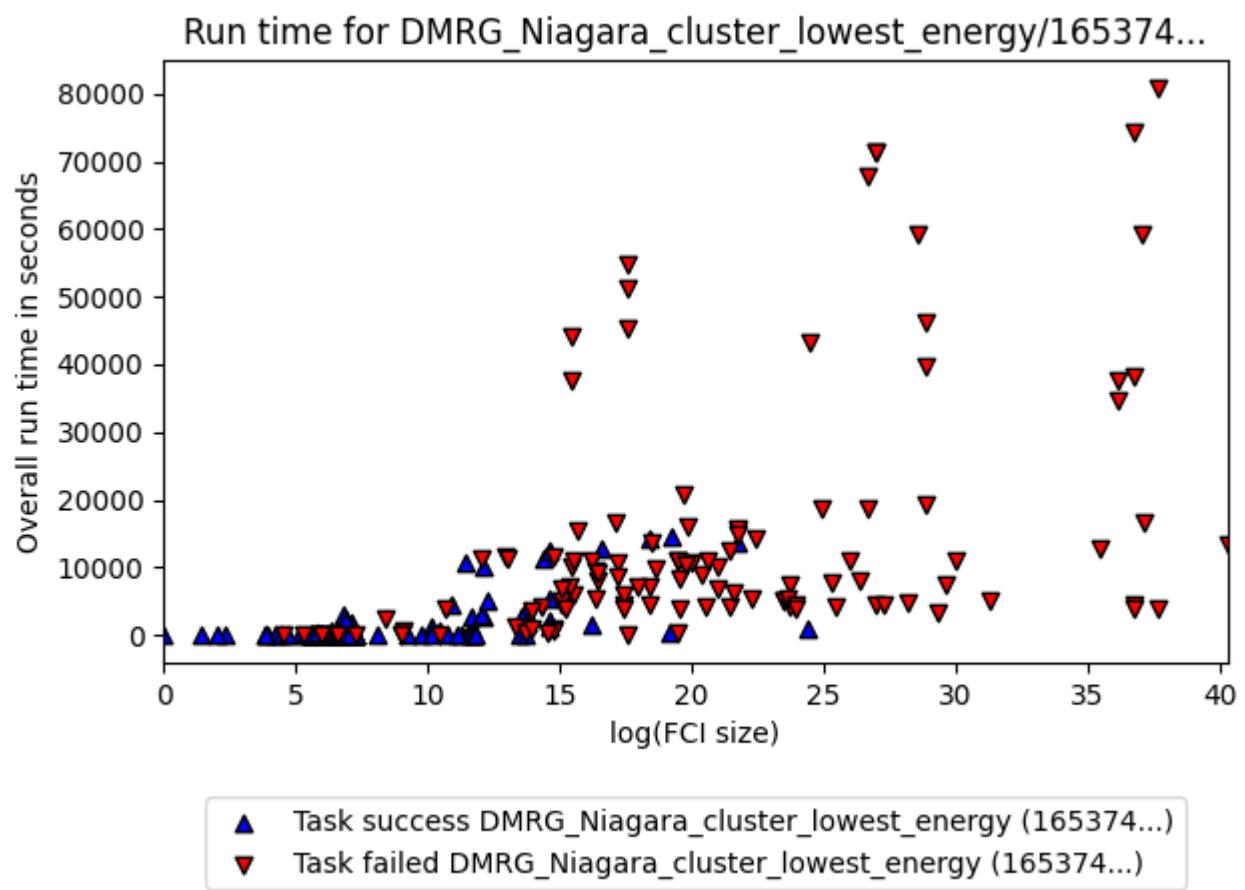
performance_metrics_uuid: 1bc901e4-ab02-4414-b4fa-daaf368a889c

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 13
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 107
number_of_tasks_solved_within_run_time_limit: 228
number_of_tasks_solved_within_accuracy_threshold: 107
max_run_time_of_attempted_tasks: 80820.729907066
sum_of_run_time_of_attempted_tasks: 1841774.710900084
solvability_ratio: 0.4126
comments: solvability ratio based on PCA embedding.
f1_score: [0.9130434782608695, 0.9626168224299065]
ml_metrics_calculator_version: 1



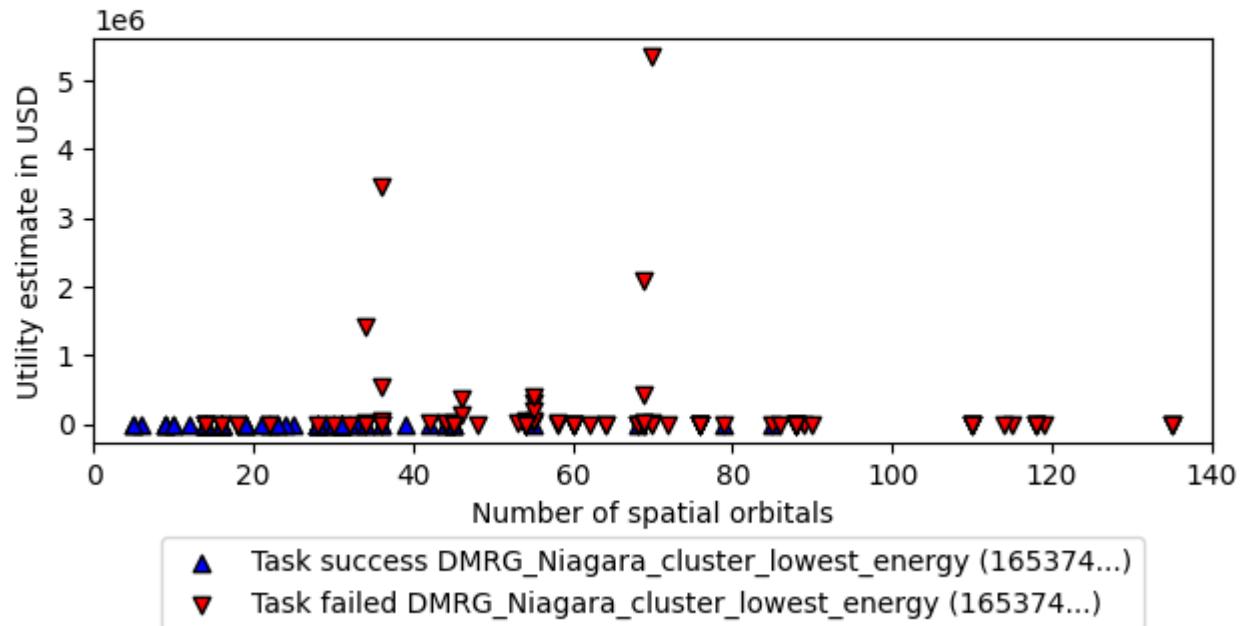
Note: plot only contains attempted tasks.



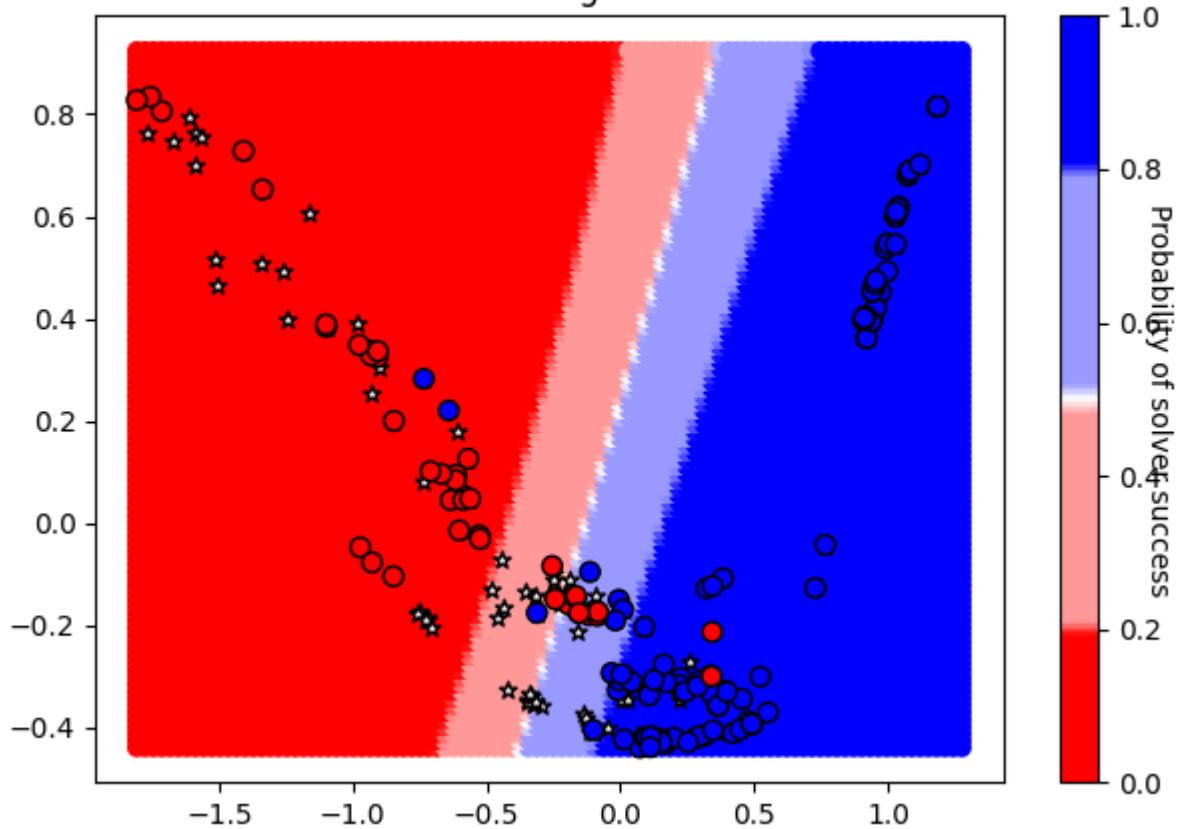
Note: plot only contains attempted tasks.

Utility capture from DMRG_Niagara_cluster_lowest_energy/165374

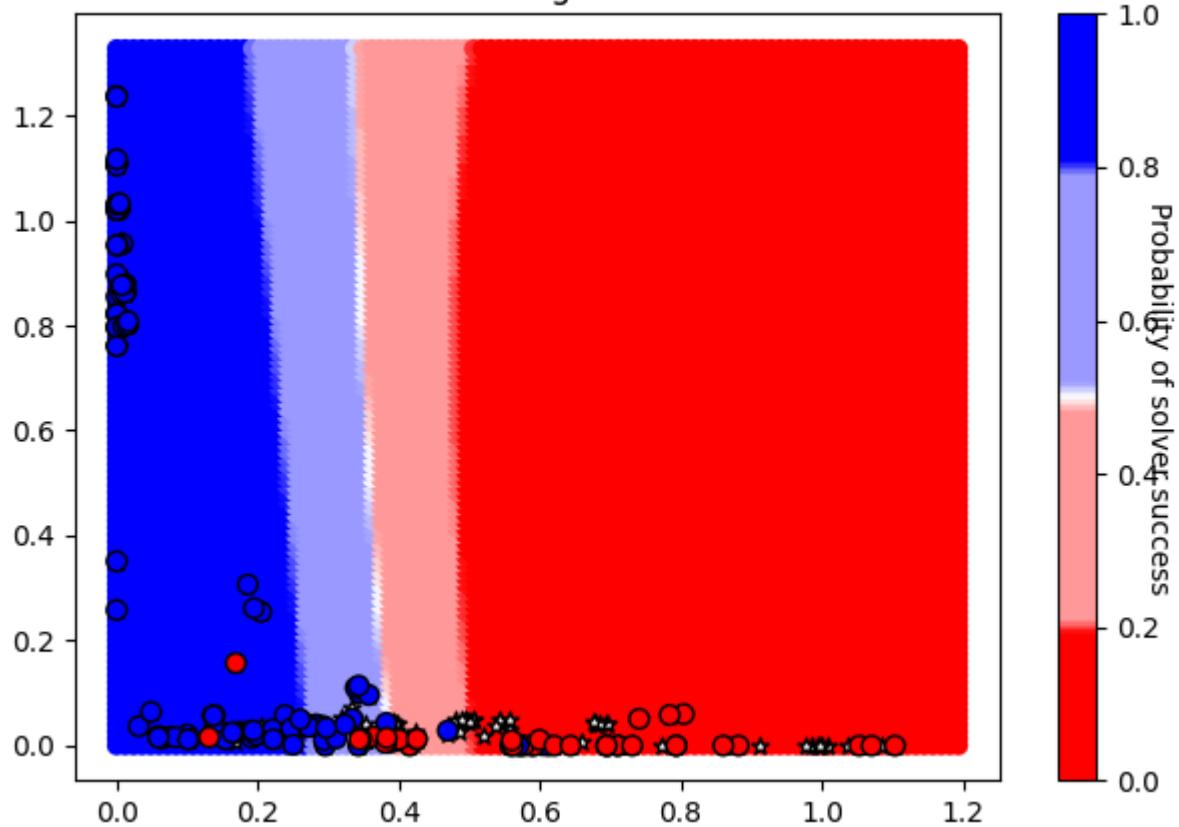
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



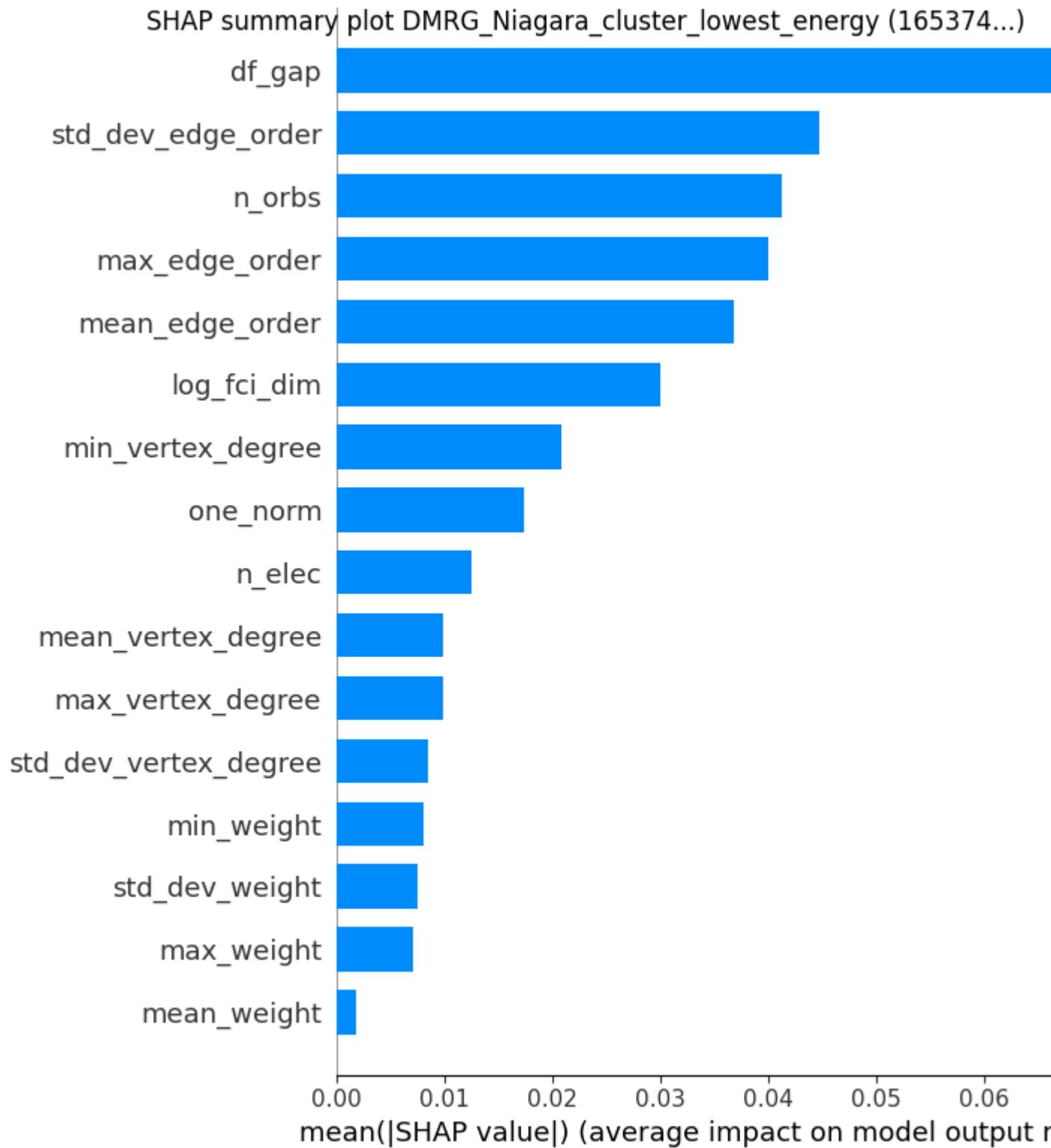
Solver DMRG_Niagara_cluster_lowest_energy (165374...)
Embedding: PCA



Solver DMRG_Niagara_cluster_lowest_energy (165374...)
Embedding: NNMF



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



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

solver_uuid:7c8ef984-4d3a-4468-8900-e0da3bd8b22d

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_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 the optimistic model described in https://arxiv.org/abs/2011.03494.', 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.0001, 'cycle_time_microseconds': 1}}

logical_resource_estimate_solution_uuid: 36607deb-5926-4a05-9121-7299e371d1e6

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

performance_metrics_uuid: 4a5c63ad-147c-401c-827f-99dcaf6d6d1f

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 4

number_of_problem_instances_solved: 1

number_of_tasks: 228

number_of_tasks_attempted: 24

number_of_tasks_solved: 1

number_of_tasks_solved_within_run_time_limit: 1

number_of_tasks_solved_within_accuracy_threshold: 24

max_run_time_of_attempted_tasks: 451622221.769206

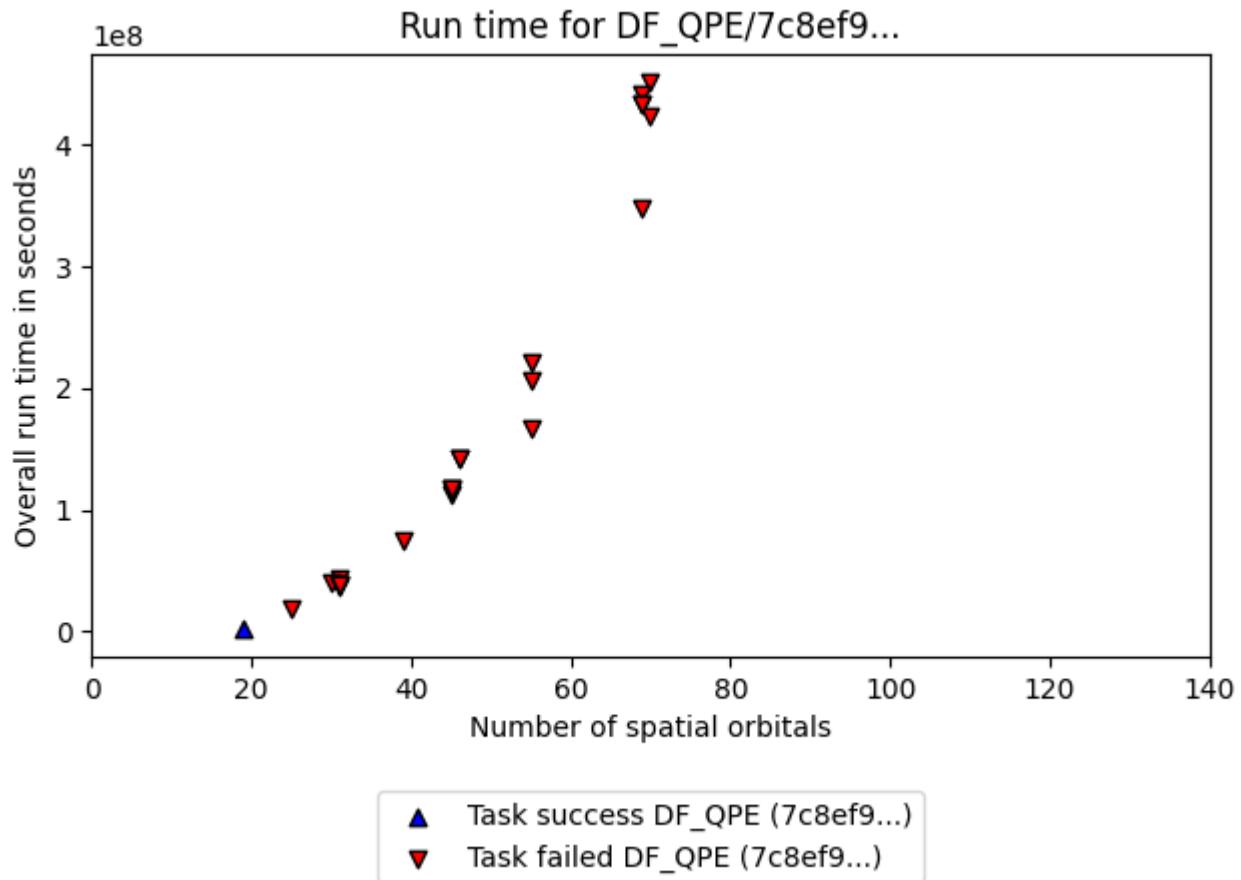
sum_of_run_time_of_attempted_tasks: 4206142119.5542016

solvability_ratio: 0.0

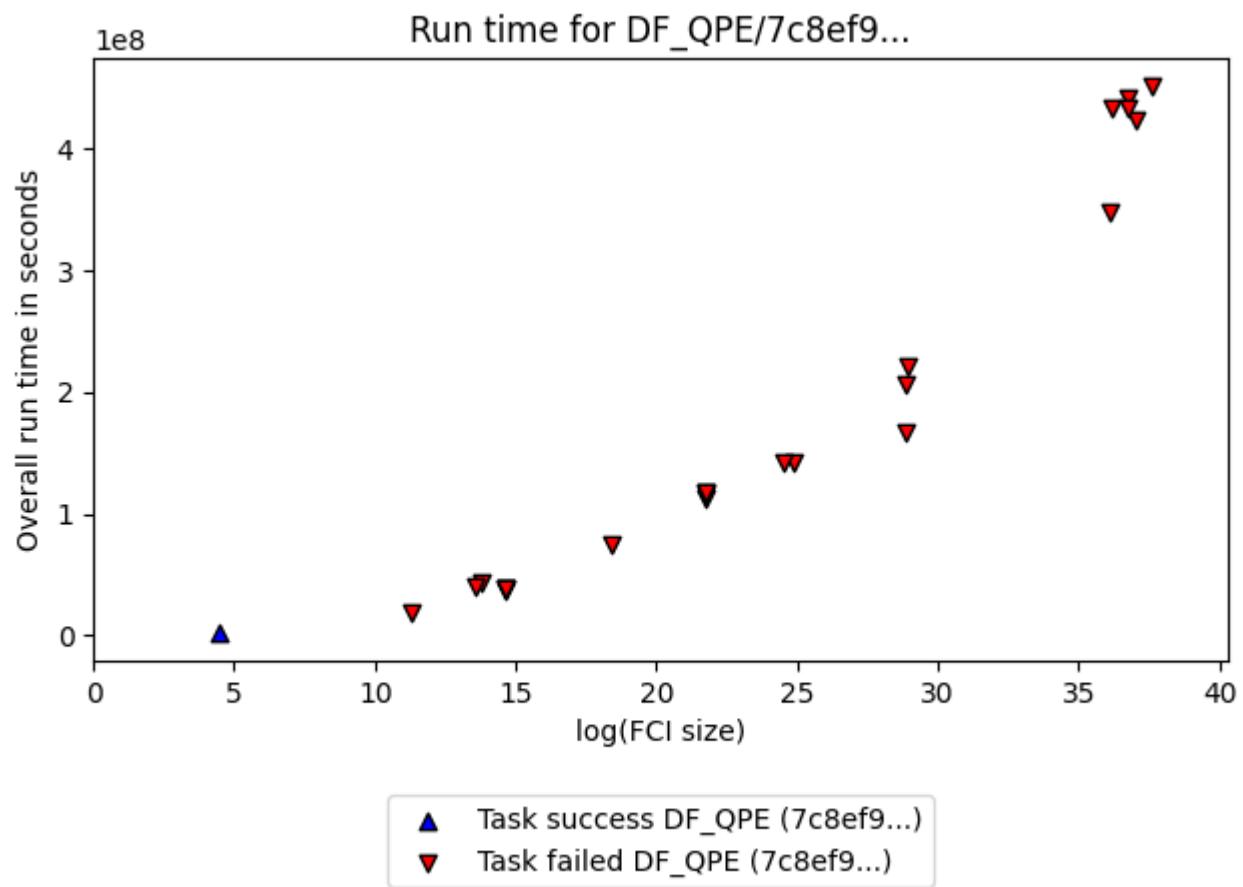
comments: solvability ratio based on PCA embedding., ML model calculated without GridSearchCV

f1_score: [0.9370629370629371, 0.1]

ml_metrics_calculator_version: 1



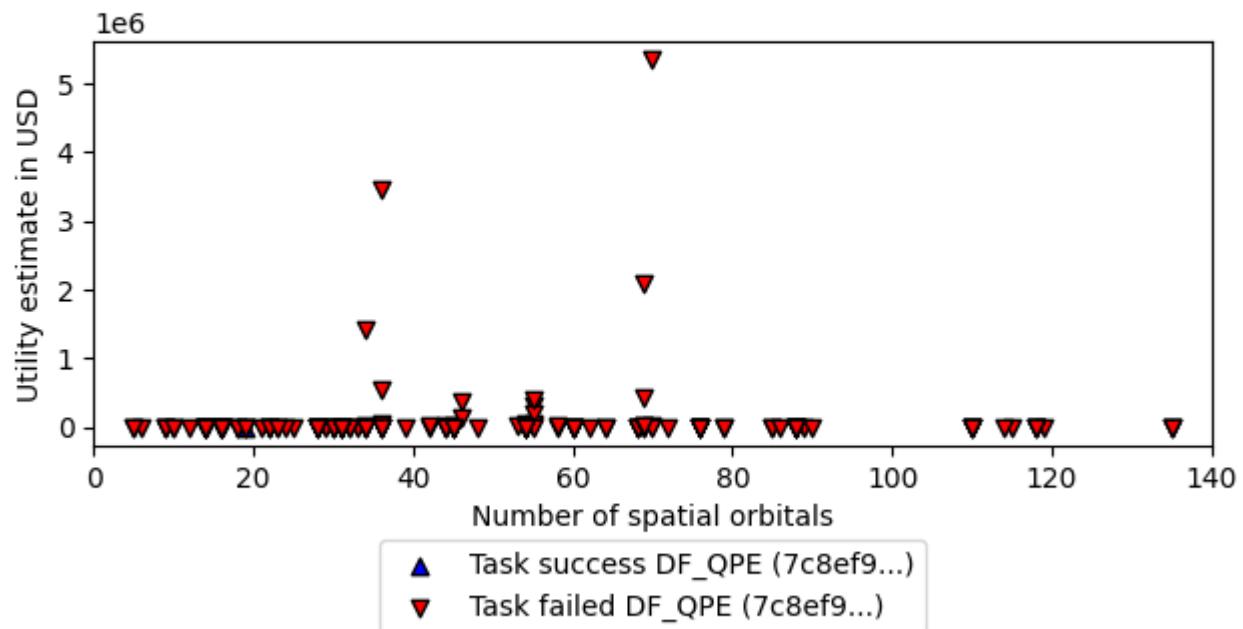
Note: plot only contains attempted tasks.



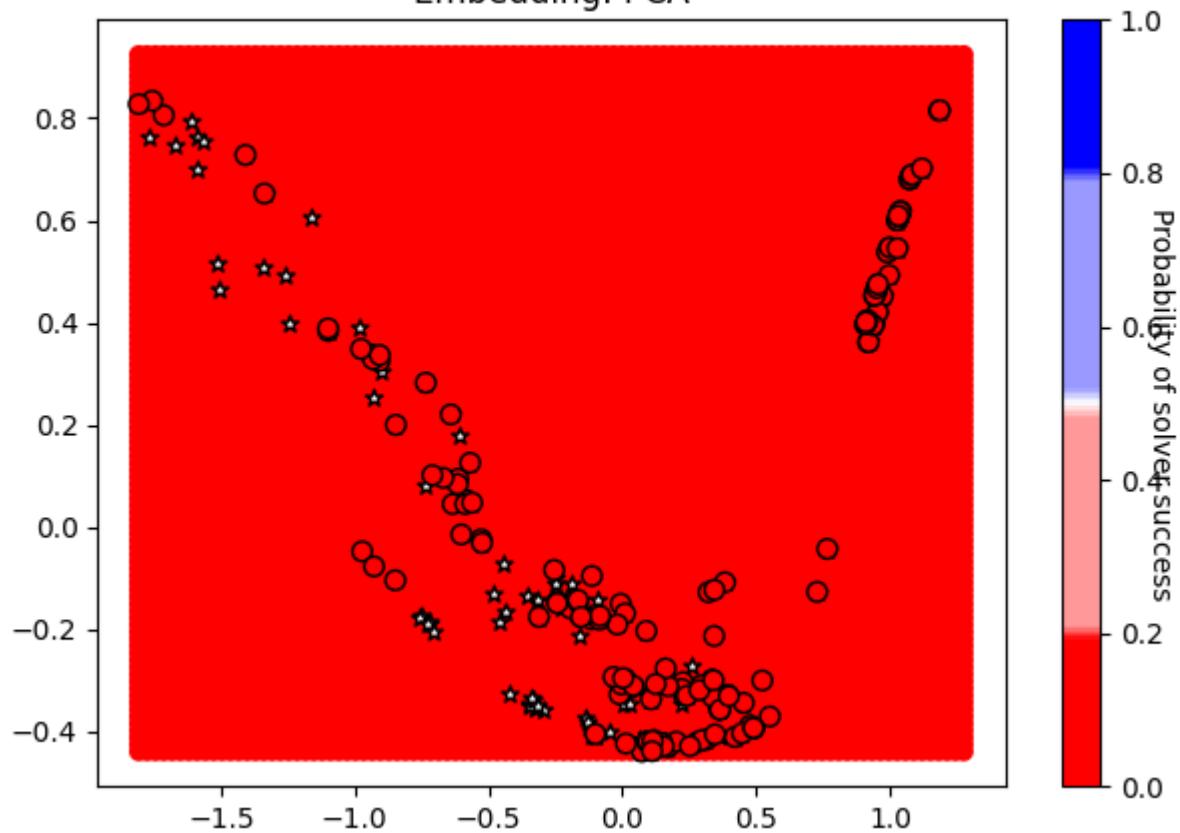
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/7c8ef9...

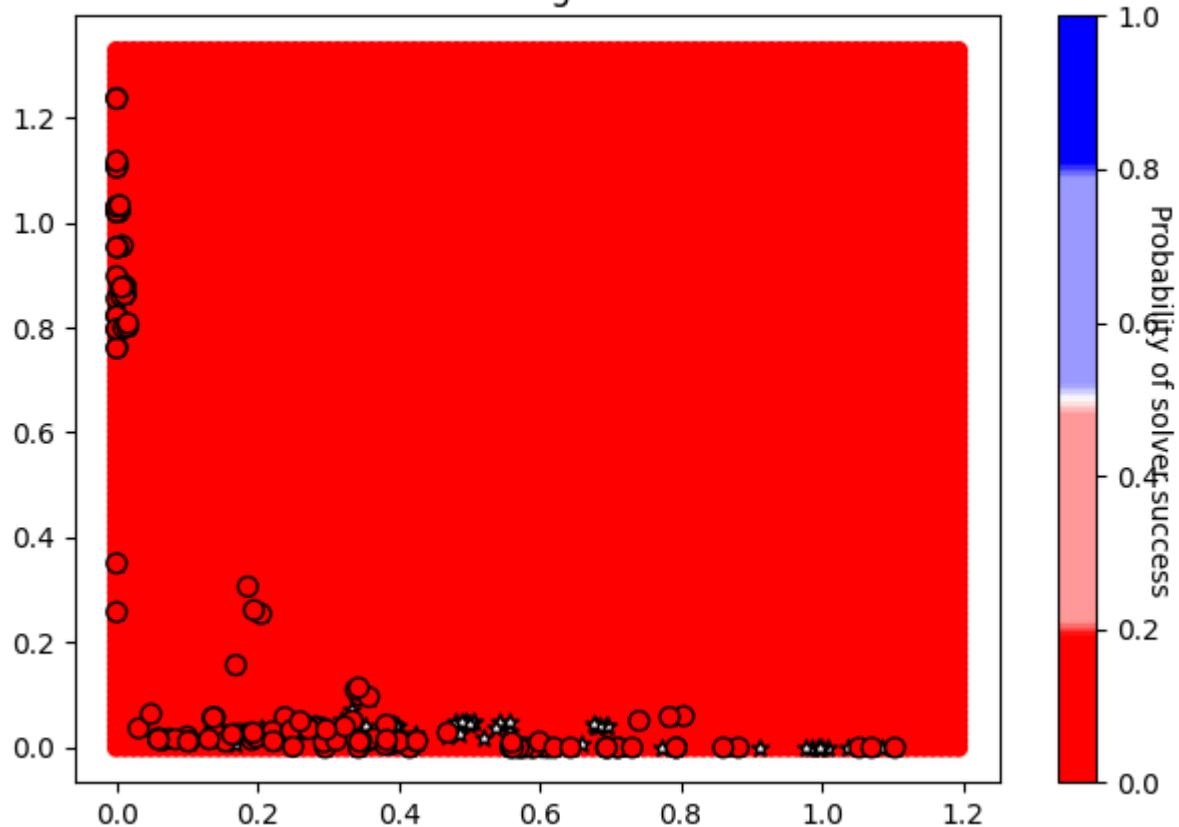
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



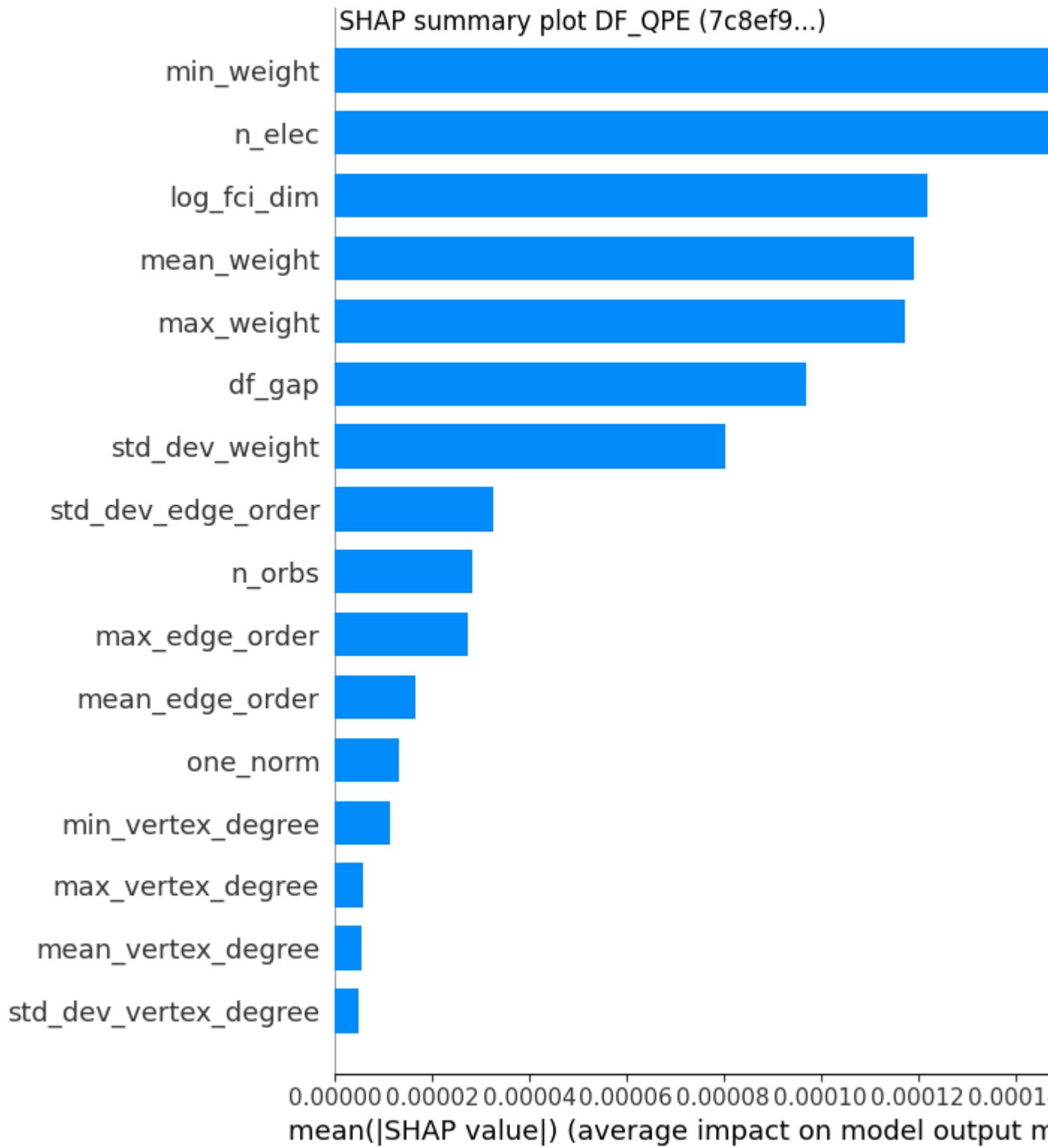
Solver DF_QPE (7c8ef9...)
Embedding: PCA



Solver DF_QPE (7c8ef9...)
Embedding: NNMF



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



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

solver_uuid:f6b36bde-be4a-4eee-975b-2c5f7e553f5f

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70}}

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

quantum_hardware_details:{'quantum_hardware_description': 'Ultra-optimistic hardware model based on the superconducting architecture described in https://arxiv.org/abs/2011.03494.'}, 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 1e-06, 'cycle_time_microseconds': 0.1, 'parallelize_shots': False}}

logical_resource_estimate_solution_uuid:0b52167c-c35a-4cf9-a0ad-bc85c06fac5f

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

performance_metrics_uuid: fa89b48e-4300-4ca4-885e-27477228d154

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 24

number_of_problem_instances_solved: 4

number_of_tasks: 228

number_of_tasks_attempted: 137

number_of_tasks_solved: 5

number_of_tasks_solved_within_run_time_limit: 5

number_of_tasks_solved_within_accuracy_threshold: 137

max_run_time_of_attempted_tasks: 7188148035230.209

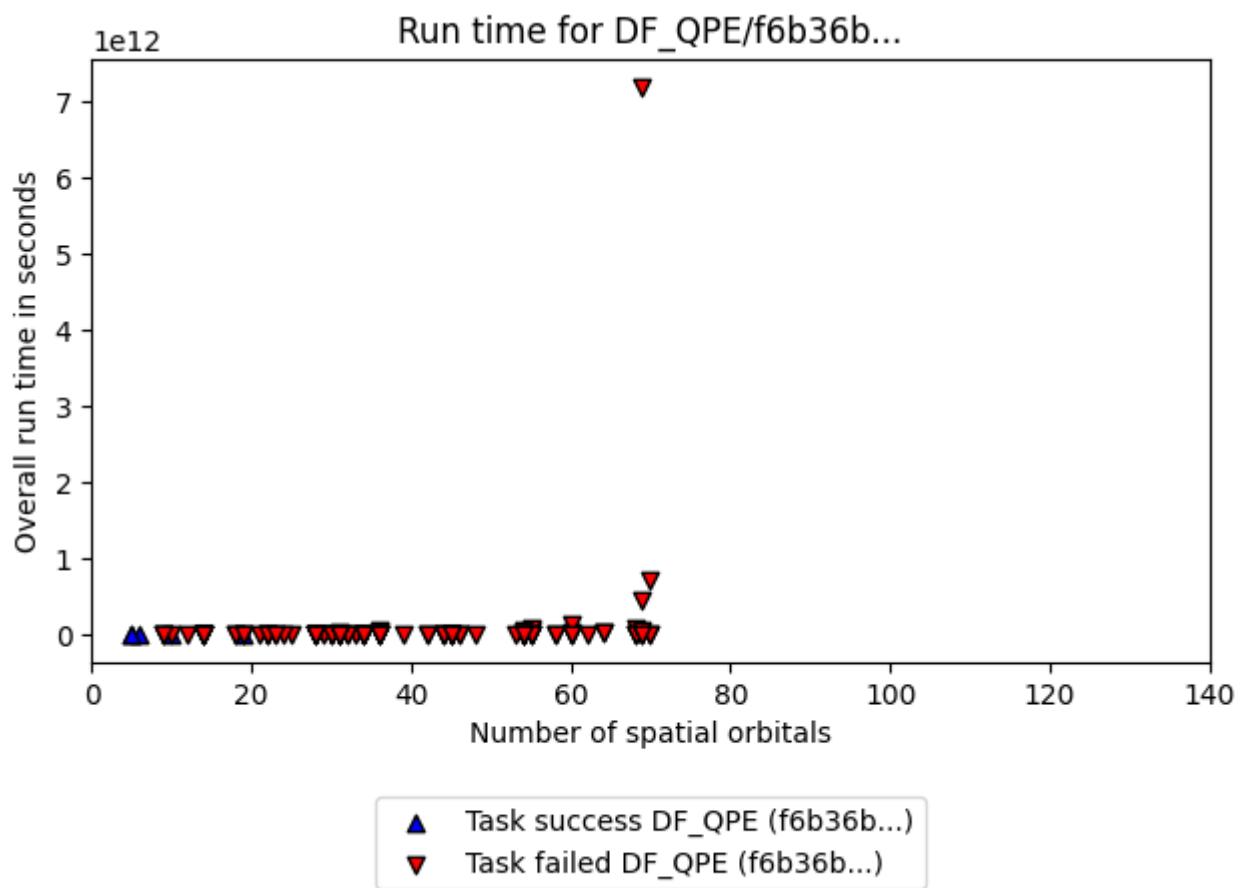
sum_of_run_time_of_attempted_tasks: 9230378074762.195

solvability_ratio: 0.013

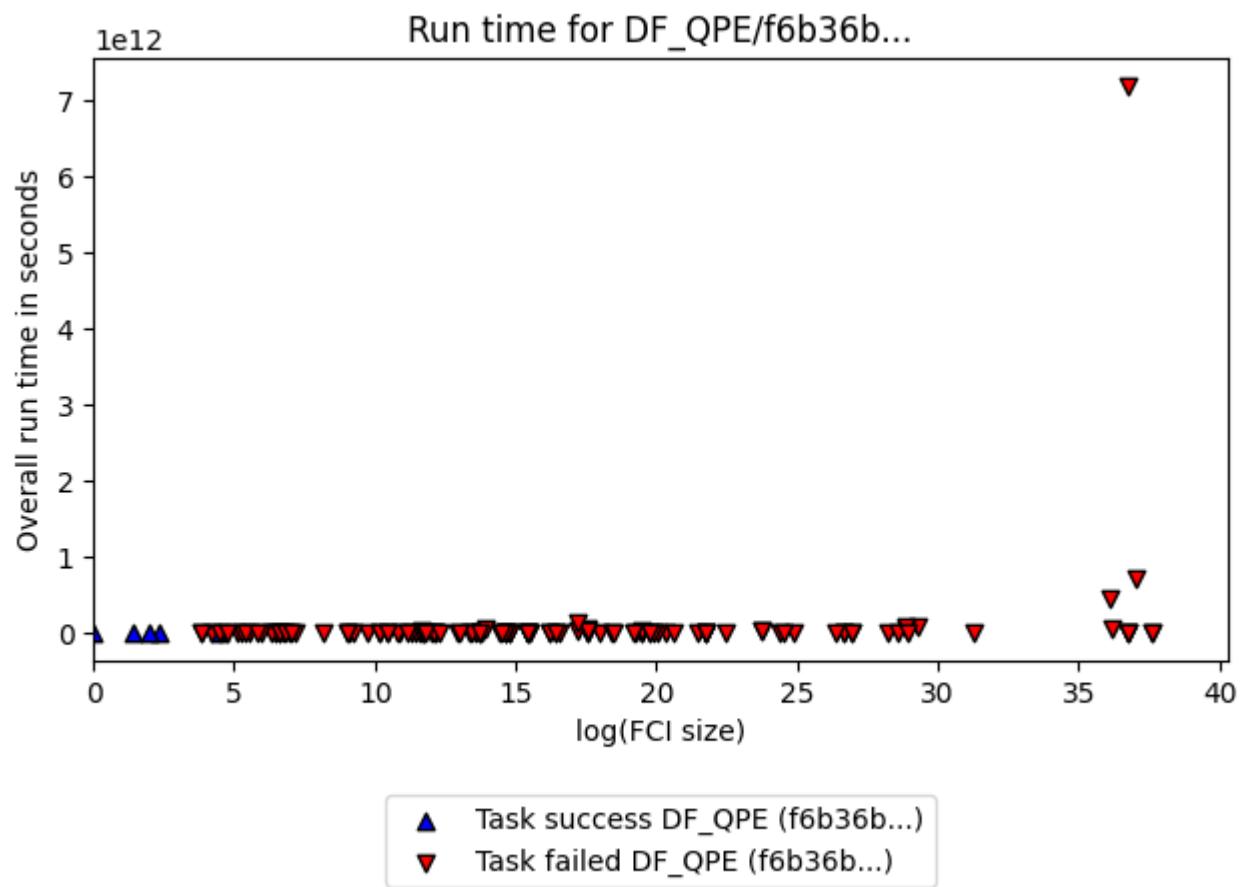
comments: solvability ratio based on PCA embedding.

f1_score: [0.9931972789115646, 0.8333333333333334]

ml_metrics_calculator_version: 1



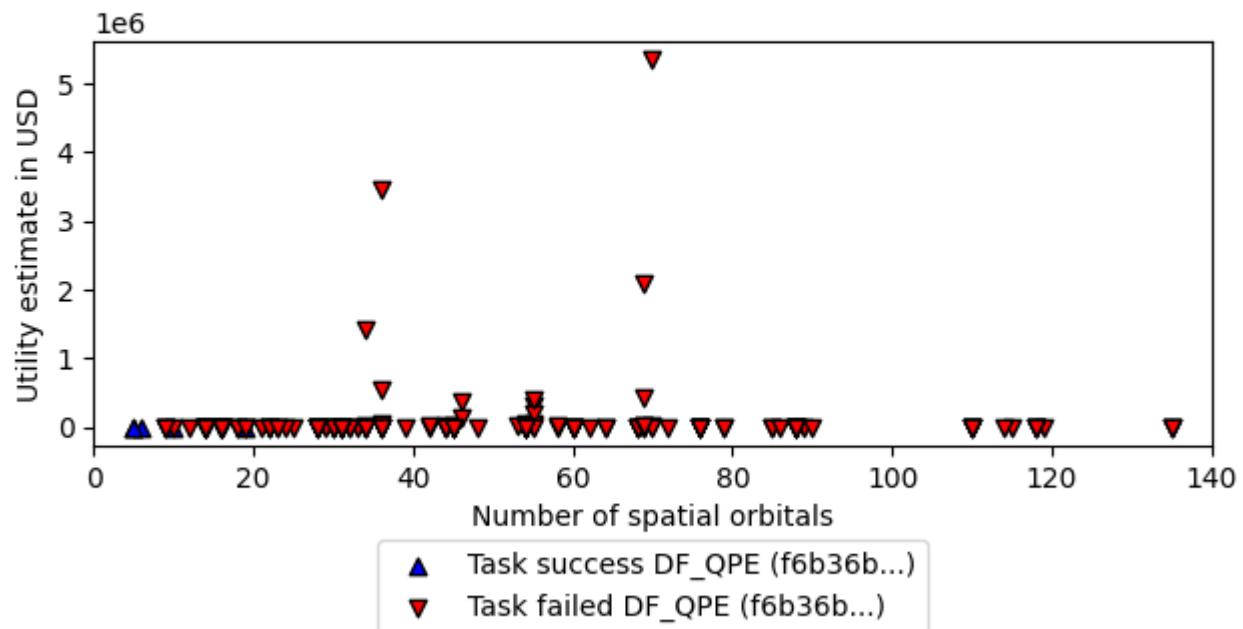
Note: plot only contains attempted tasks.



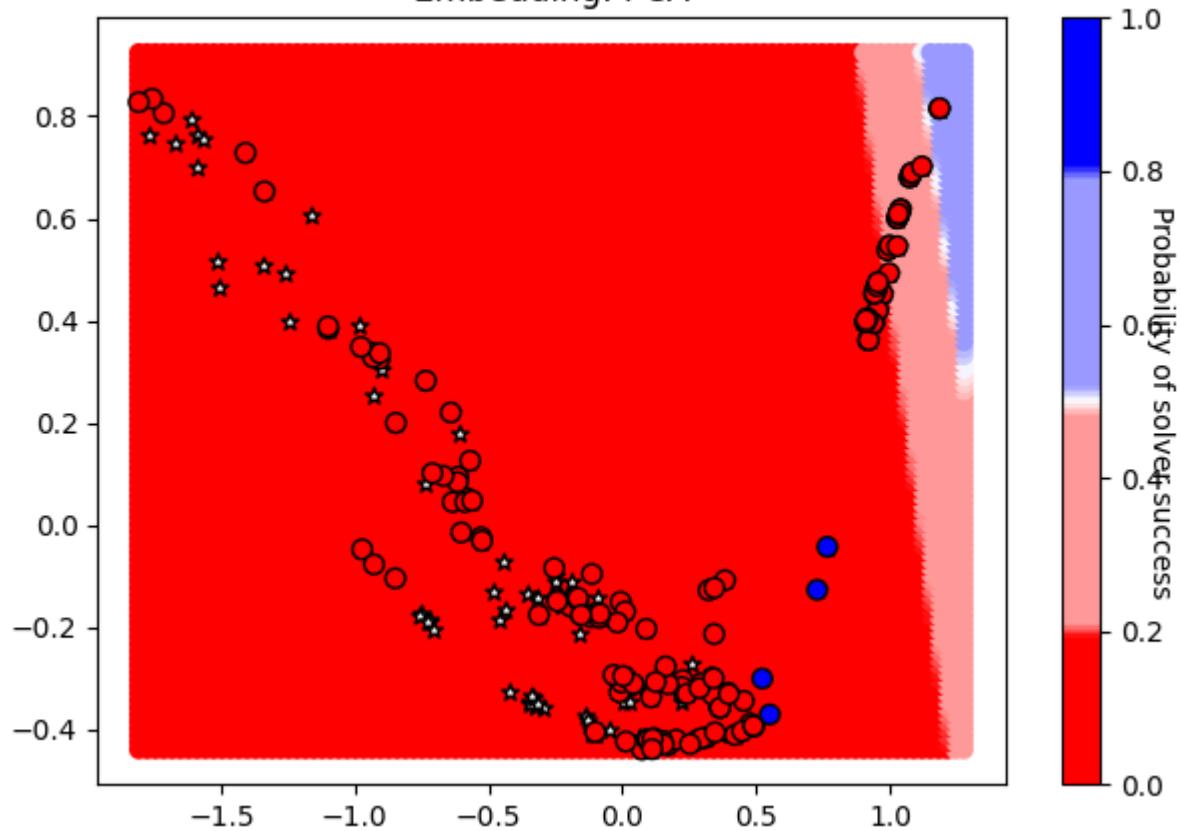
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/f6b36b...

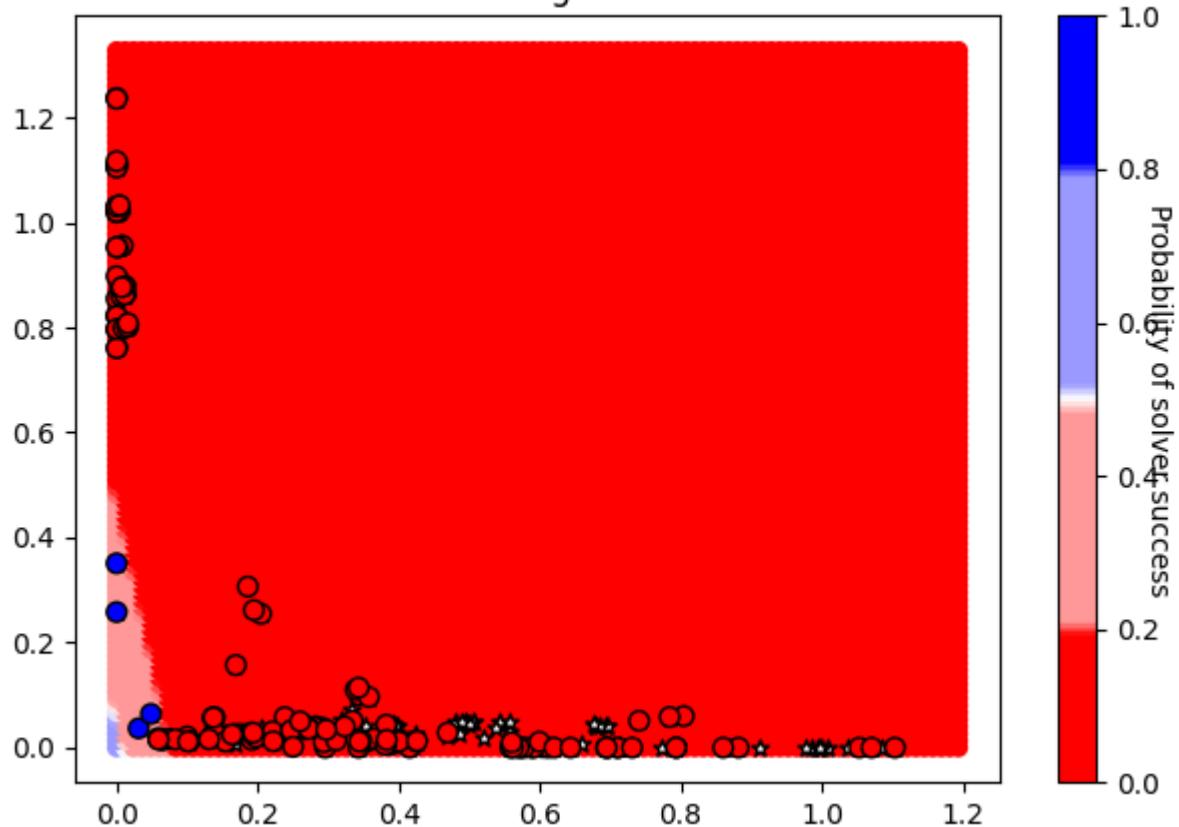
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



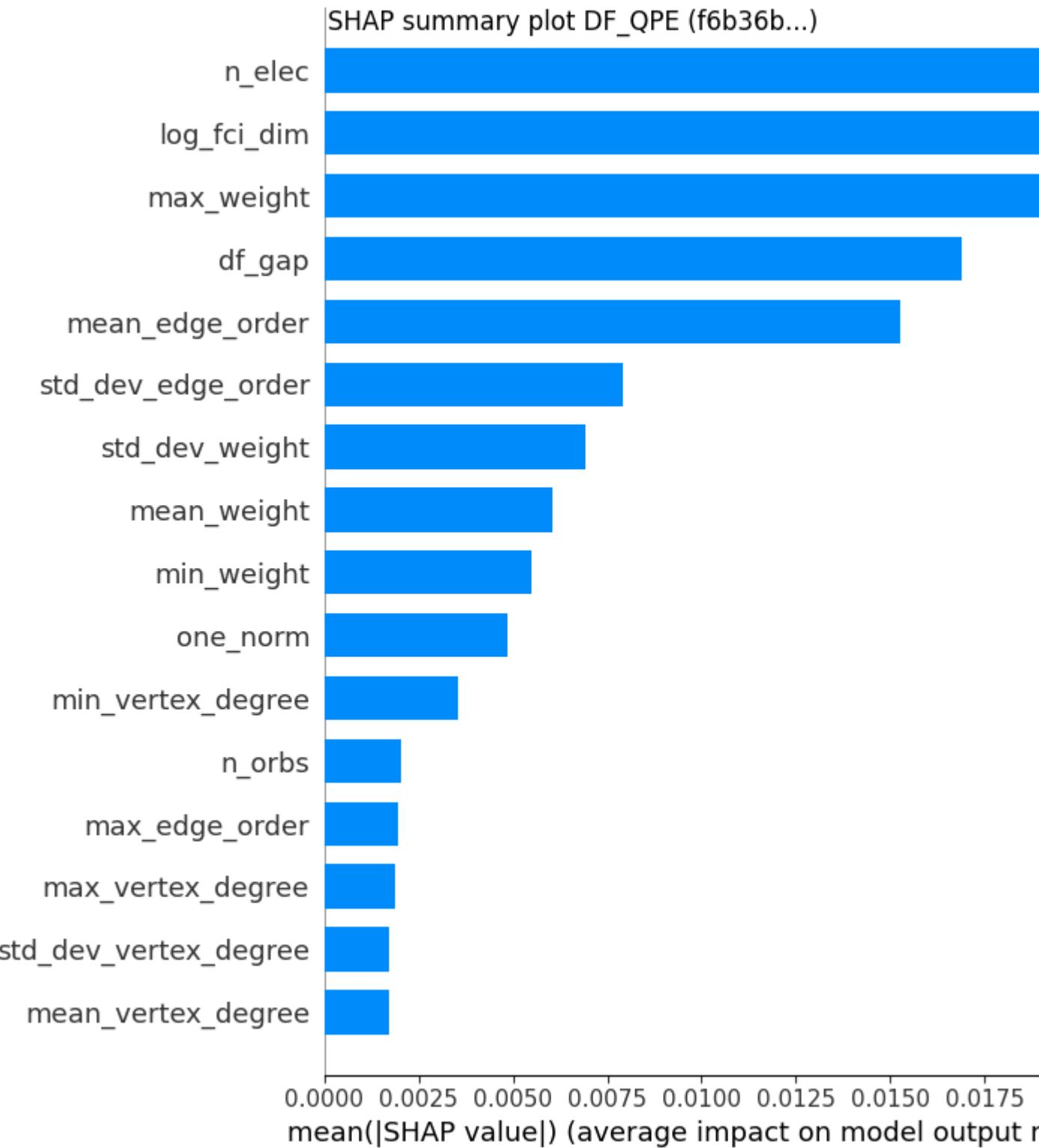
Solver DF_QPE (f6b36b...)
Embedding: PCA



Solver DF_QPE (f6b36b...)
Embedding: NNMF



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



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

solver_uuid:5d768520-b3d0-4292-bbb4-9776fa128107

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70}}

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

quantum.hardware_details:{'quantum.hardware_description': 'Superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494 with an extremely optimistic physical error rate.', 'quantum.hardware_parameters': {'num_factories': 4, 'physical_error_rate': 1e-06, 'cycle_time_microseconds': 1, 'parallelize_shots': False}}

logical_resource_estimate_solution_uuid:0b52167c-c35a-4cf9-a0ad-bc85c06fac5f

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

performance_metrics_uuid: 6f7eacb5-5565-474a-9d2a-fb46ba16dd45

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 24

number_of_problem_instances_solved: 2

number_of_tasks: 228

number_of_tasks_attempted: 137

number_of_tasks_solved: 2

number_of_tasks_solved_within_run_time_limit: 2

number_of_tasks_solved_within_accuracy_threshold: 137

max_run_time_of_attempted_tasks: 71881480309947.6

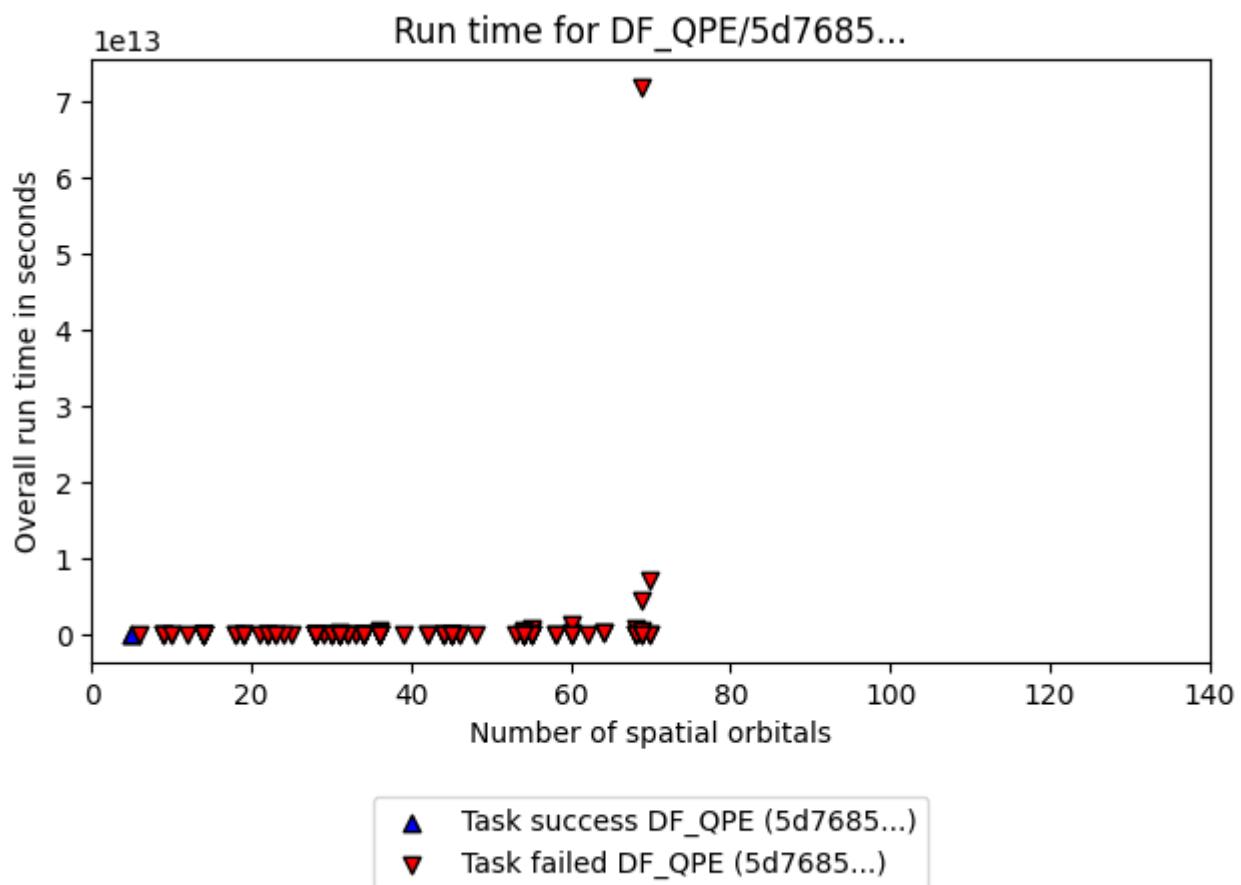
sum_of_run_time_of_attempted_tasks: 92303779447162.08

solvability_ratio: 0.0394

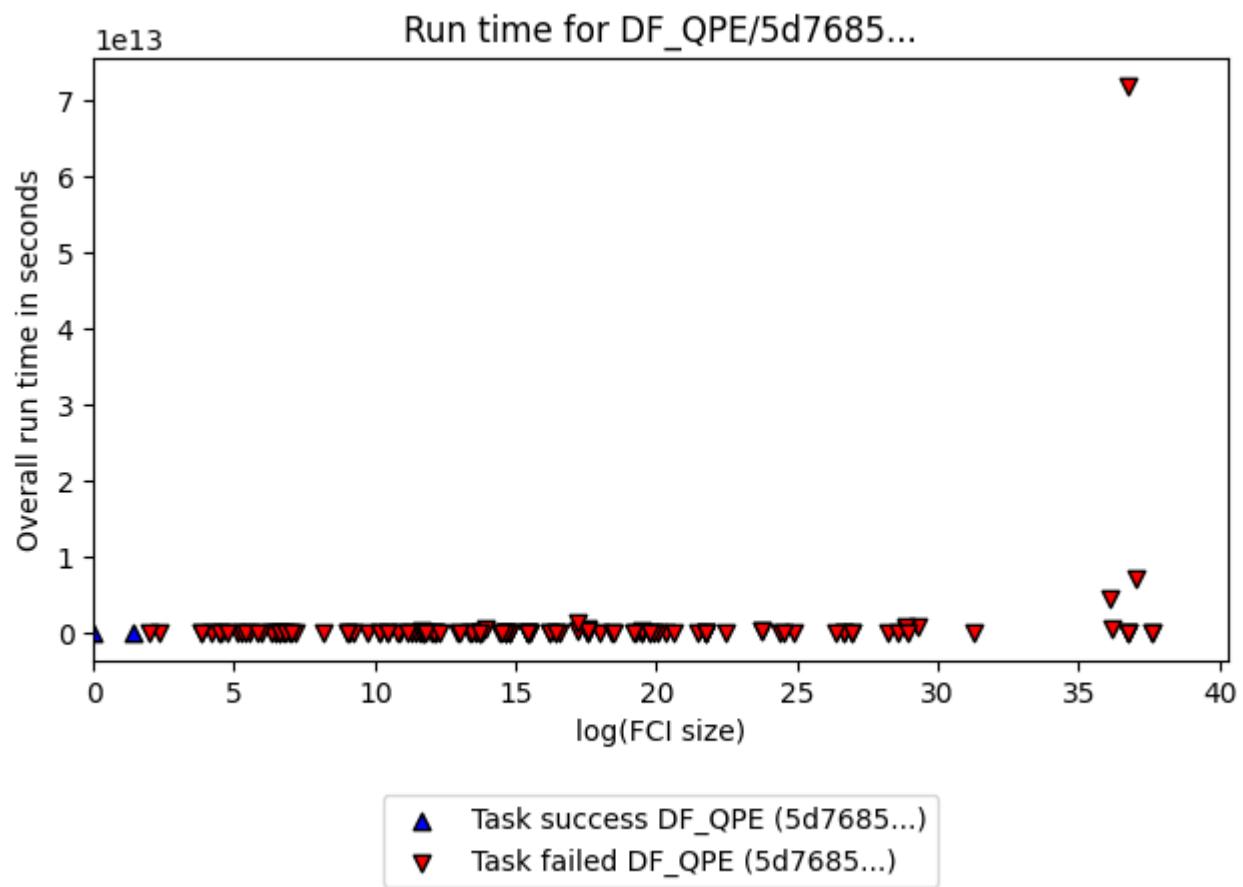
comments: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



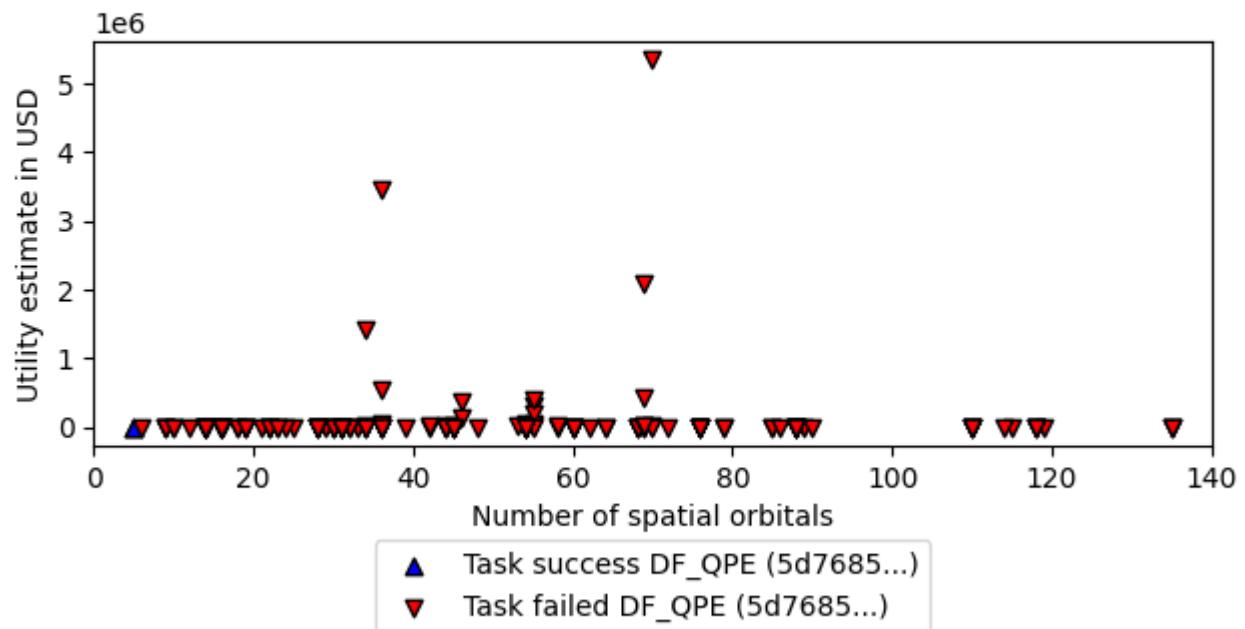
Note: plot only contains attempted tasks.



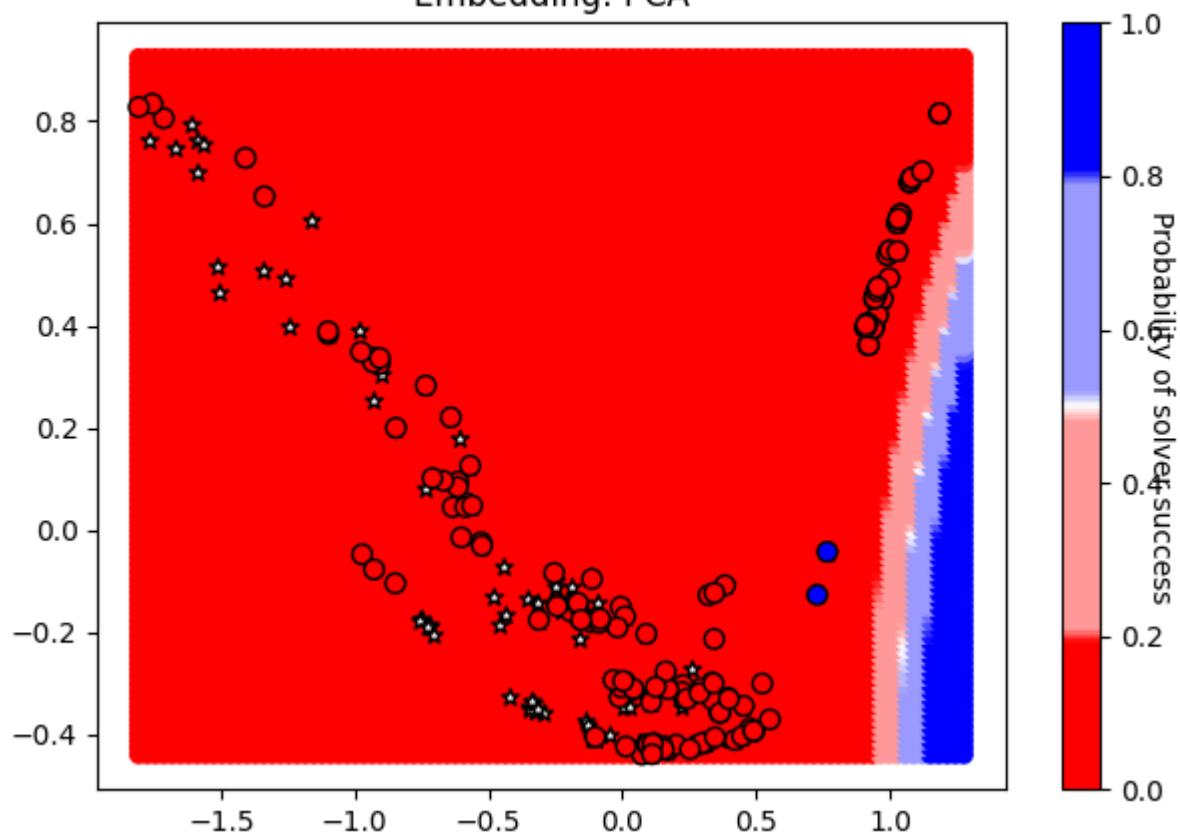
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5d7685...

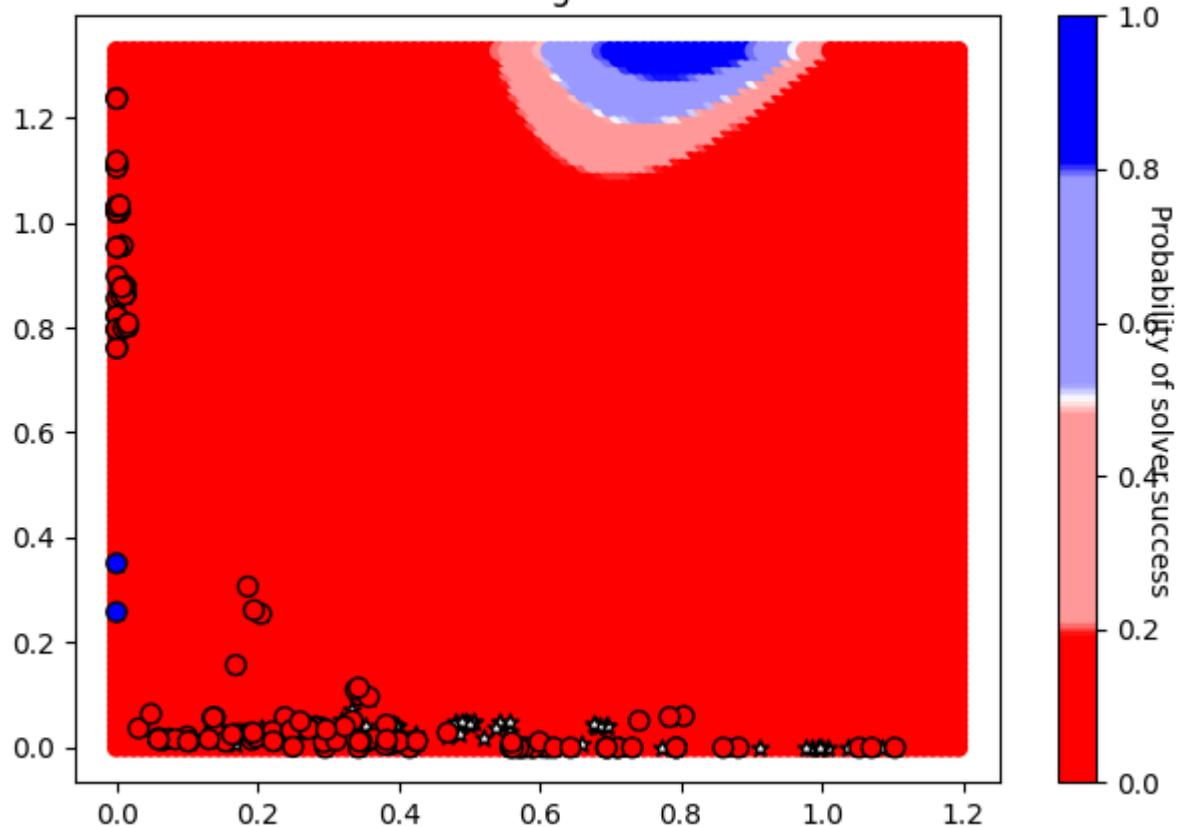
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



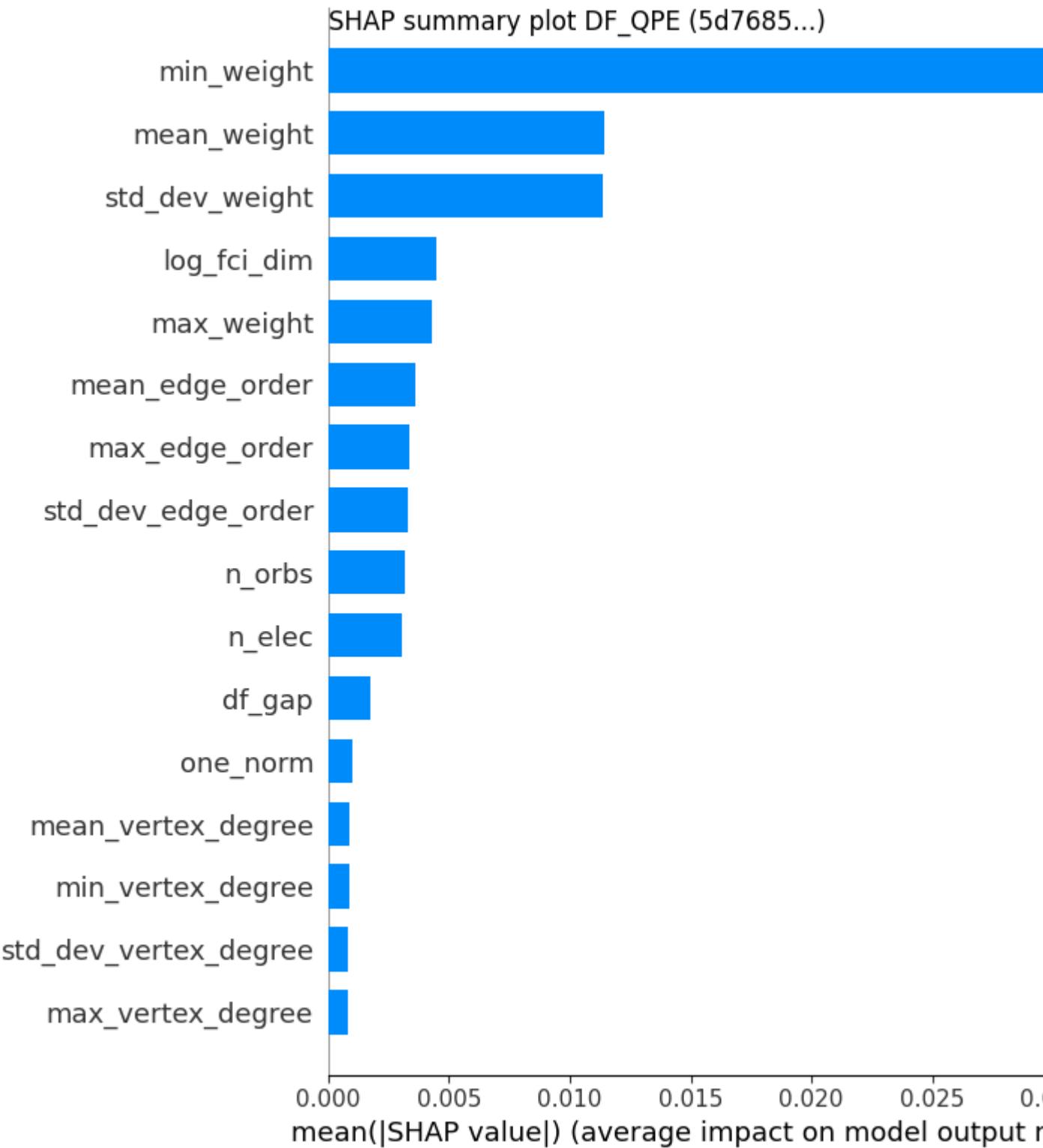
Solver DF_QPE (5d7685...)
Embedding: PCA



Solver DF_QPE (5d7685...)
Embedding: NMF



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



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

solver_uuid:2610d8de-bd3a-469e-9a80-473e8988755f

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70}}

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

quantum_hardware_details:{'quantum_hardware_description': 'Ultra-optimistic hardware model based on the superconducting architecture described in https://arxiv.org/abs/2011.03494.'}, 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.0001, 'cycle_time_microseconds': 0.1, 'parallelize_shots': False}}

logical_resource_estimate_solution_uuid:32037675-e2b9-46d5-9920-ec47386ceaf3

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

performance_metrics_uuid: 340f1c34-9915-474a-98eb-53be283a7e04

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 22

number_of_problem_instances_solved: 3

number_of_tasks: 228

number_of_tasks_attempted: 131

number_of_tasks_solved: 4

number_of_tasks_solved_within_run_time_limit: 4

number_of_tasks_solved_within_accuracy_threshold: 131

max_run_time_of_attempted_tasks: 139405710024.59732

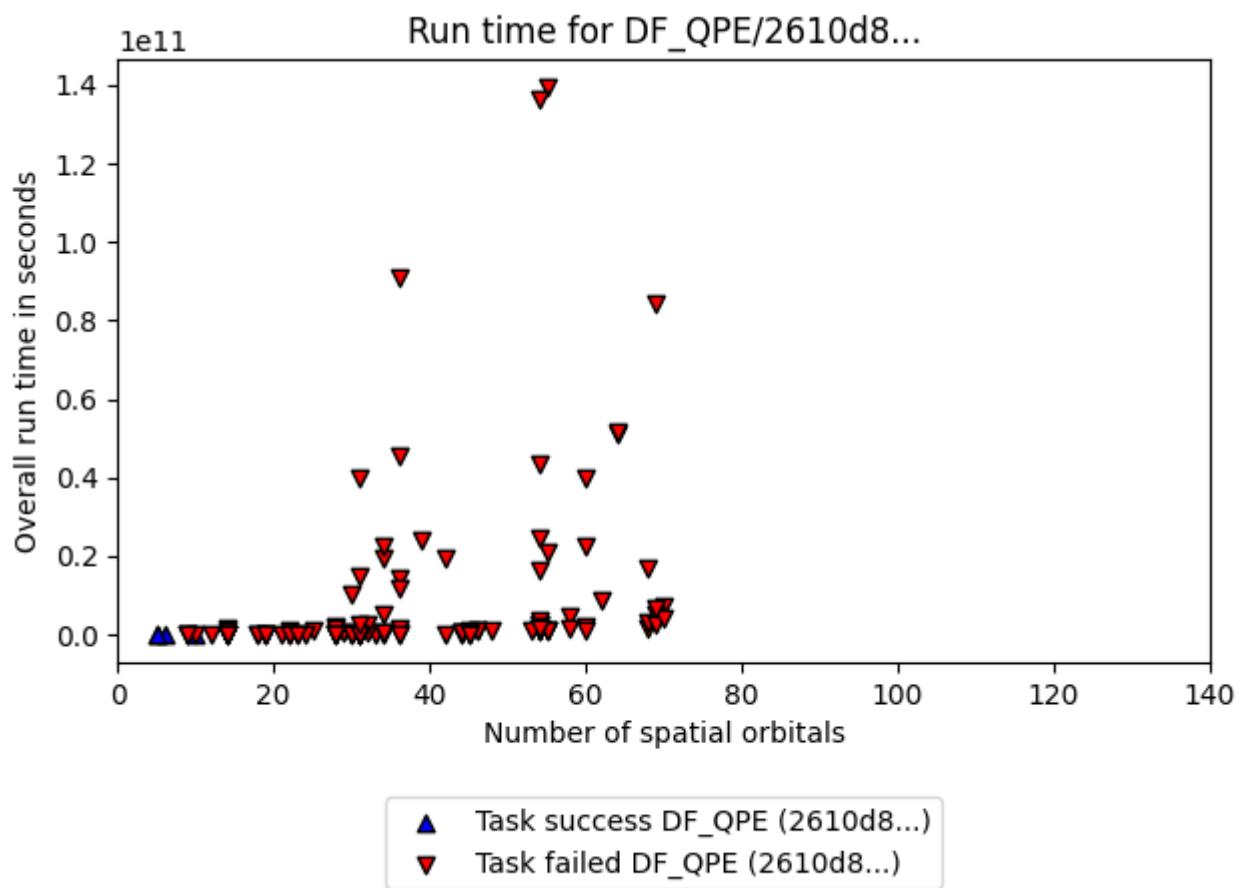
sum_of_run_time_of_attempted_tasks: 1070189510131.8345

solvability_ratio: 0.0716

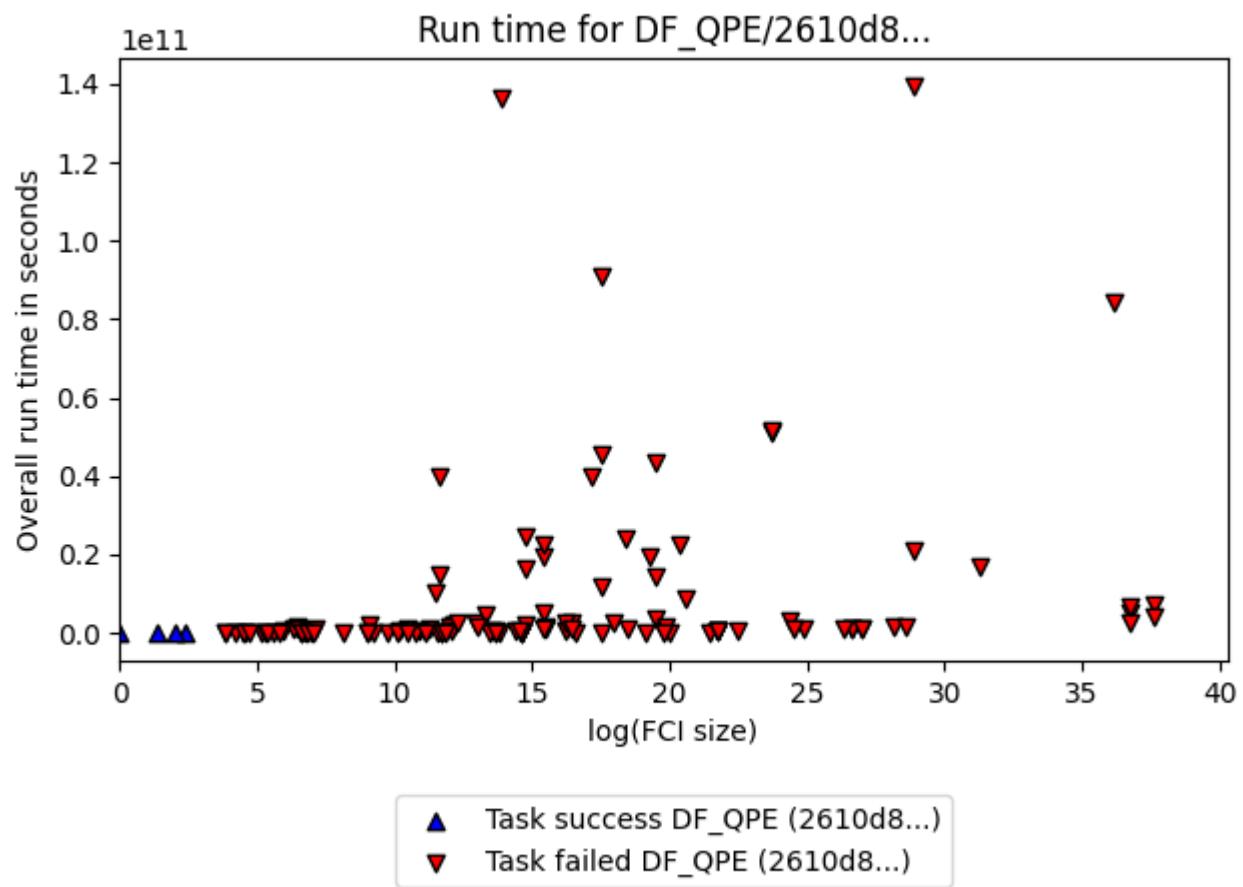
comments: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



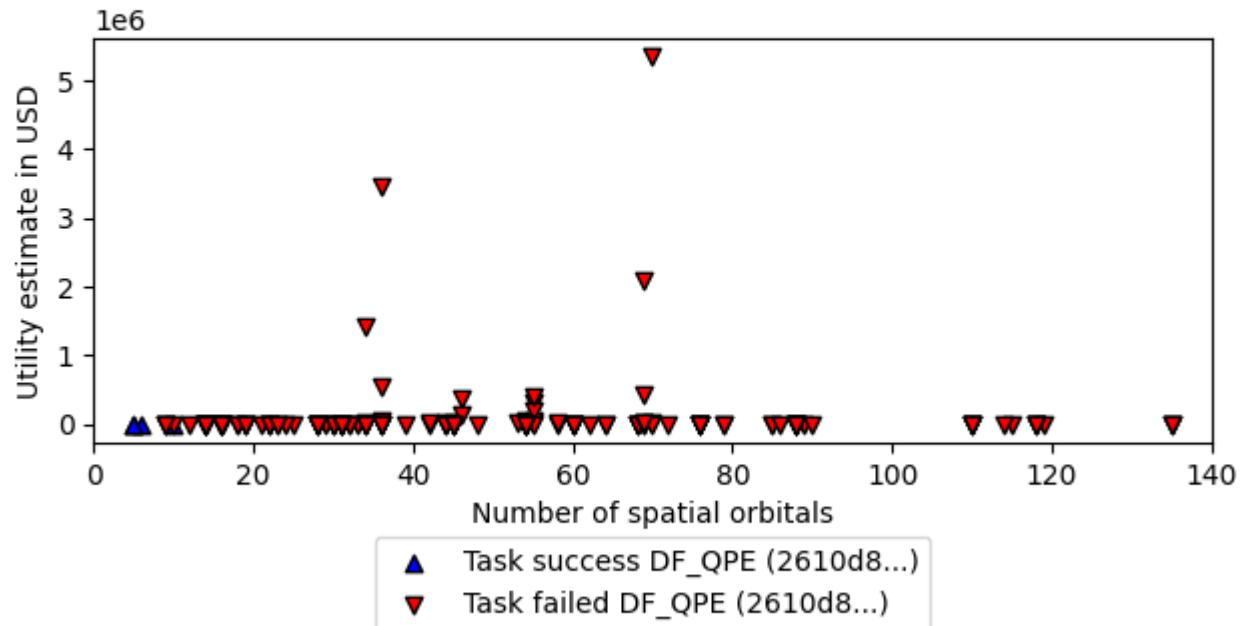
Note: plot only contains attempted tasks.



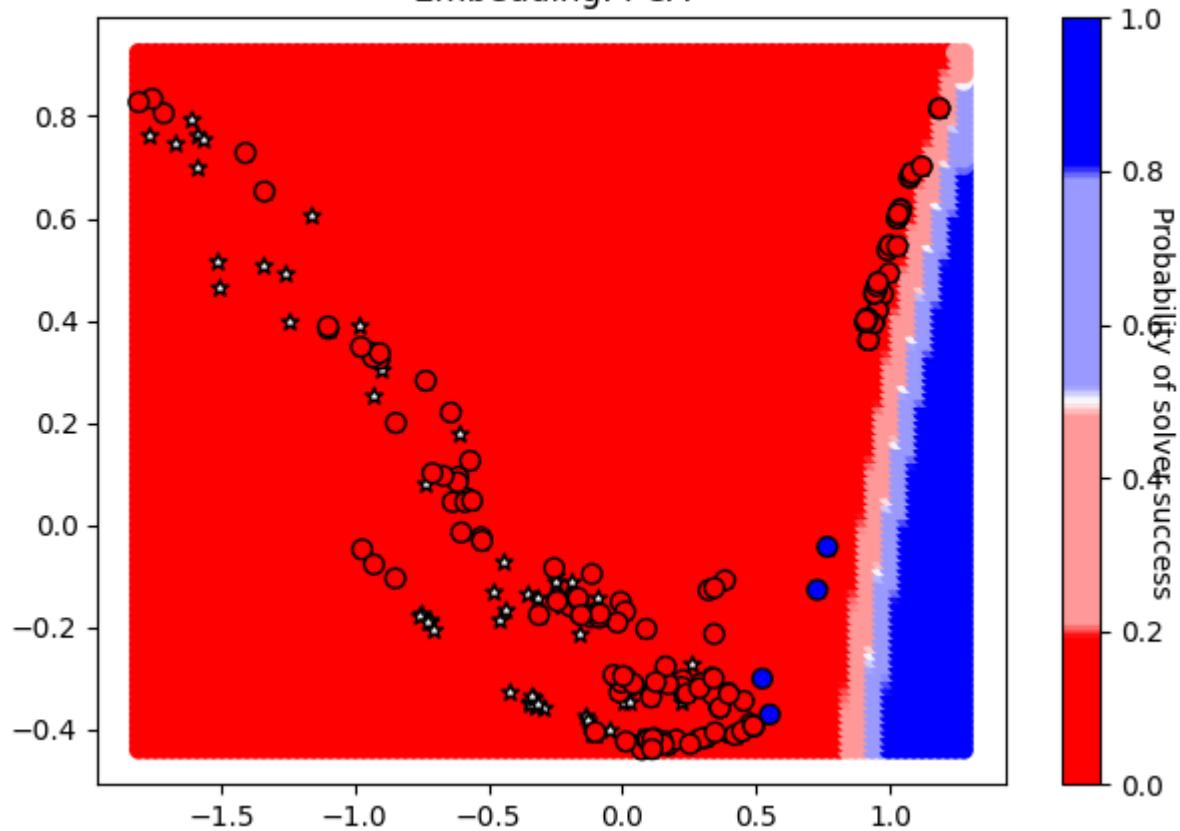
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/2610d8...

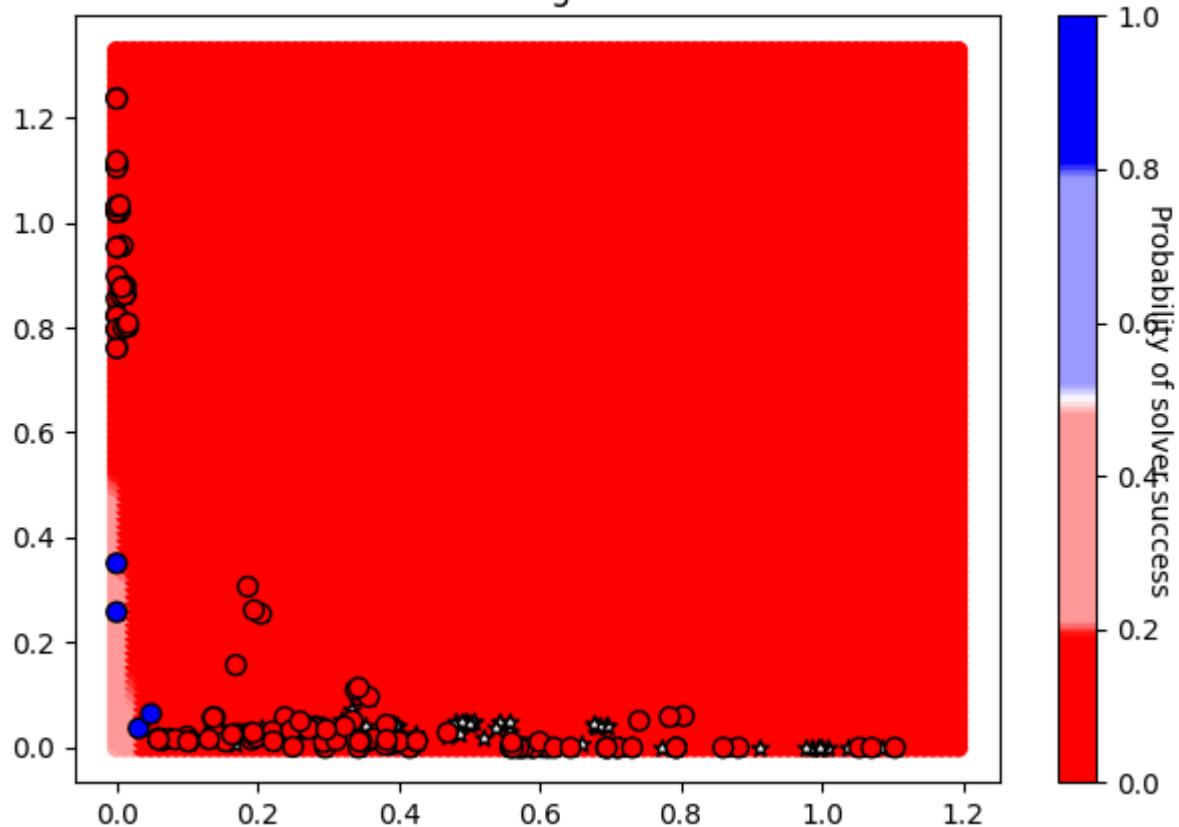
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



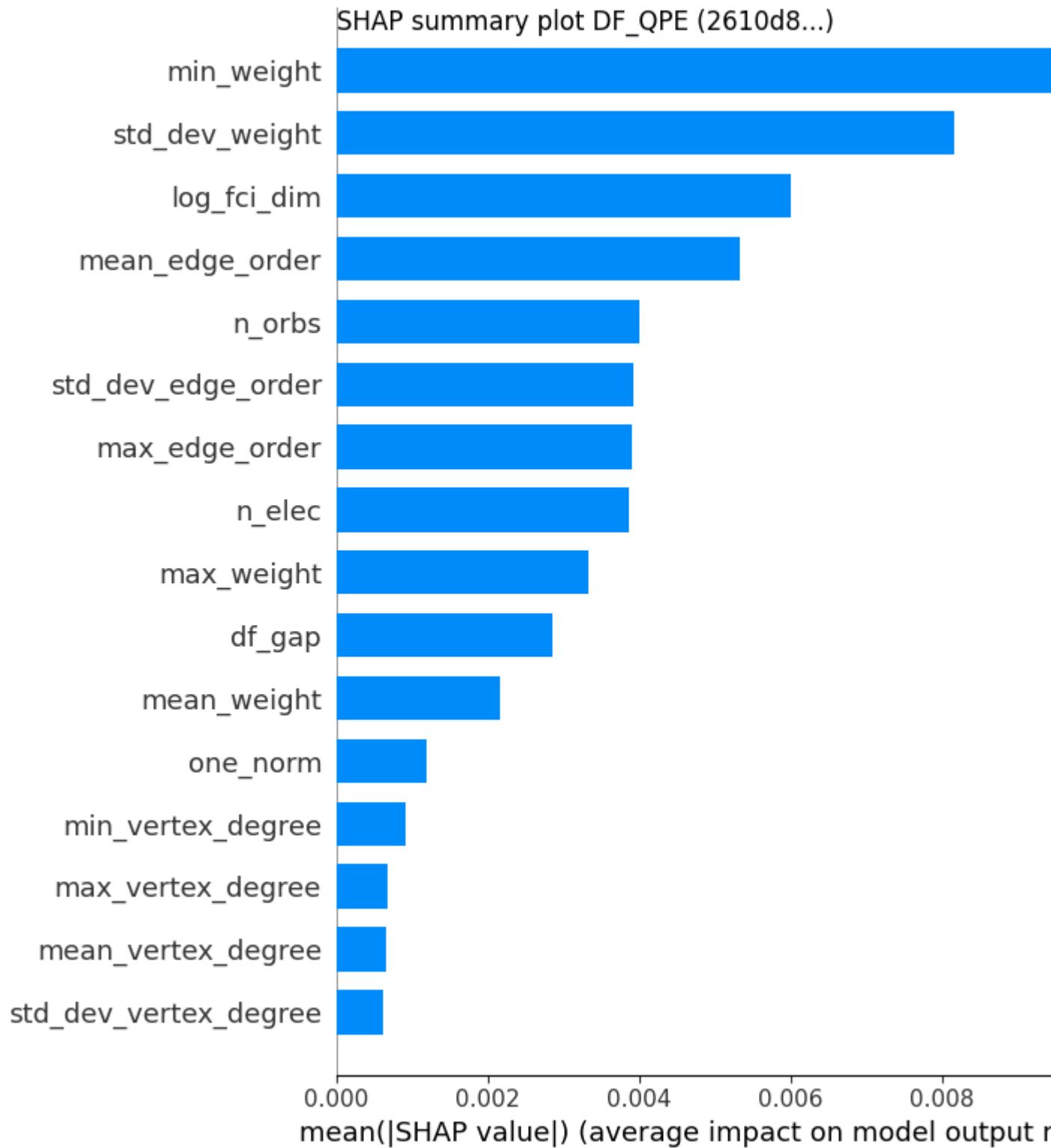
Solver DF_QPE (2610d8...)
Embedding: PCA



Solver DF_QPE (2610d8...)
Embedding: NMF



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



Solver DF_QPE, 5dad4064-cd11-412f-85cb-d722afe3b3de

solver_uuid:5dad4064-cd11-412f-85cb-d722afe3b3de

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70}}

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

quantum_hardware_details:{'quantum_hardware_description': 'Optimistic superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494.', 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.0001, 'cycle_time_microseconds': 1, 'parallelize_shots': False}}

logical_resource_estimate_solution_uuid:32037675-e2b9-46d5-9920-ec47386ceaf3

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

performance_metrics_uuid: aa79a488-9f5e-4ef4-a37d-7e3c0d93604f

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 22

number_of_problem_instances_solved: 2

number_of_tasks: 228

number_of_tasks_attempted: 131

number_of_tasks_solved: 2

number_of_tasks_solved_within_run_time_limit: 2

number_of_tasks_solved_within_accuracy_threshold: 131

max_run_time_of_attempted_tasks: 1394057080220.9934

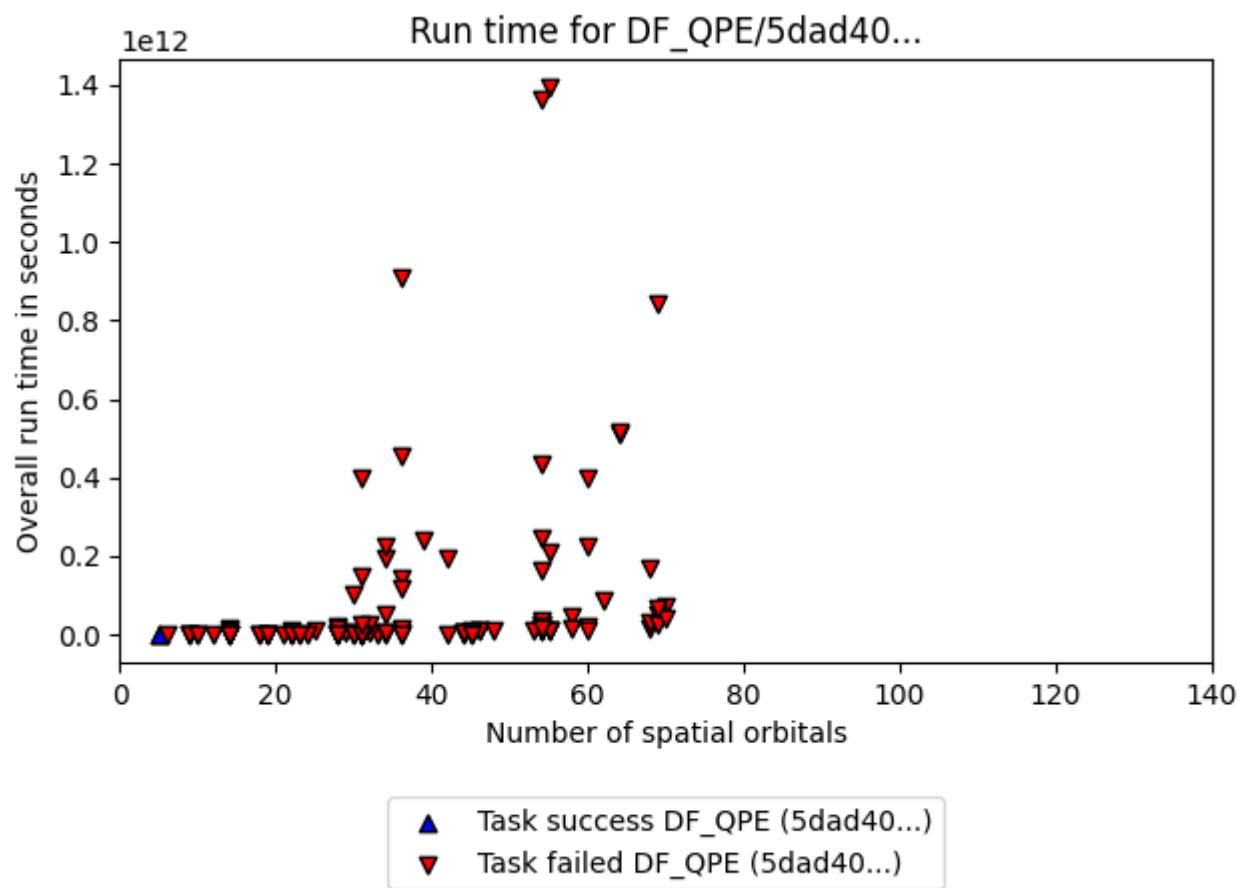
sum_of_run_time_of_attempted_tasks: 10701894024019.273

solvability_ratio: 0.0394

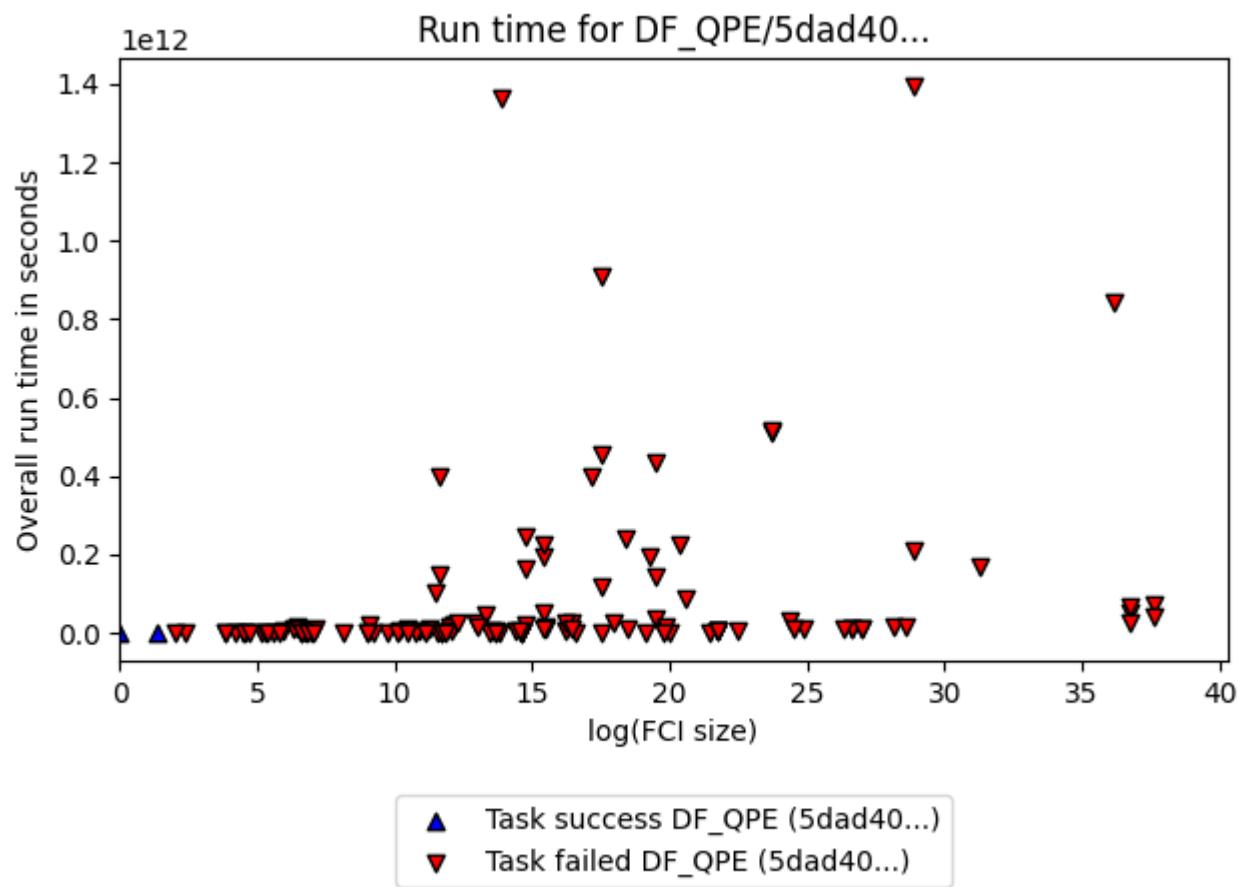
comments: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



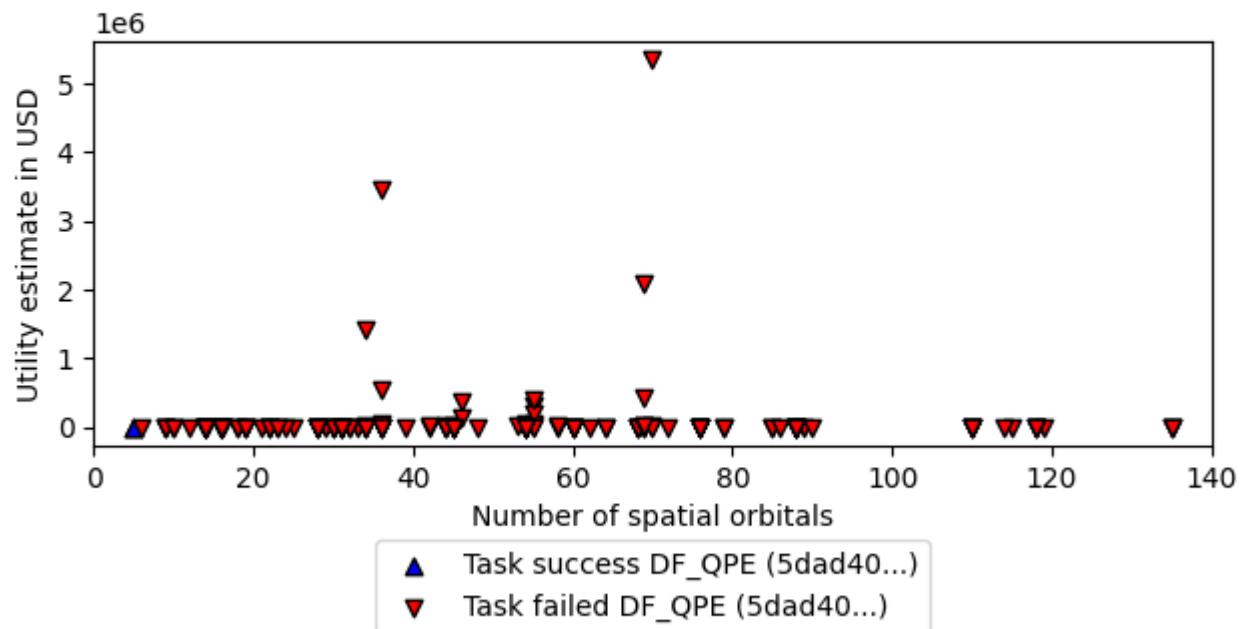
Note: plot only contains attempted tasks.



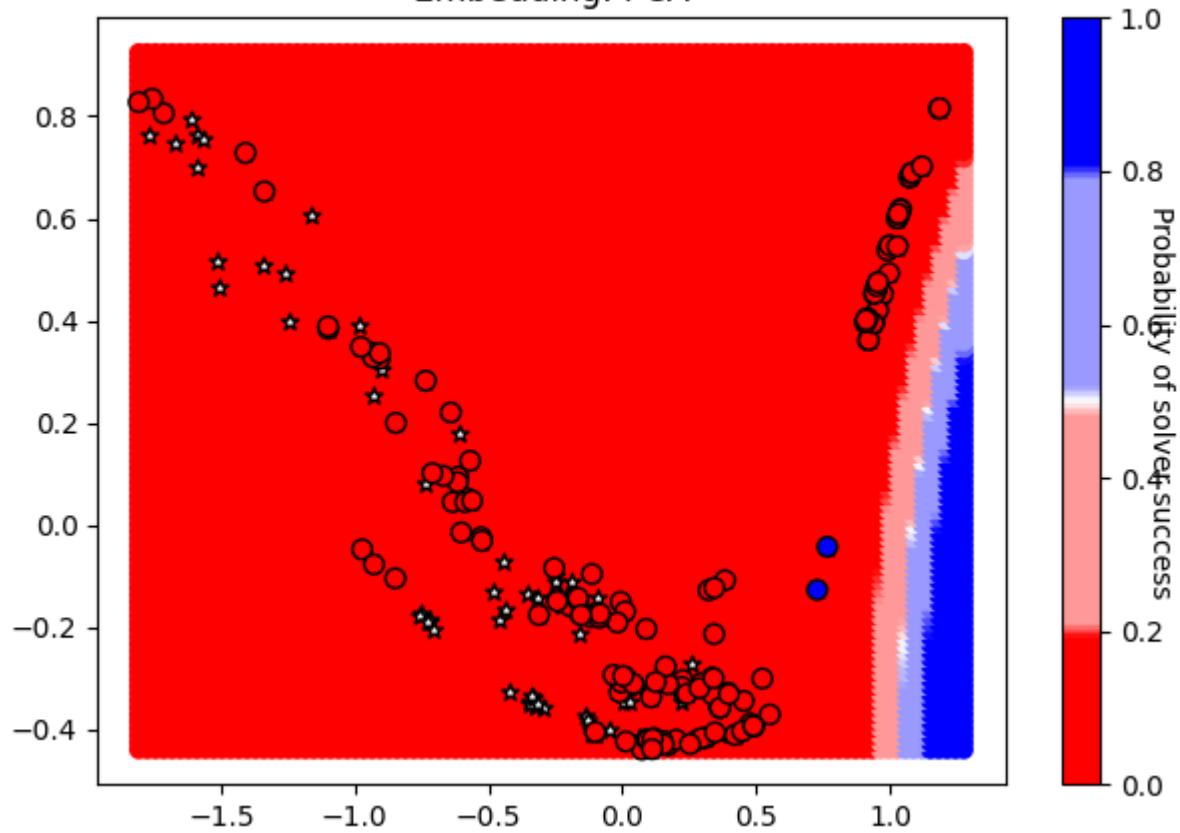
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5dad40...

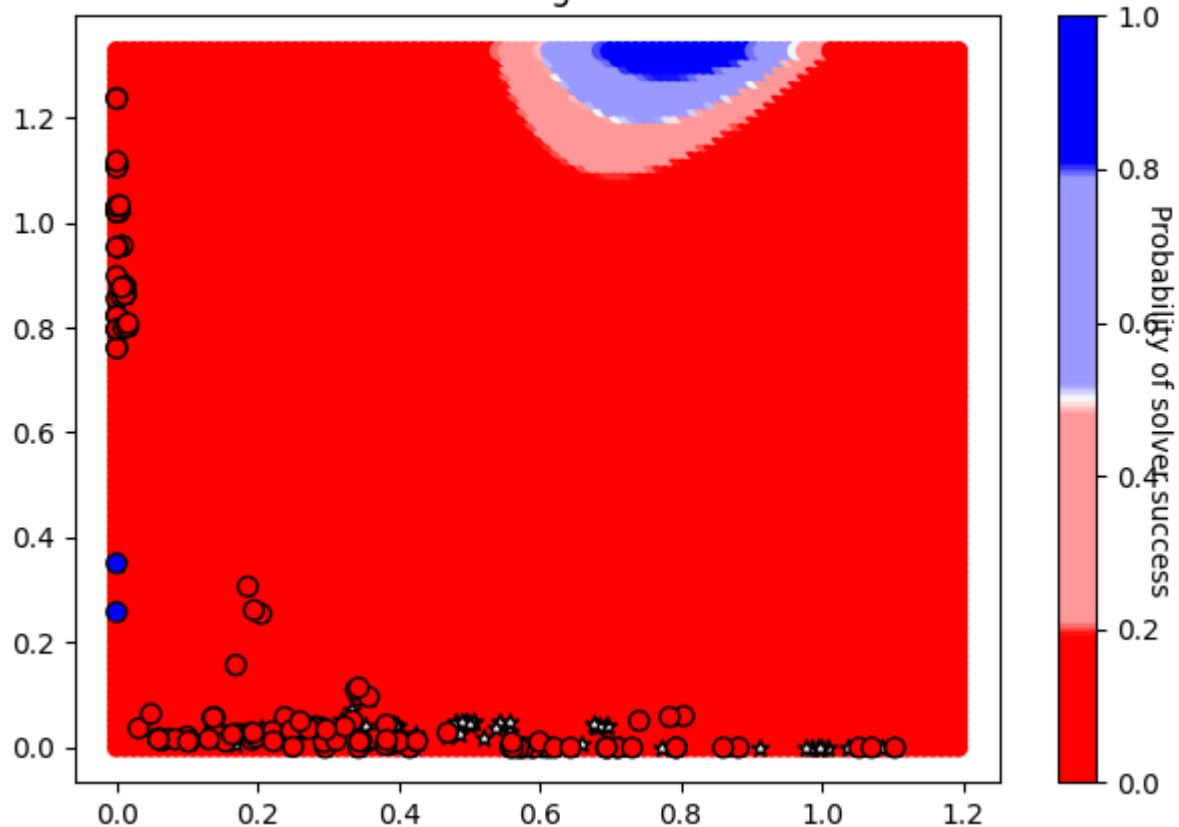
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



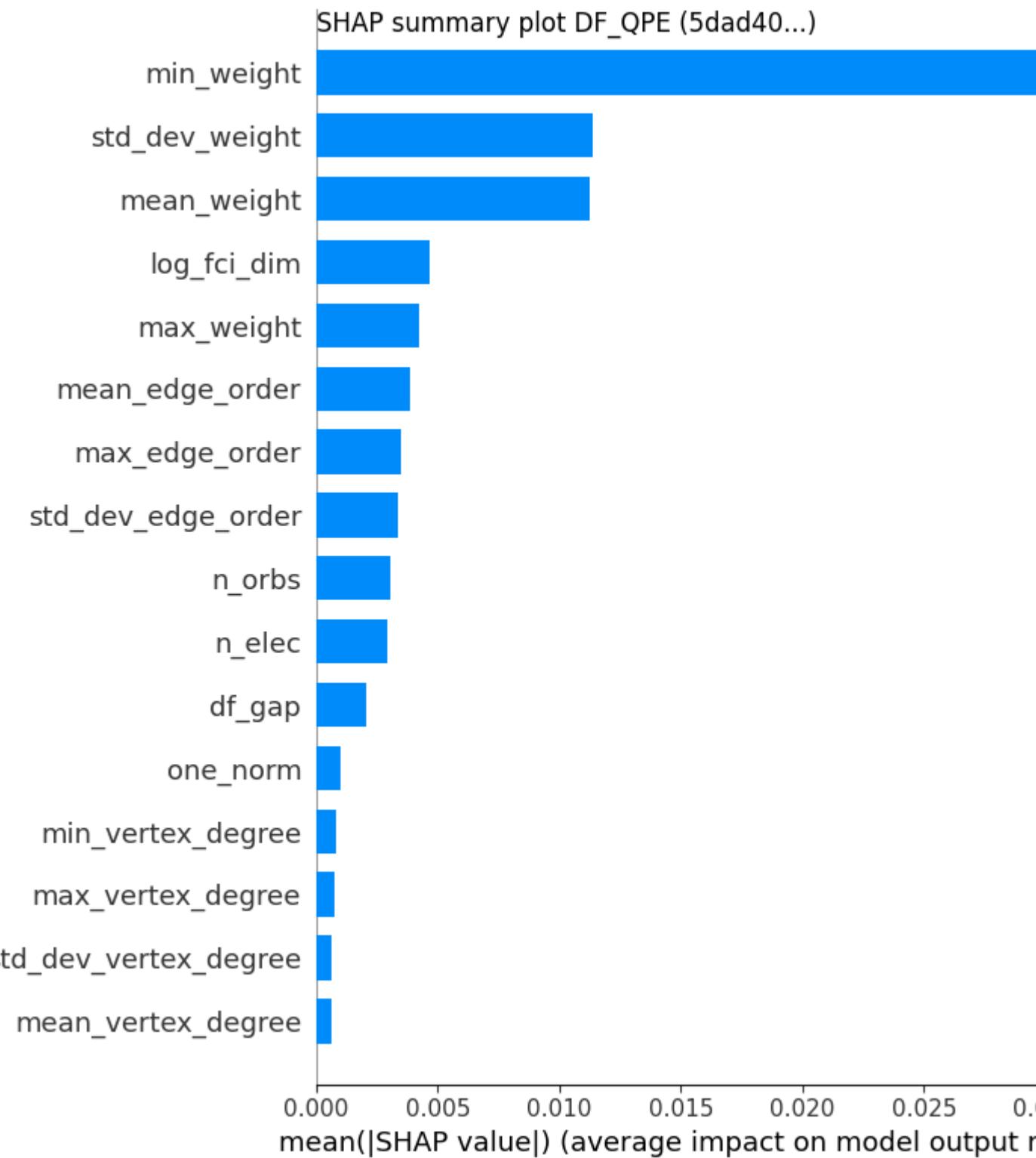
Solver DF_QPE (5dad40...)
Embedding: PCA



Solver DF_QPE (5dad40...)
Embedding: NMF



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



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

solver_uuid:4b07b89f-c66f-4e72-8c24-df3e4222cb41

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70}}

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

quantum.hardware_details:{'quantum.hardware_description': 'Optimistic superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494. Assumes that enough QPUs are available to run all shots in parallel.', 'quantum.hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.0001, 'cycle_time_microseconds': 1, 'parallelize_shots': True}}

logical_resource_estimate_solution_uuid:32037675-e2b9-46d5-9920-ec47386ceaf3

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

performance_metrics_uuid: a5a3e609-4155-4cb6-ab87-9febc872972d

creation_timestamp: 2025-06-12T20:42:55.603395+00:00

number_of_problem_instances: 68

number_of_problem_instances_attempted: 22

number_of_problem_instances_solved: 3

number_of_tasks: 228

number_of_tasks_attempted: 131

number_of_tasks_solved: 3

number_of_tasks_solved_within_run_time_limit: 3

number_of_tasks_solved_within_accuracy_threshold: 131

max_run_time_of_attempted_tasks: 26774753292.953506

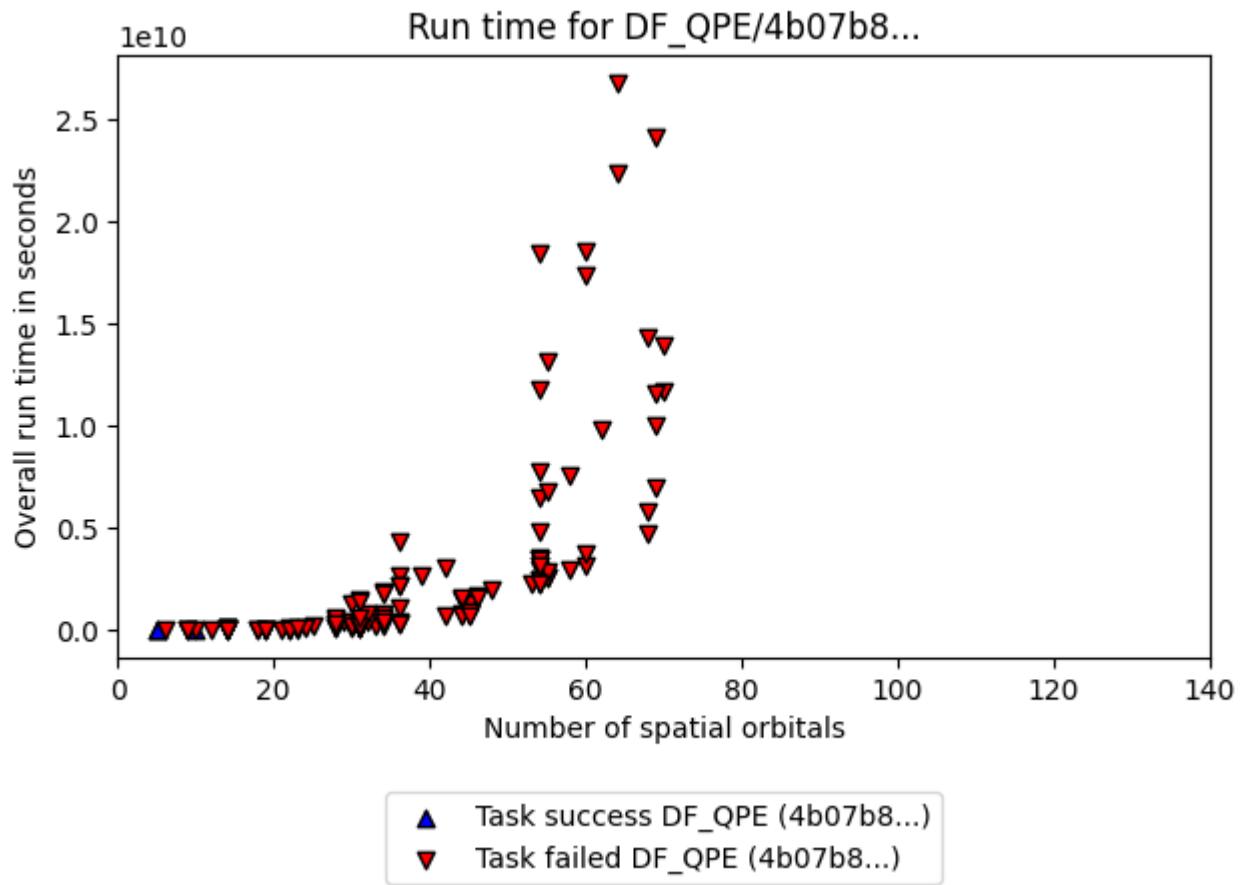
sum_of_run_time_of_attempted_tasks: 381759348210.49603

solvability_ratio: 0.0

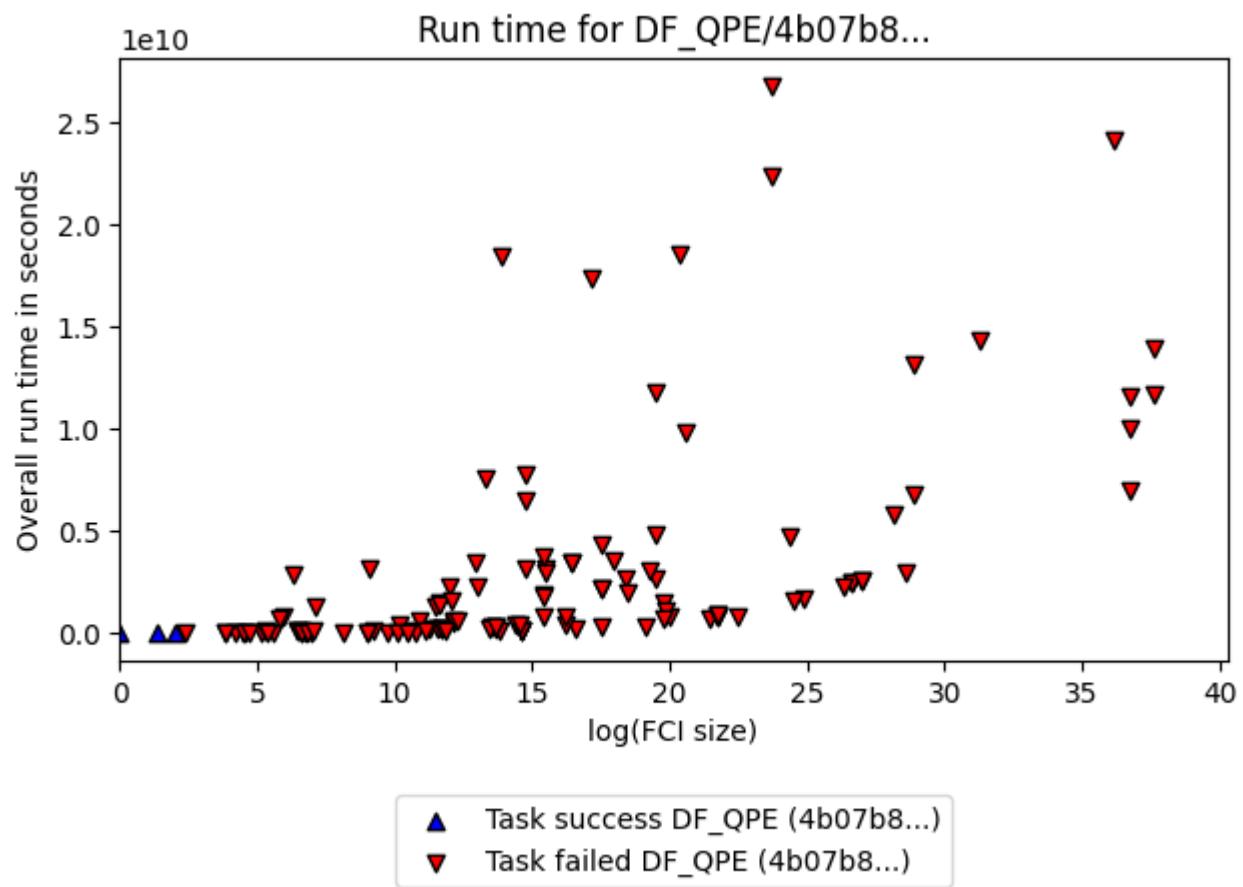
comments: solvability ratio based on PCA embedding.

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1



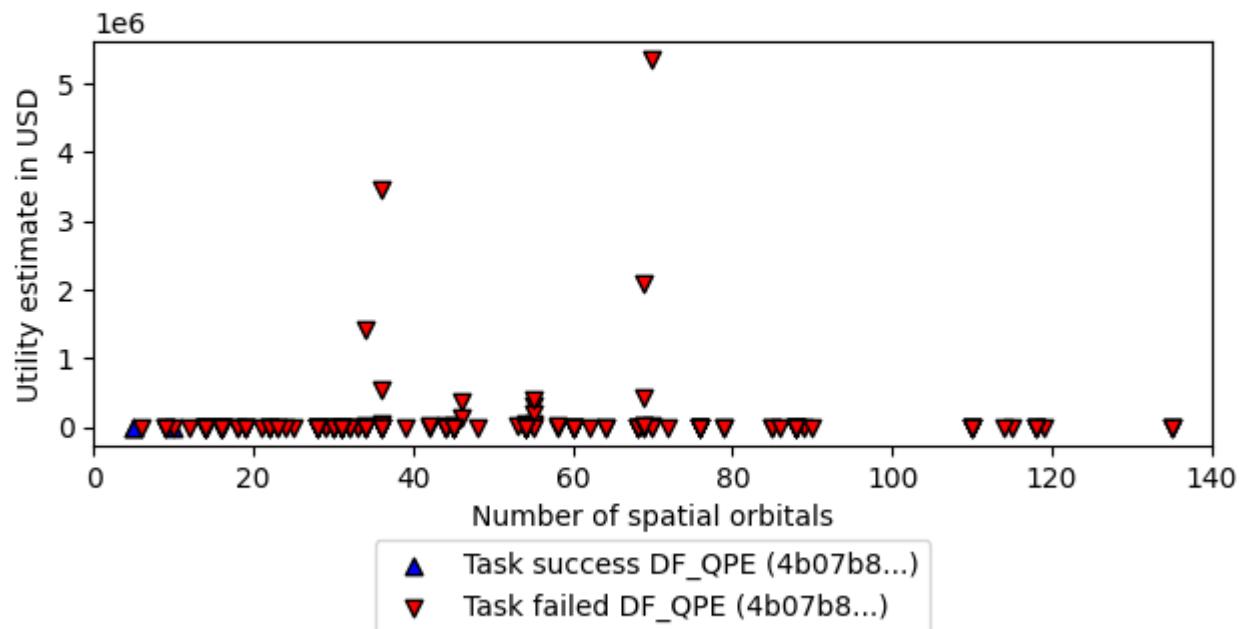
Note: plot only contains attempted tasks.



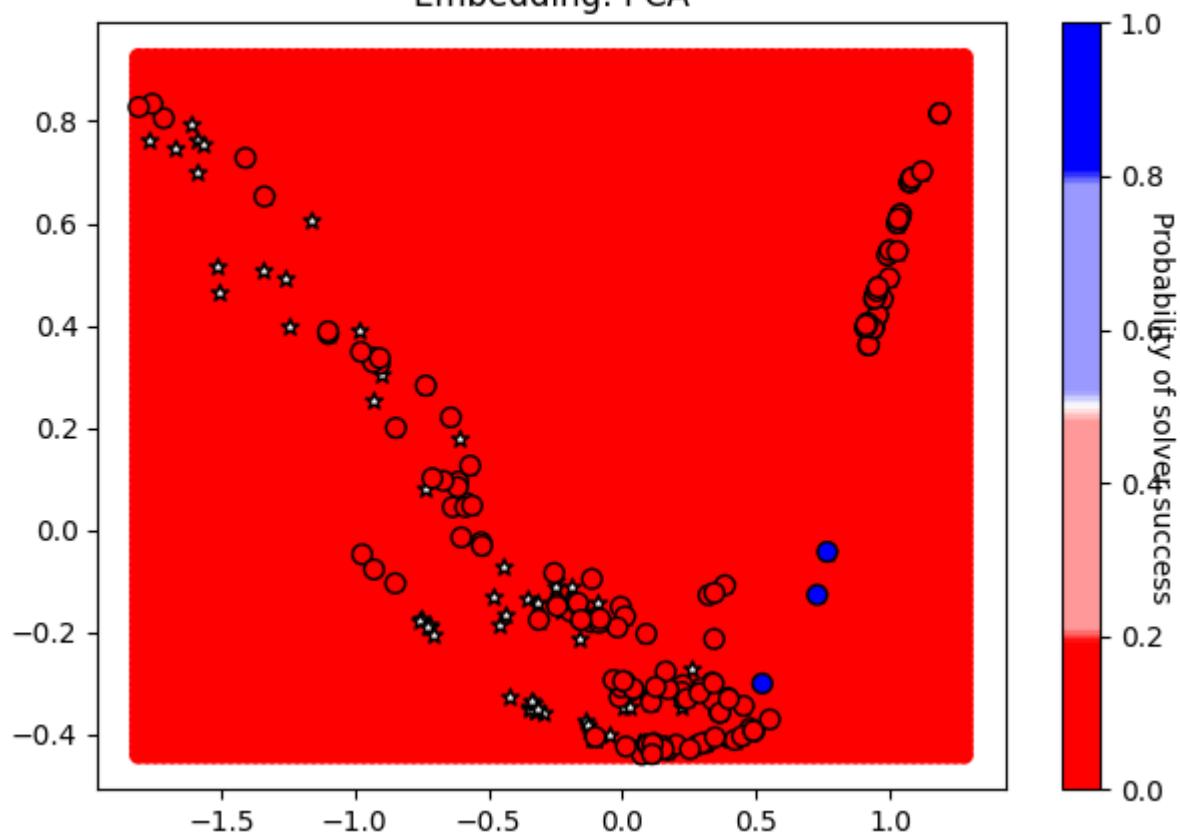
Note: plot only contains attempted tasks.

Utility capture from DF_QPE/4b07b8...

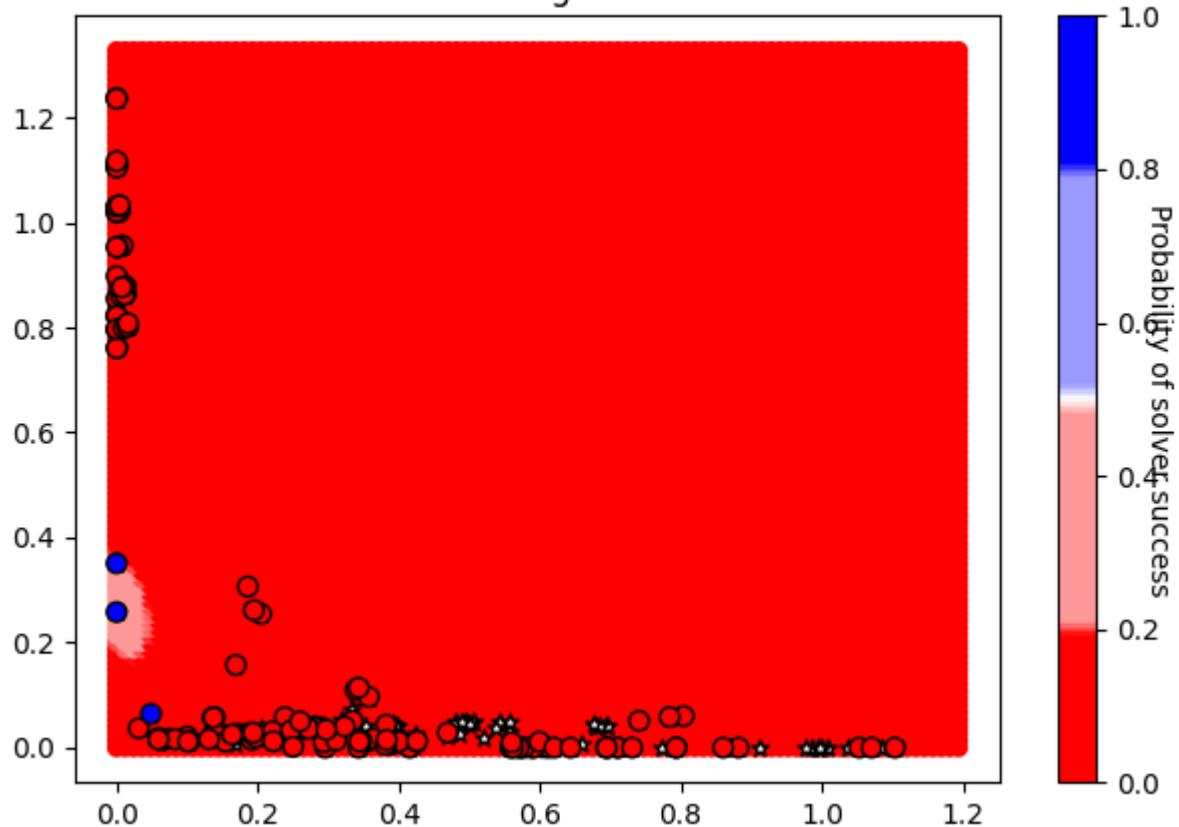
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



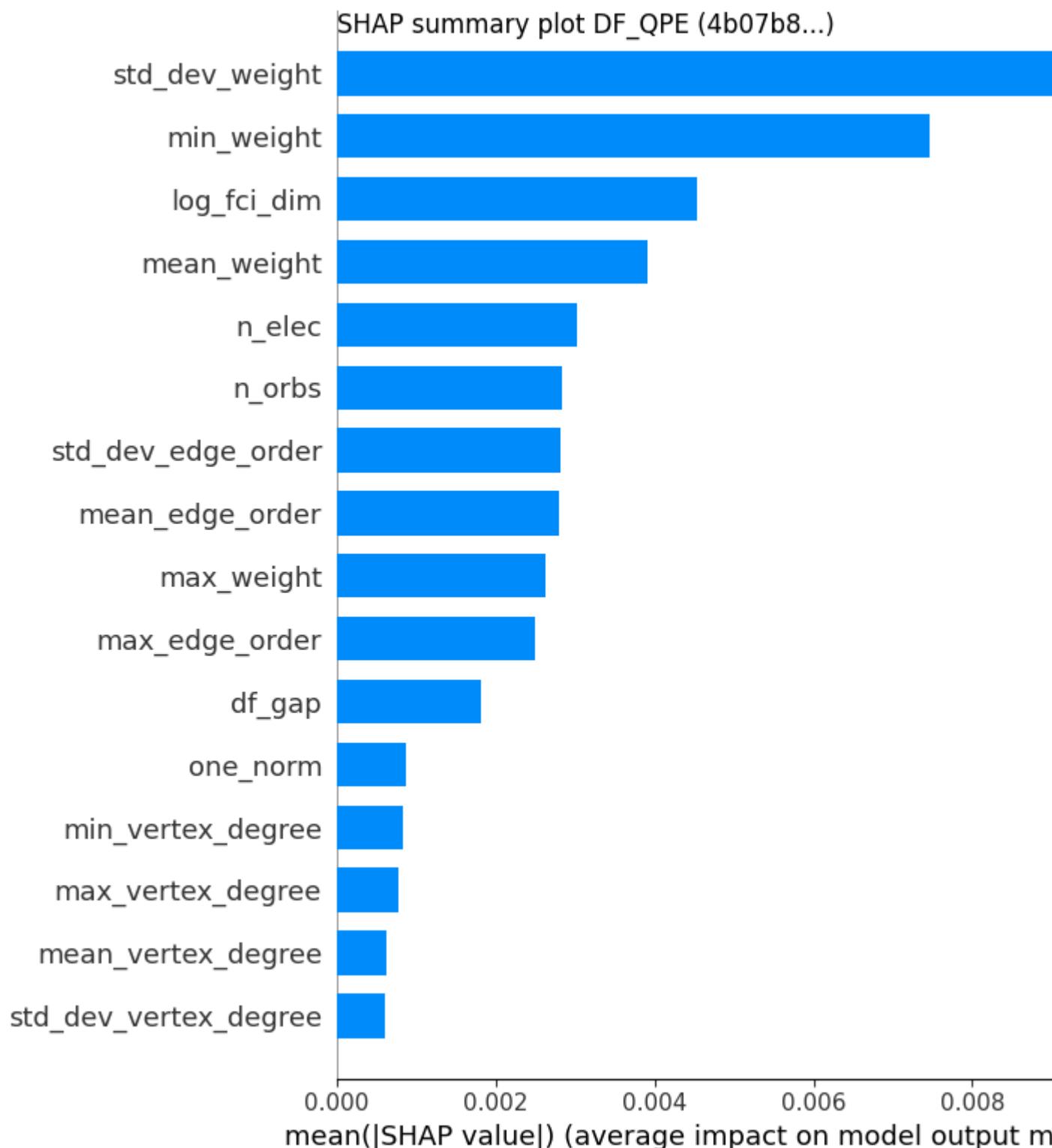
Solver DF_QPE (4b07b8...)
Embedding: PCA



Solver DF_QPE (4b07b8...)
Embedding: NNMF



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



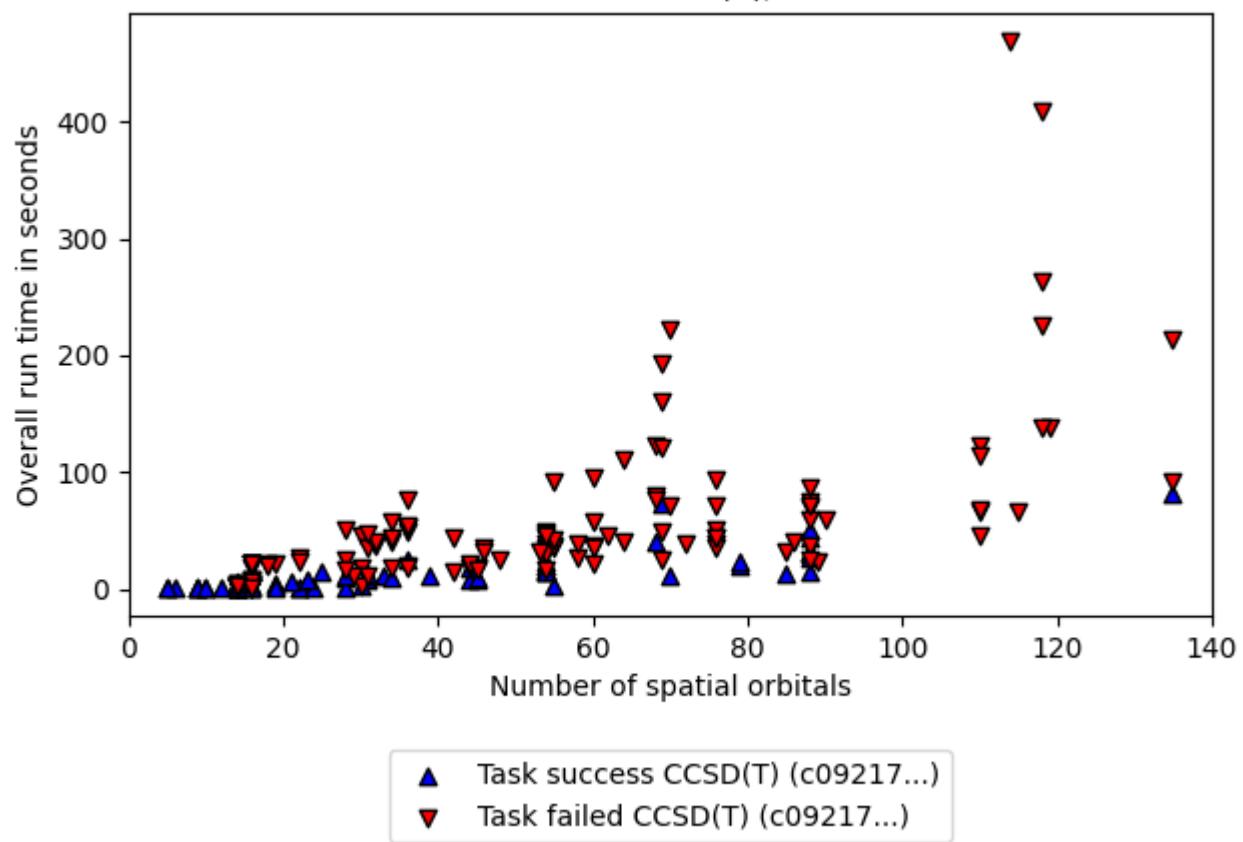
Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878

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

solver_short_name:CCSD(T)

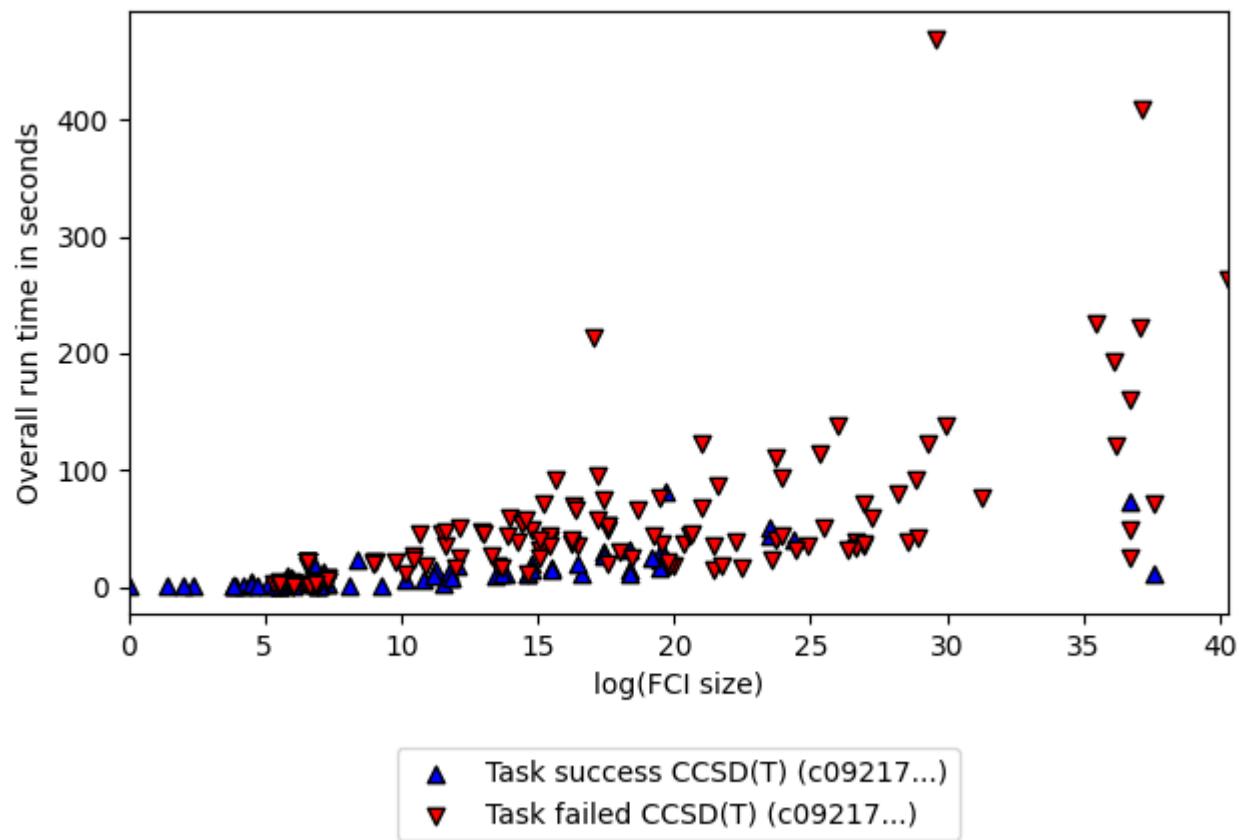
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD(T)
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 1d0304da-c8cb-422c-ae15-8b494ecd1fb6
creation_timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 64
number_of_problem_instances_solved: 23
number_of_tasks: 228
number_of_tasks_attempted: 217
number_of_tasks_solved: 71
number_of_tasks_solved_within_run_time_limit: 217
number_of_tasks_solved_within_accuracy_threshold: 71
max_run_time_of_attempted_tasks: 469.1432478427887
sum_of_run_time_of_attempted_tasks: 7918.634609699249
solvability_ratio: 0.2847
comments: solvability ratio based on PCA embedding.
f1_score: [0.9685534591194969, 0.9659863945578231]
ml_metrics_calculator_version: 1

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



Note: plot only contains attempted tasks.

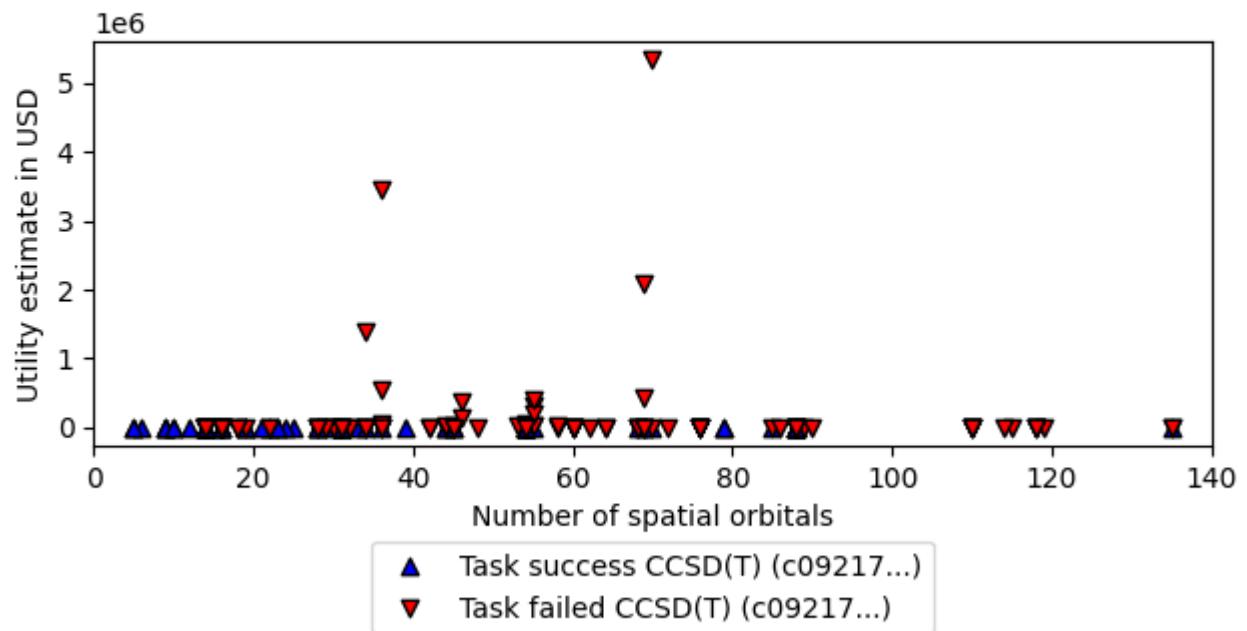
Run time for CCSD(T)/c09217...



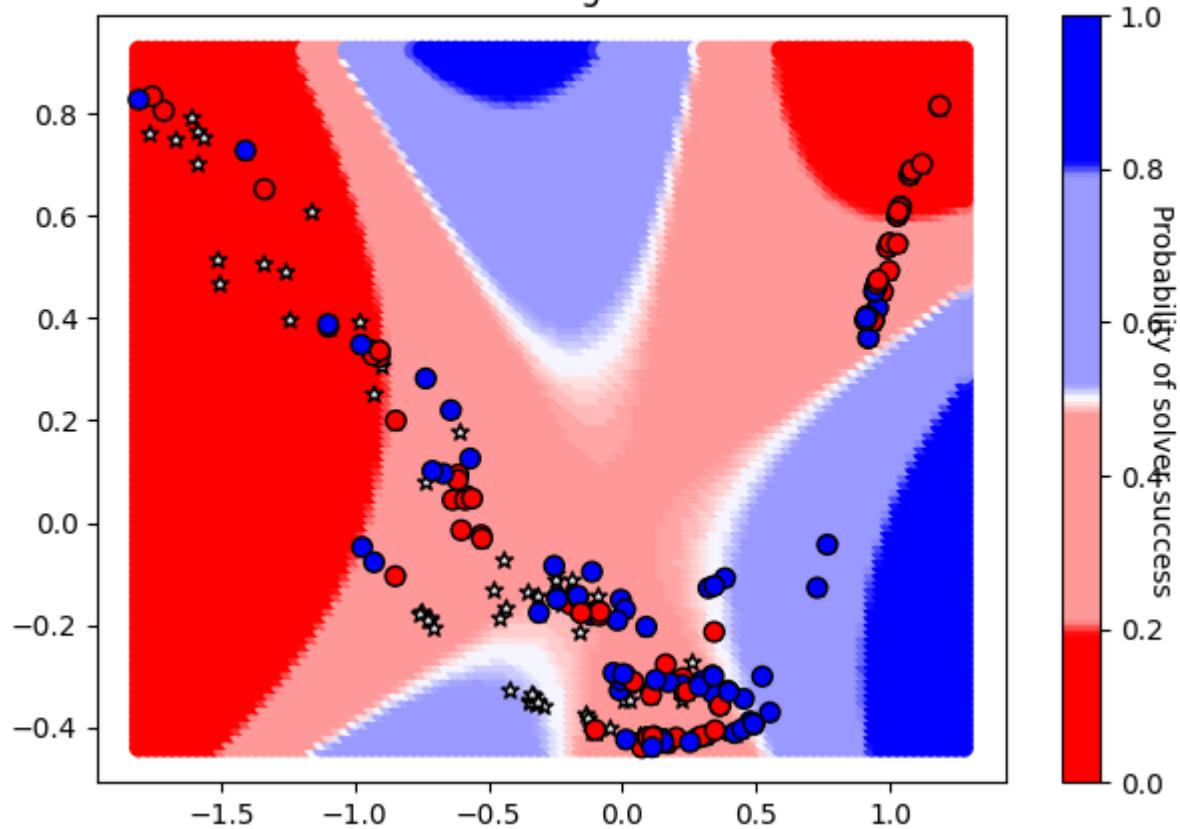
Note: plot only contains attempted tasks.

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

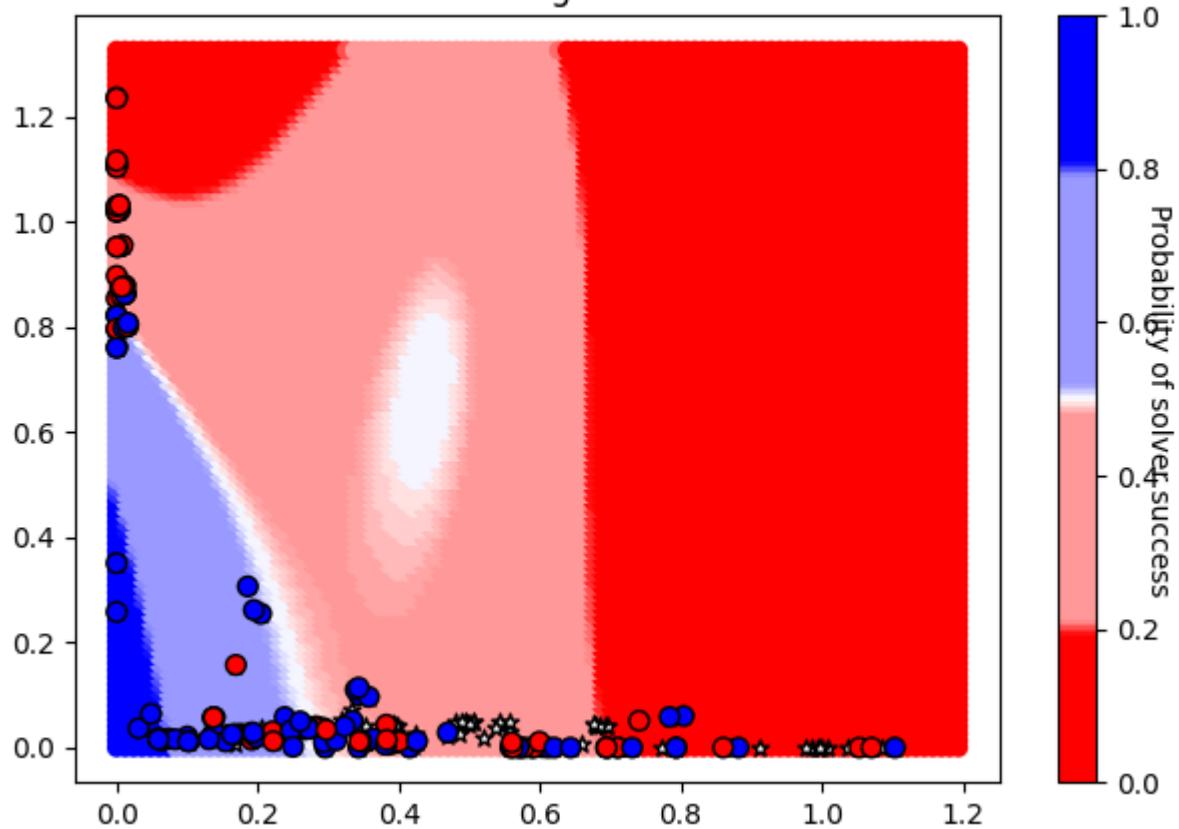
(captured: $\$1.8e+02/1.5e+07$, approximately $1.2e-03\%$)



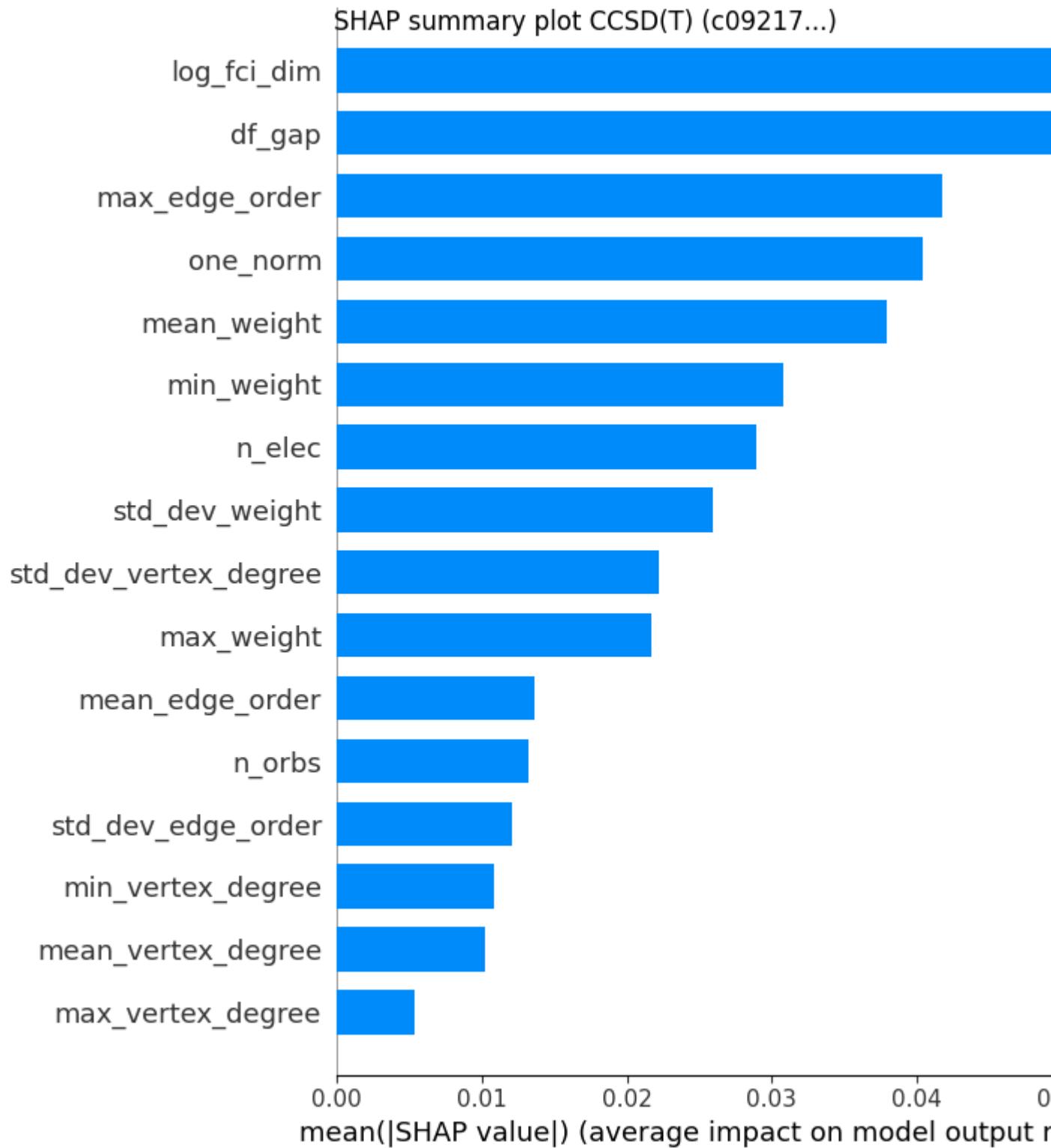
Solver CCSD(T) (c09217...)
Embedding: PCA



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



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



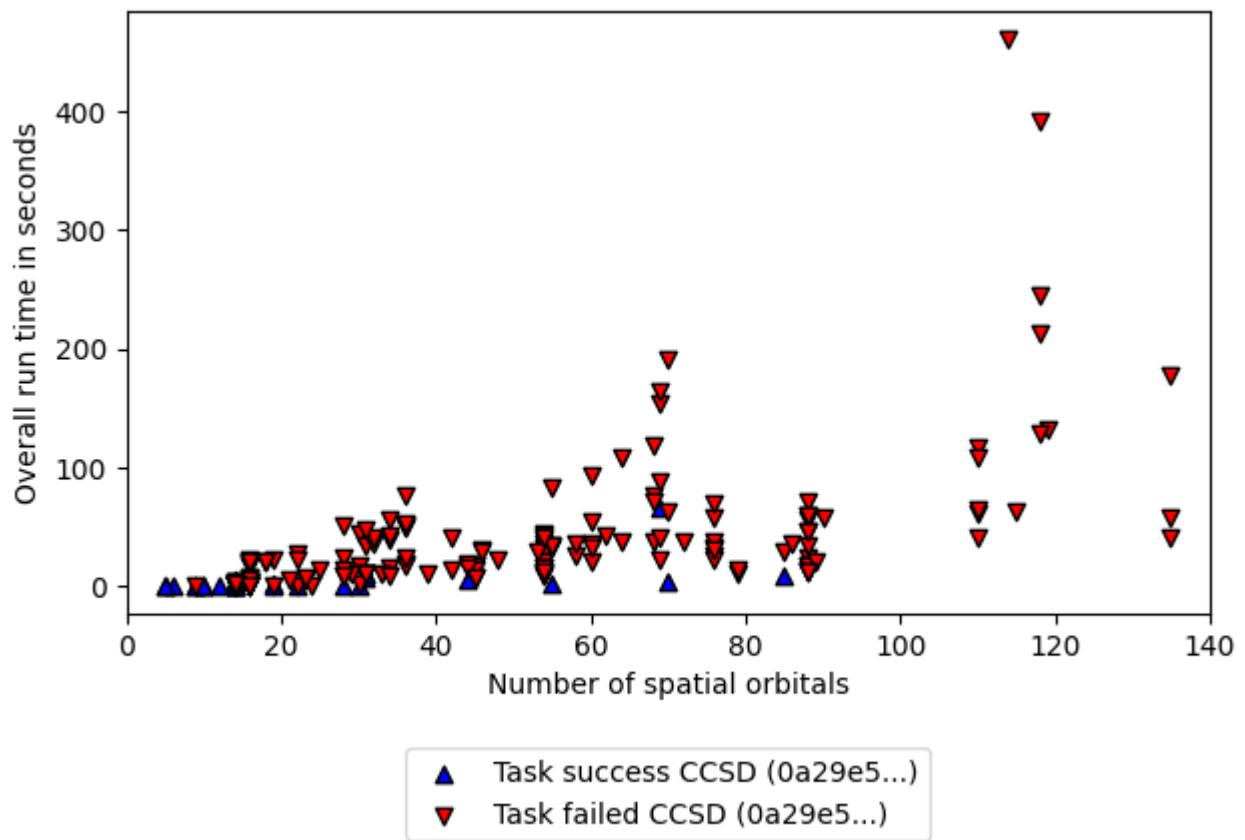
Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

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

solver_short_name:CCSD

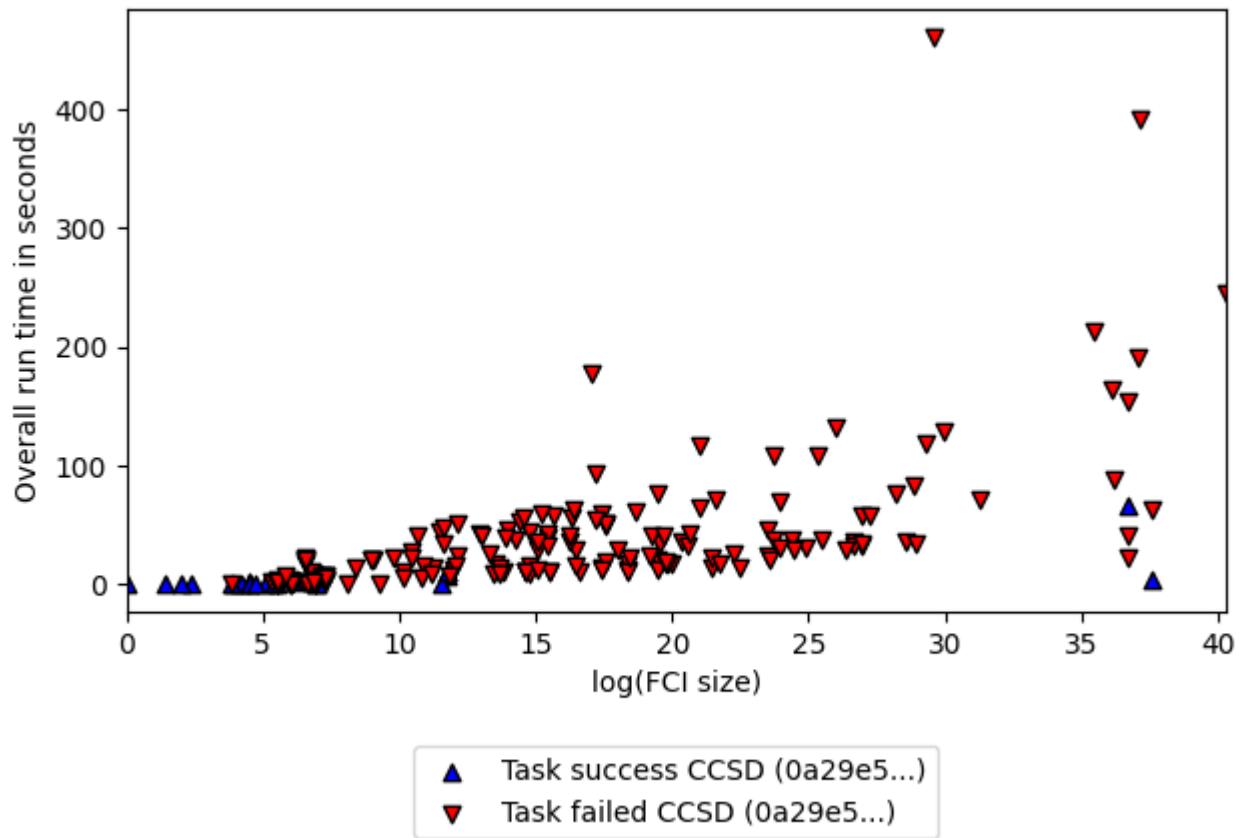
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 570268fe-a401-4b16-ba5a-fdcf40f90882
creation_timestamp: 2025-06-12T20:42:55.603395+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: 217
number_of_tasks_solved: 27
number_of_tasks_solved_within_run_time_limit: 217
number_of_tasks_solved_within_accuracy_threshold: 27
max_run_time_of_attempted_tasks: 460.71552085876465
sum_of_run_time_of_attempted_tasks: 7096.755430221558
solvability_ratio: 0.011
comments: solvability ratio based on PCA embedding.
f1_score: [0.9879518072289156, 0.9473684210526315]
ml_metrics_calculator_version: 1

Run time for CCSD/0a29e5...



Note: plot only contains attempted tasks.

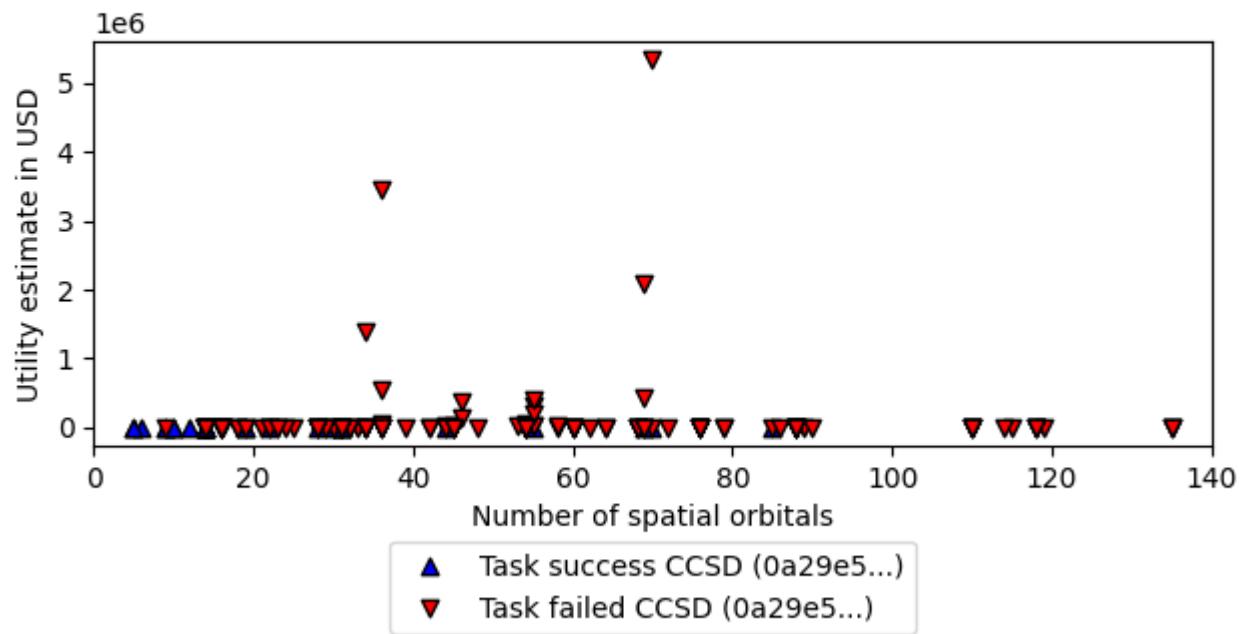
Run time for CCSD/0a29e5...



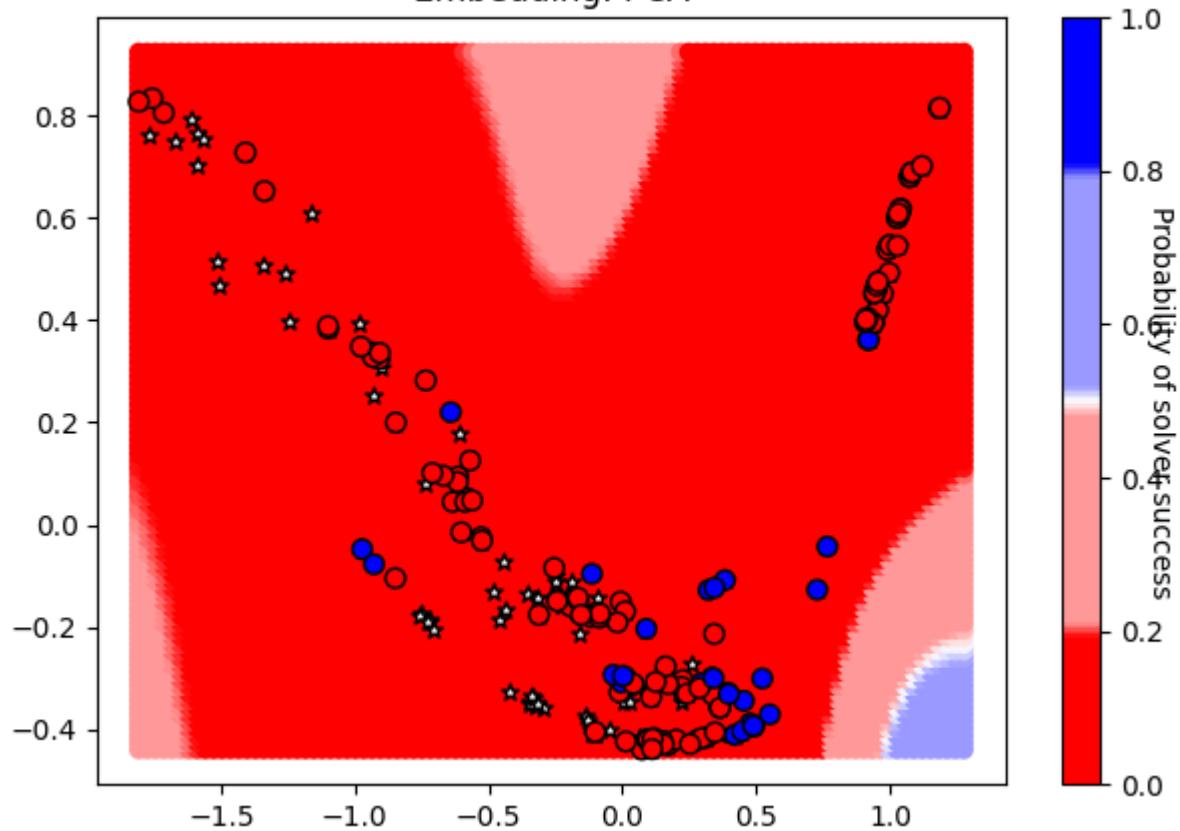
Note: plot only contains attempted tasks.

Utility capture from CCSD/0a29e5...

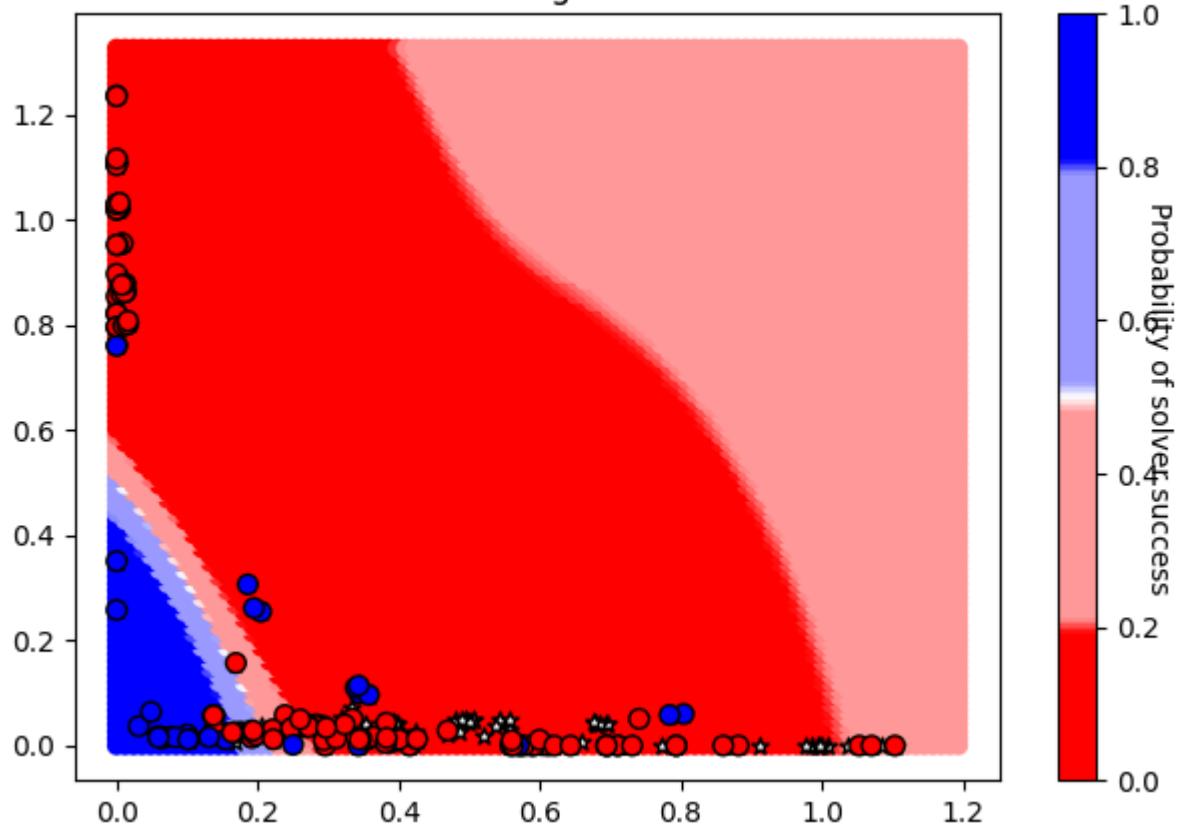
(captured: \$2.1e-02/1.5e+07, approximately 1.4e-07%)



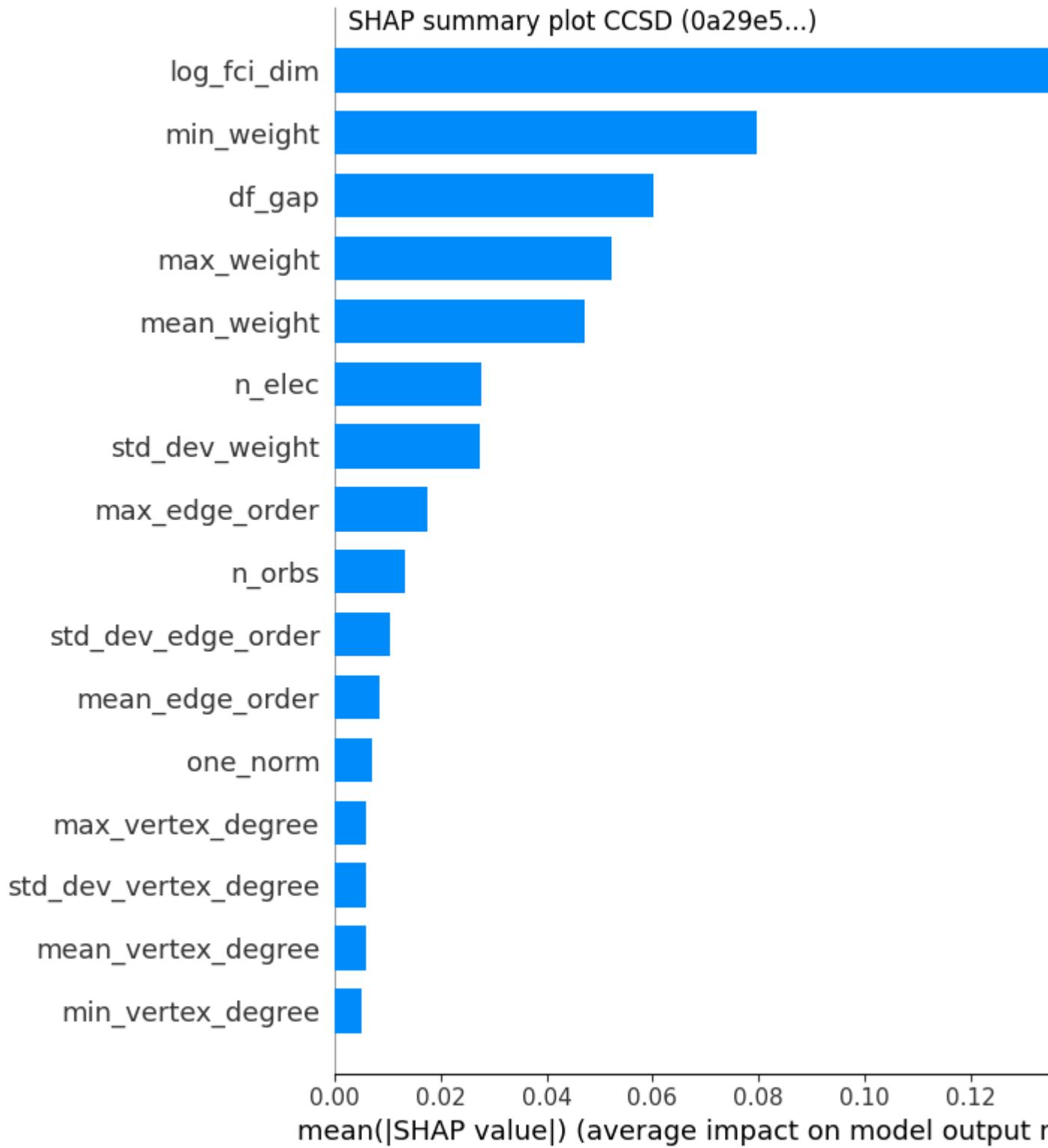
Solver CCSD (0a29e5...)
Embedding: PCA



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



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



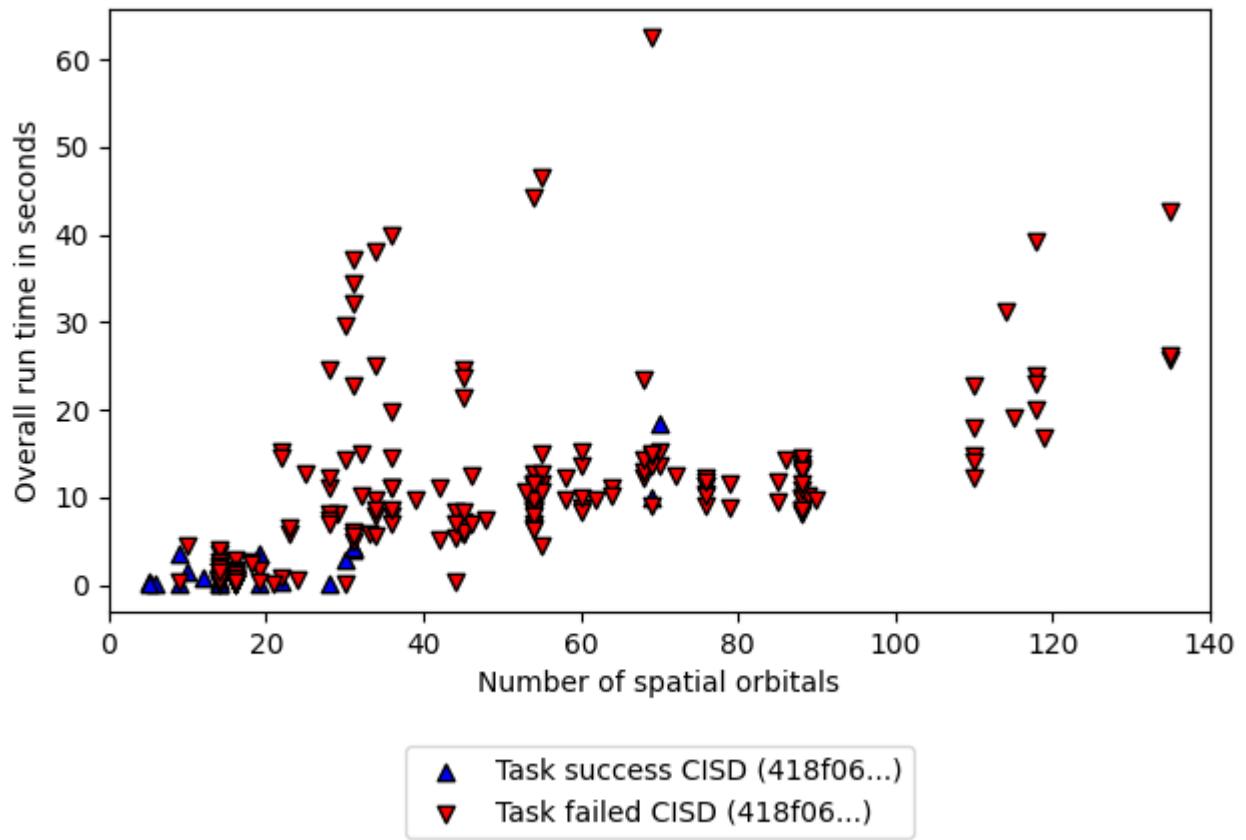
Solver CISD, 418f060e-496b-4024-8d2d-9b1f8791e76d

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

solver_short_name:CISD

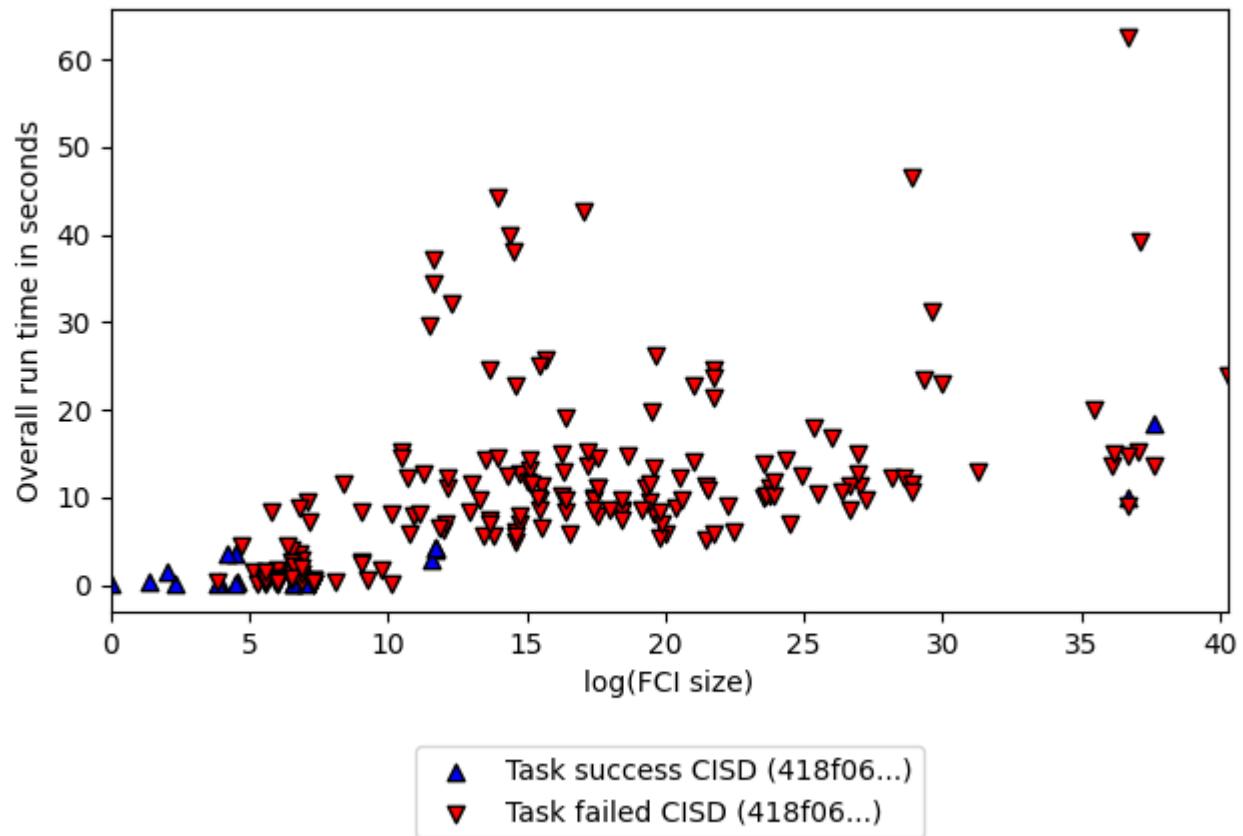
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CISD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 83456b41-c038-4fd4-8639-e5373fe394f0
creation_timestamp: 2025-06-12T20:42:55.603395+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: 21
number_of_tasks_solved_within_run_time_limit: 228
number_of_tasks_solved_within_accuracy_threshold: 21
max_run_time_of_attempted_tasks: 62.58296537399292
sum_of_run_time_of_attempted_tasks: 2147.015964984894
solvability_ratio: 0.0233
comments: solvability ratio based on PCA embedding.
f1_score: [0.9806949806949807, 0.8936170212765957]
ml_metrics_calculator_version: 1

Run time for CISD/418f06...



Note: plot only contains attempted tasks.

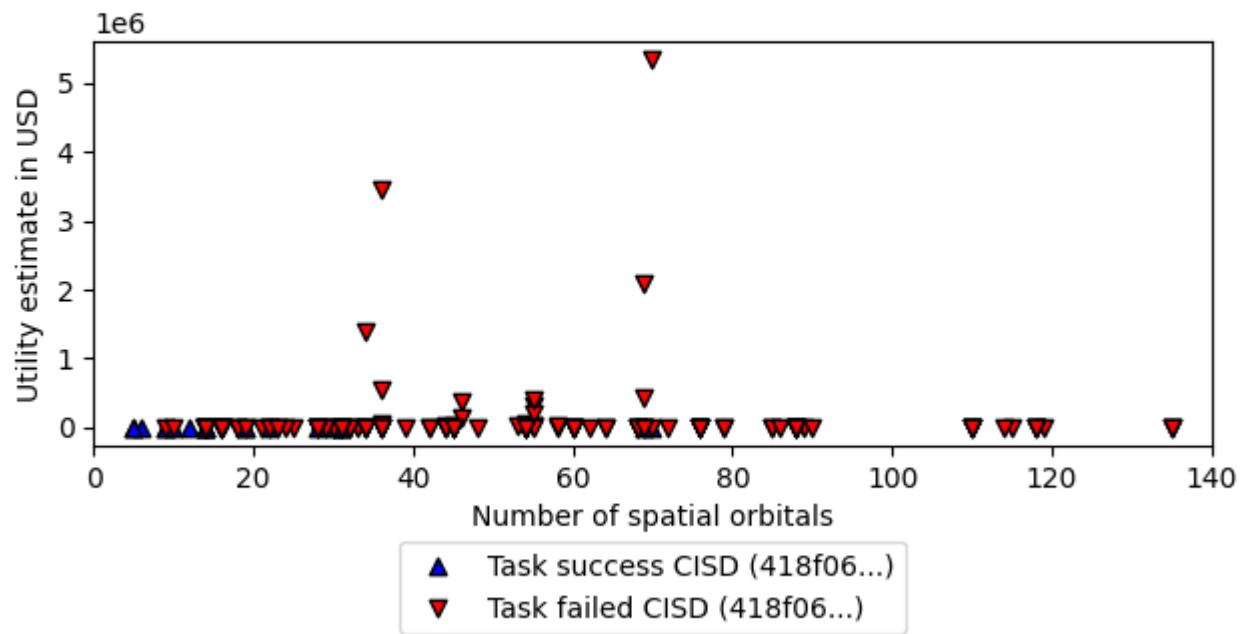
Run time for CISD/418f06...



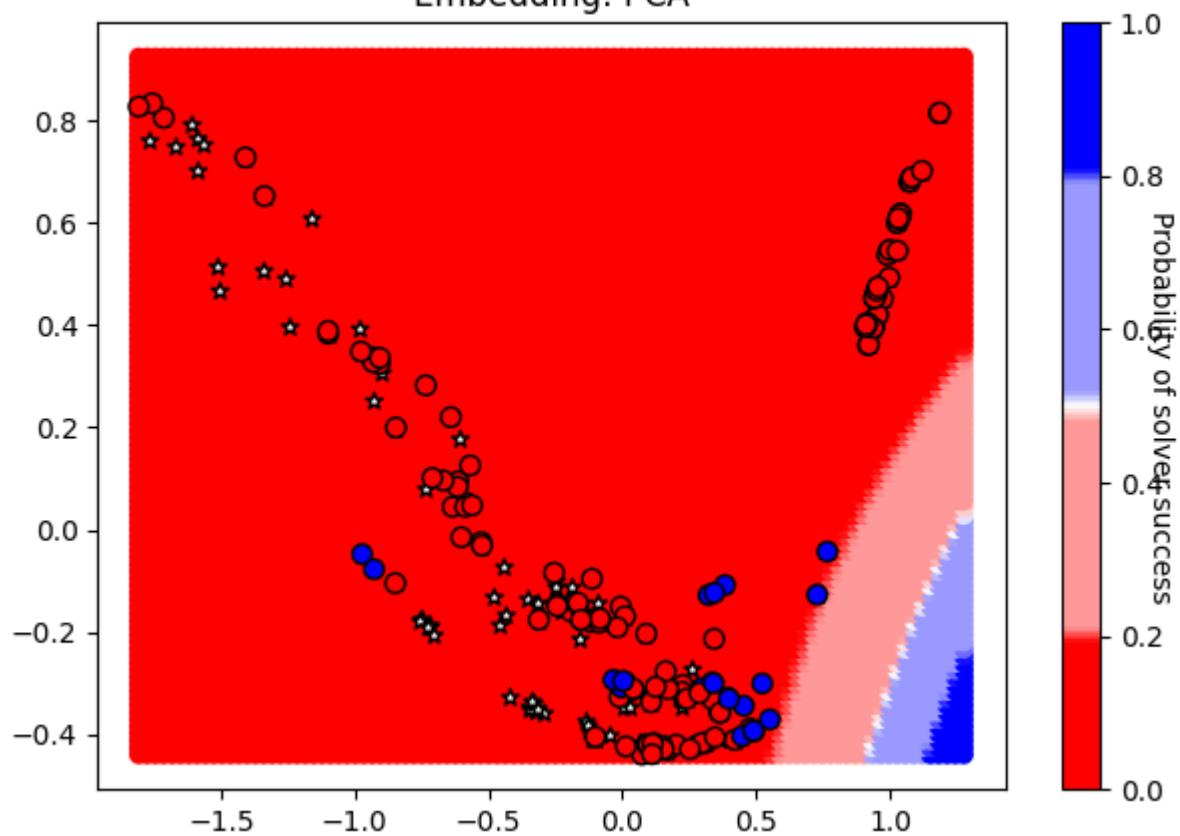
Note: plot only contains attempted tasks.

Utility capture from CISD/418f06...

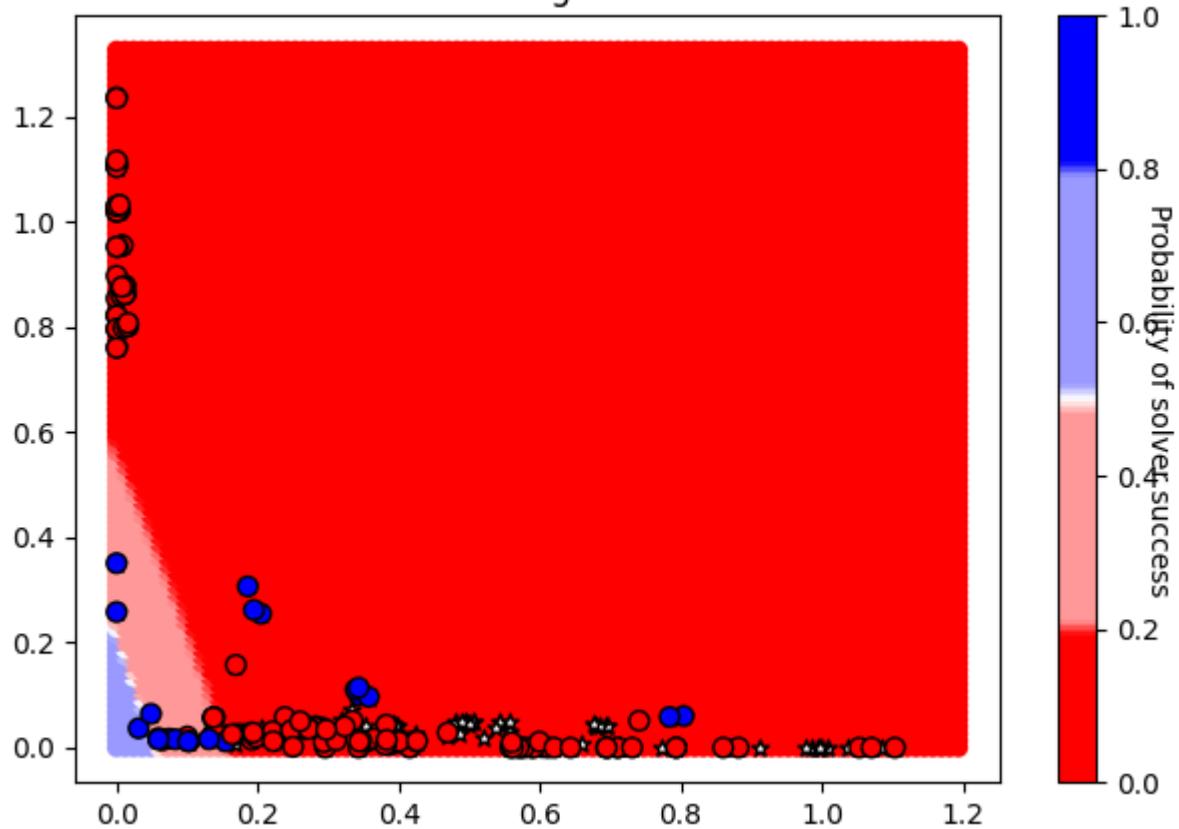
(captured: \$4.8e-03/1.5e+07, approximately 3.2e-08%)



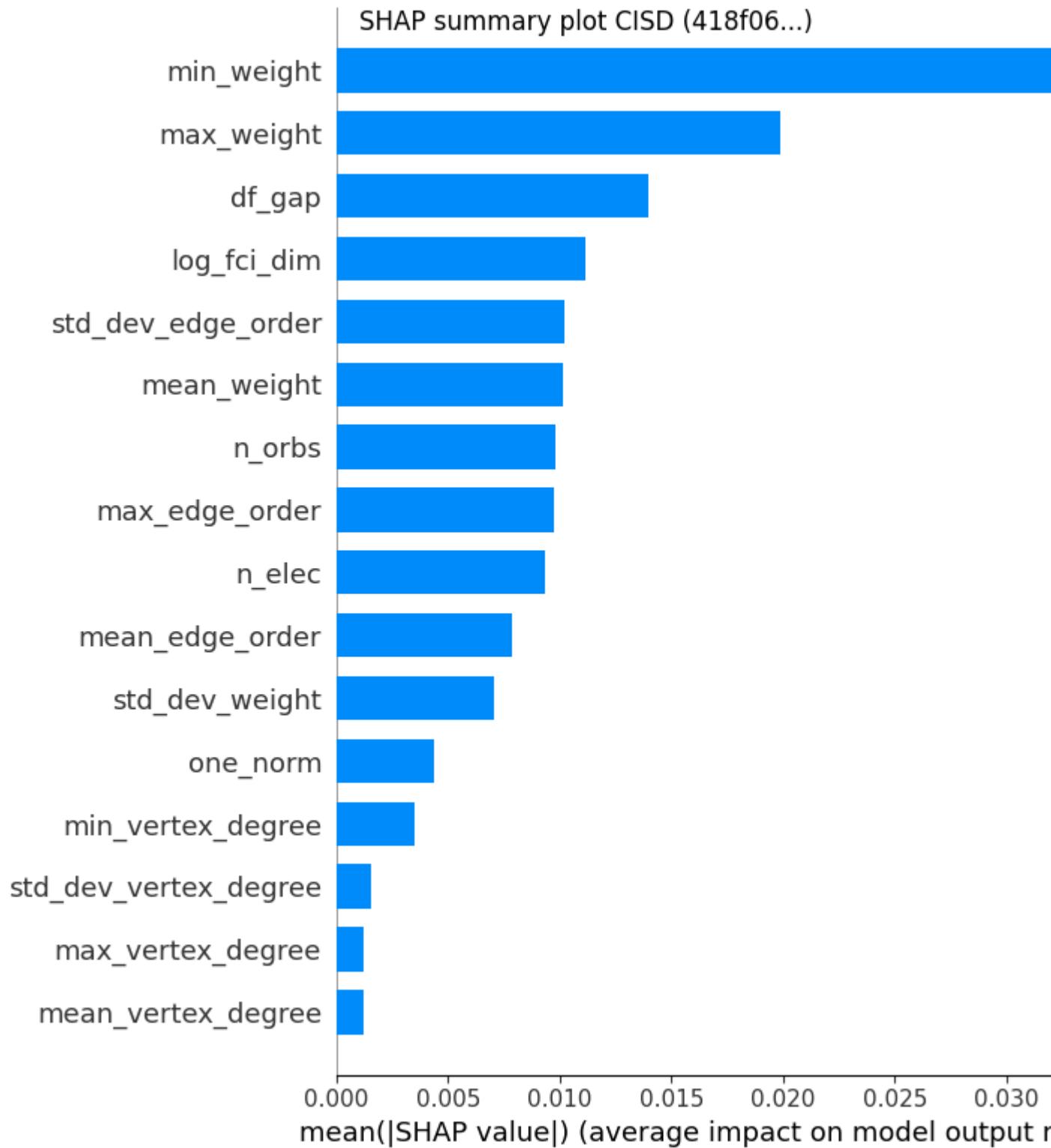
Solver CISD (418f06...)
Embedding: PCA



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



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



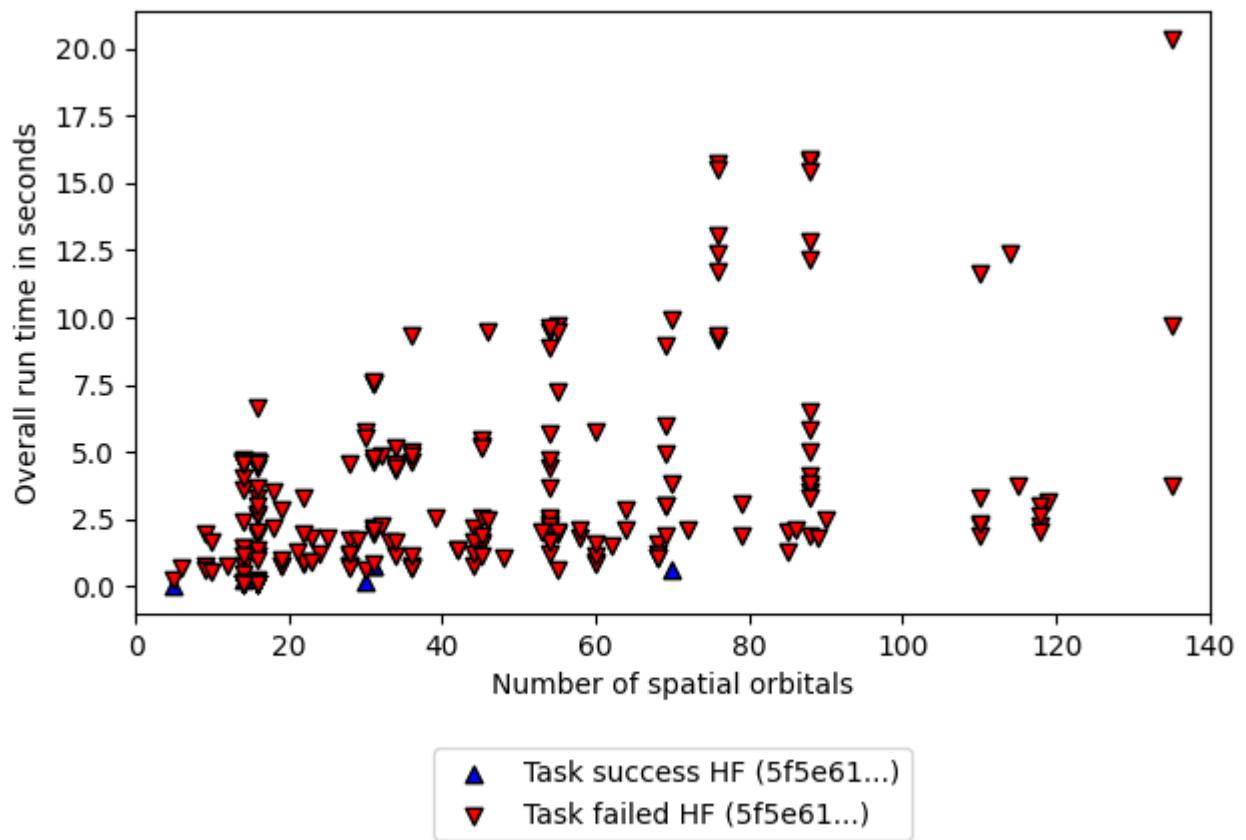
Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

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

solver_short_name:HF

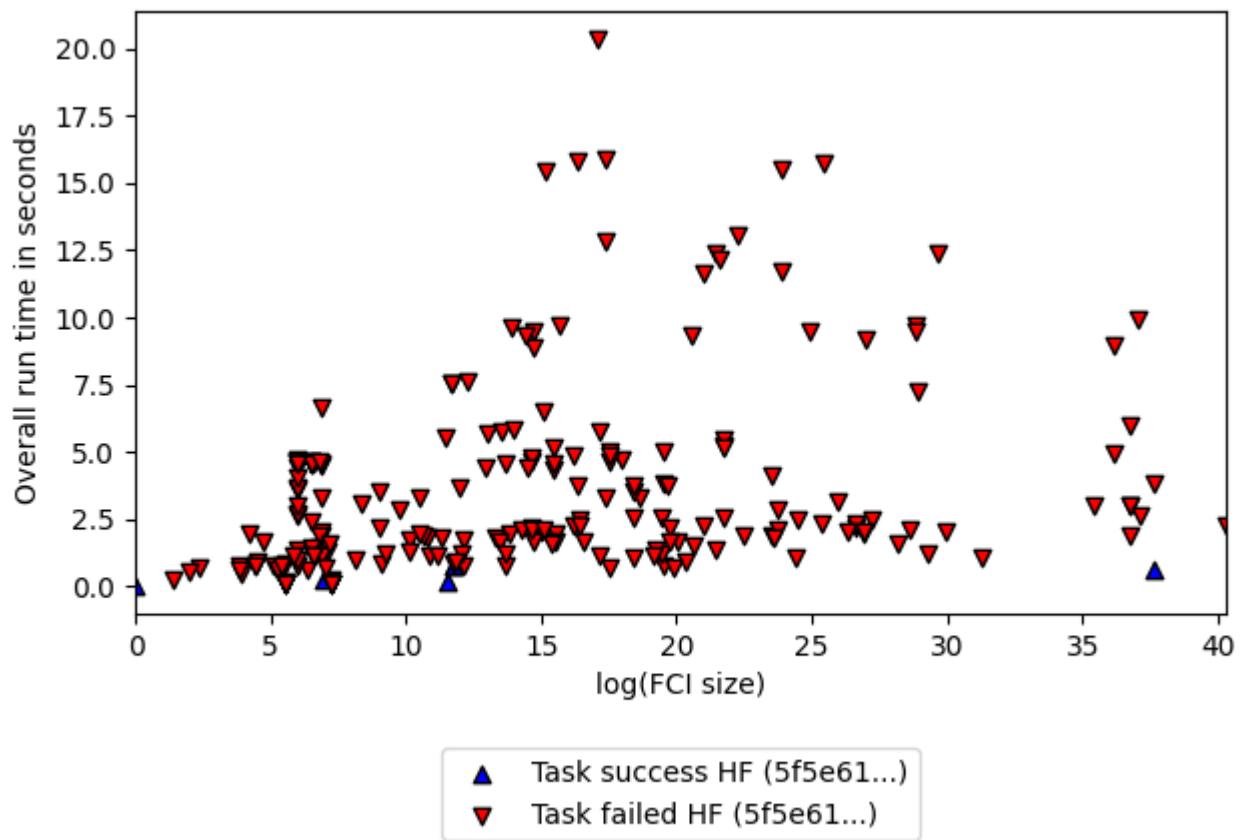
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:Hartree Fock
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 8a4b3310-3ff1-4edd-9eba-4e1ee2c65a5d
creation_timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 6
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 6
number_of_tasks_solved_within_run_time_limit: 228
number_of_tasks_solved_within_accuracy_threshold: 6
max_run_time_of_attempted_tasks: 20.338801622390747
sum_of_run_time_of_attempted_tasks: 800.5601267814636
solvability_ratio: 0.0
comments: solvability ratio based on PCA embedding.
f1_score: [0.0, 0.07547169811320754]
ml_metrics_calculator_version: 1

Run time for HF/5f5e61...



Note: plot only contains attempted tasks.

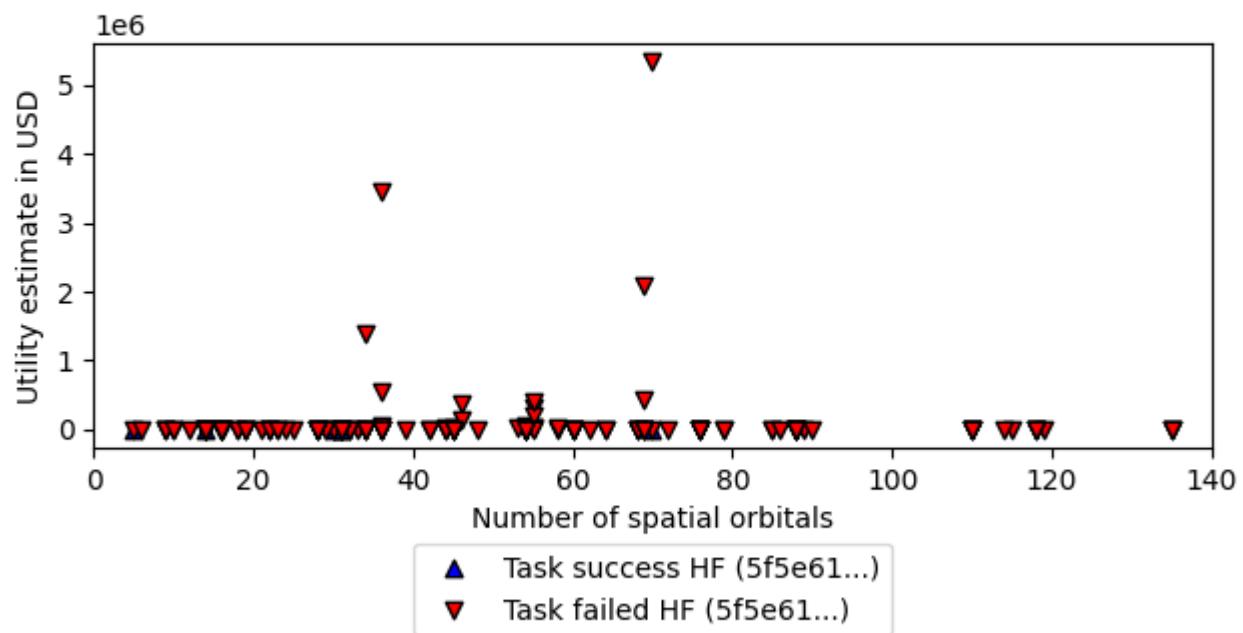
Run time for HF/5f5e61...



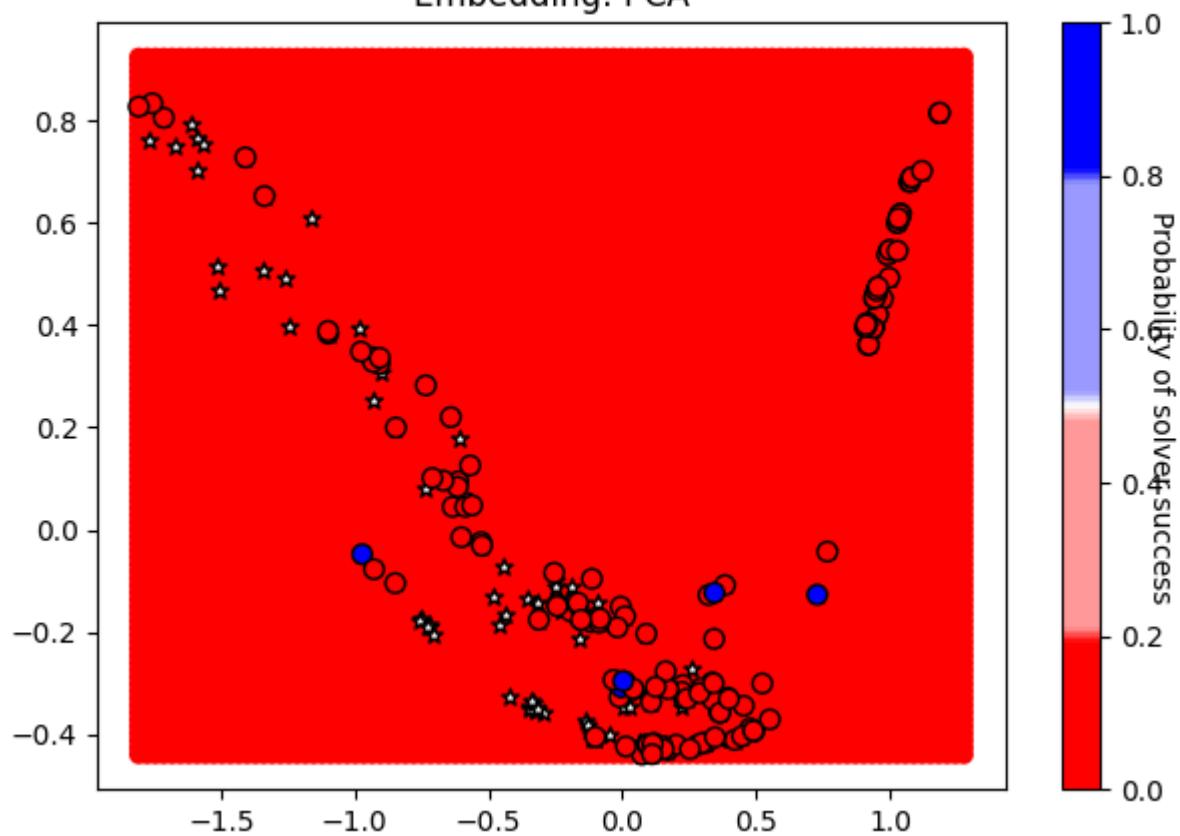
Note: plot only contains attempted tasks.

Utility capture from HF/5f5e61...

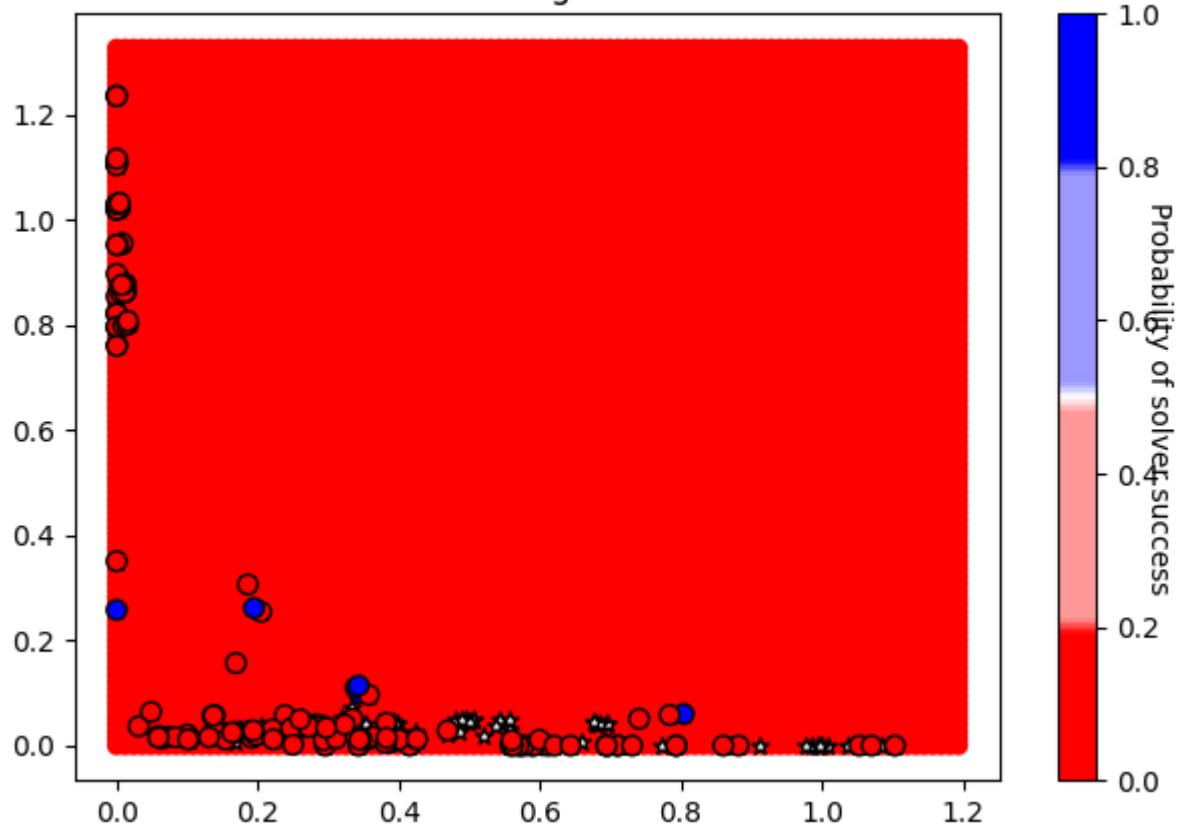
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



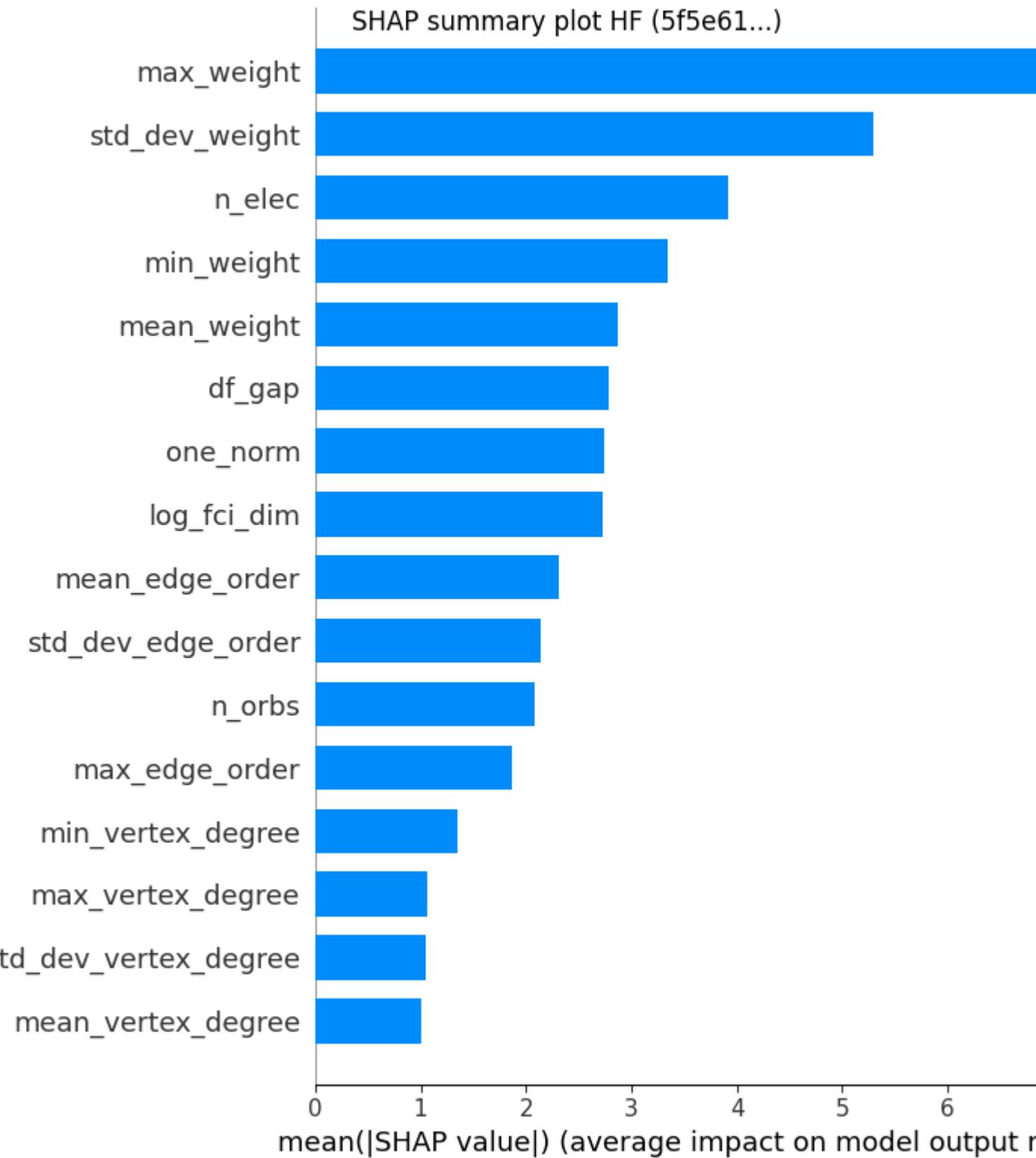
Solver HF (5f5e61...)
Embedding: PCA



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



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



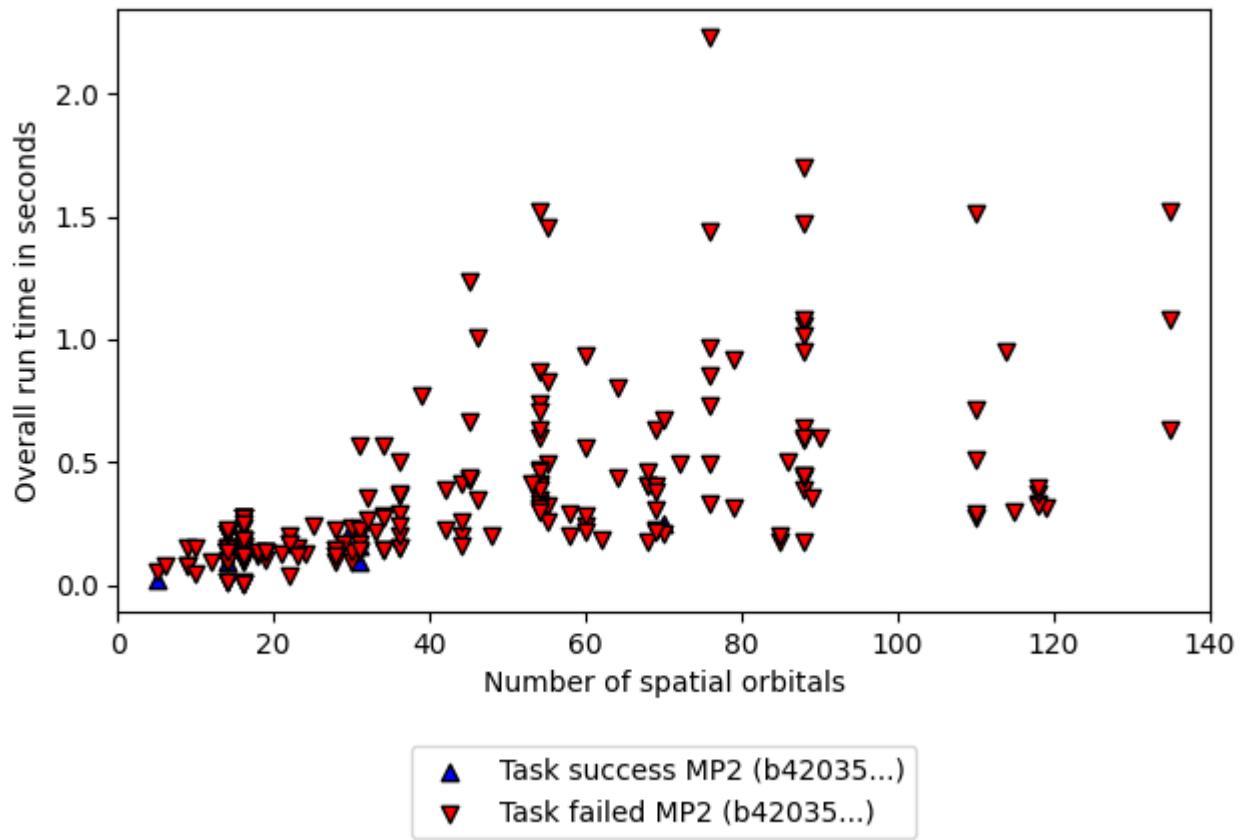
Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aecd2

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

solver_short_name:MP2

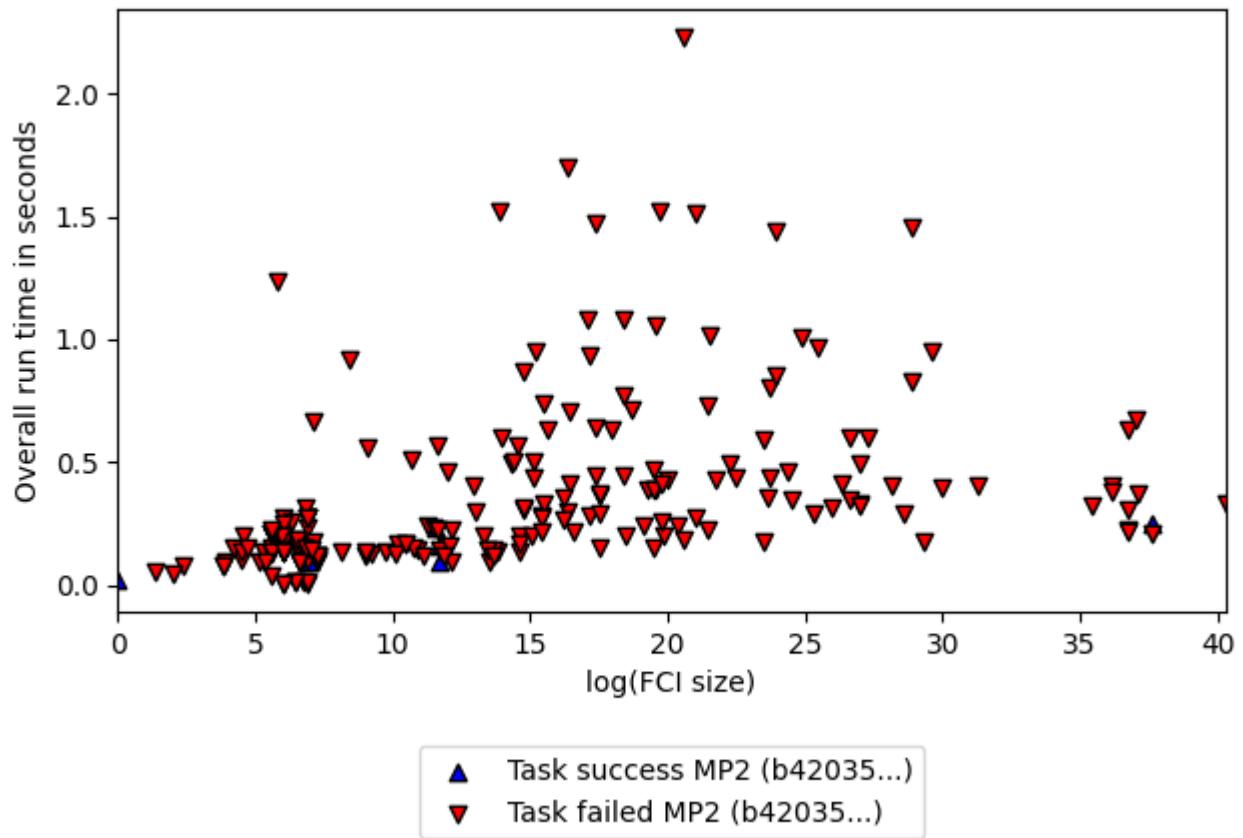
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:MP2
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: c8e8b995-8d22-48d4-9737-a44486bdc217
creation_timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 65
number_of_problem_instances_solved: 6
number_of_tasks: 228
number_of_tasks_attempted: 220
number_of_tasks_solved: 6
number_of_tasks_solved_within_run_time_limit: 220
number_of_tasks_solved_within_accuracy_threshold: 6
max_run_time_of_attempted_tasks: 2.230440139770508
sum_of_run_time_of_attempted_tasks: 78.57580351829529
solvability_ratio: 0.0
comments: solvability ratio based on PCA embedding.
f1_score: [0.0, 0.07547169811320754]
ml_metrics_calculator_version: 1

Run time for MP2/b42035...



Note: plot only contains attempted tasks.

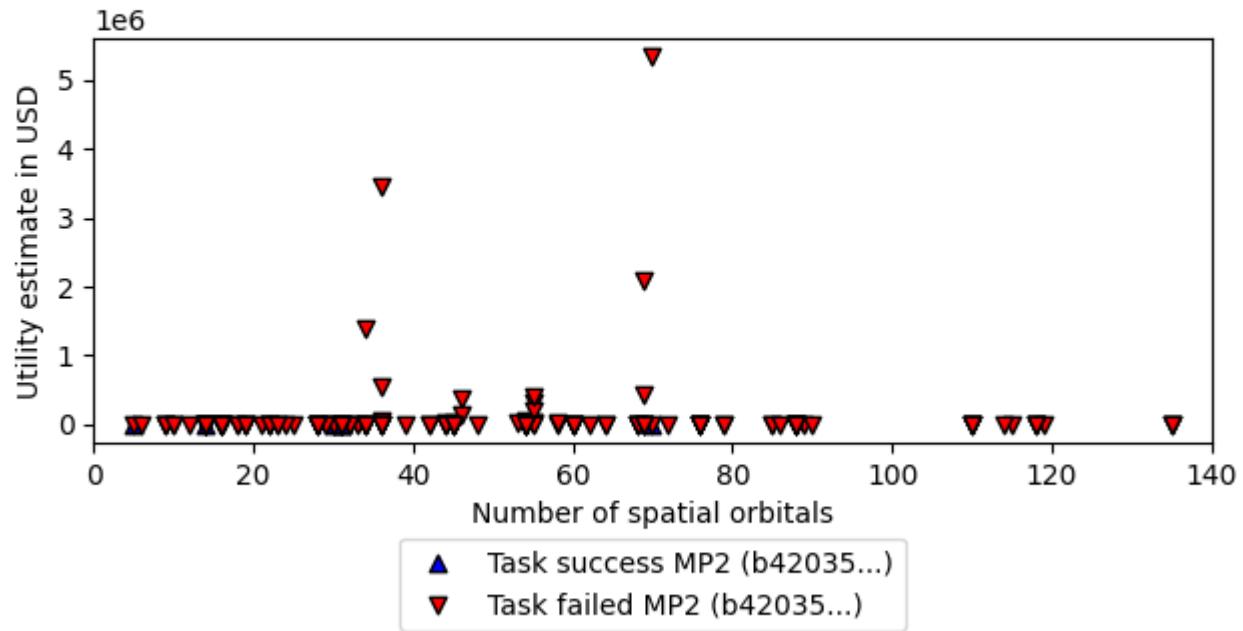
Run time for MP2/b42035...



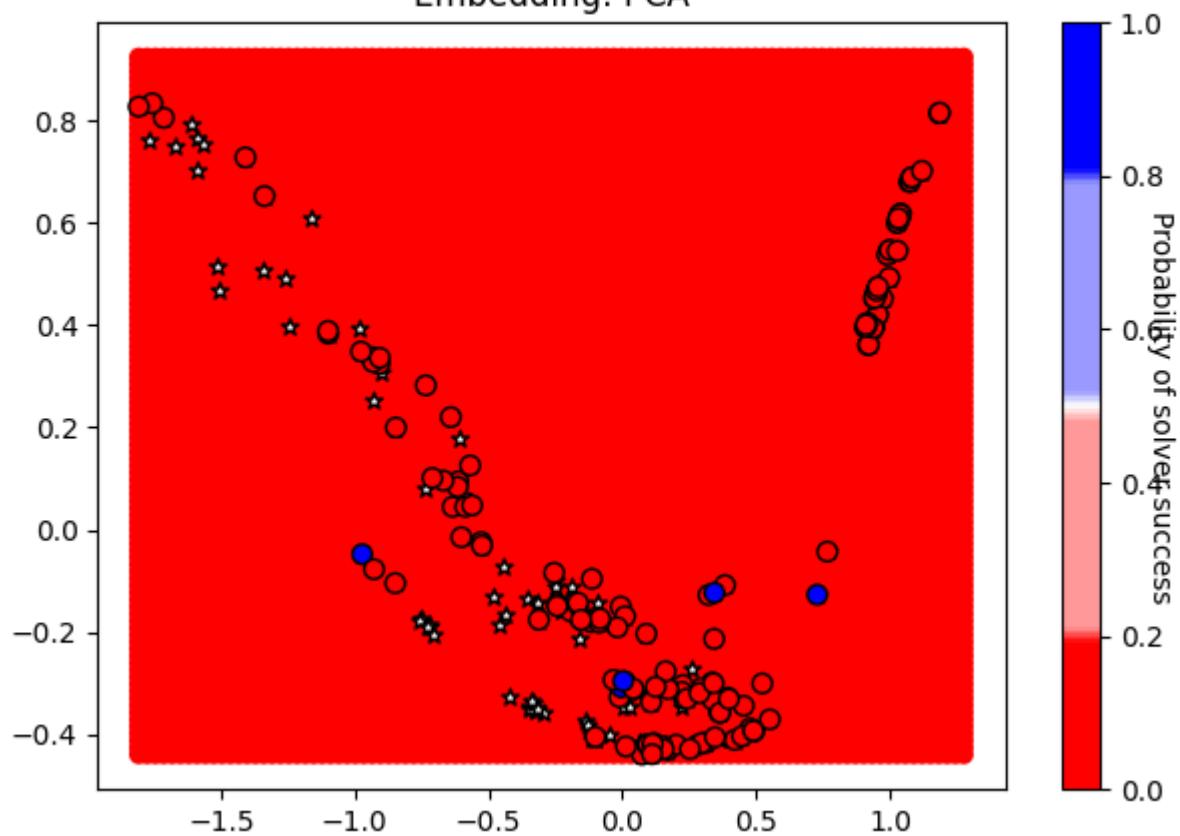
Note: plot only contains attempted tasks.

Utility capture from MP2/b42035...

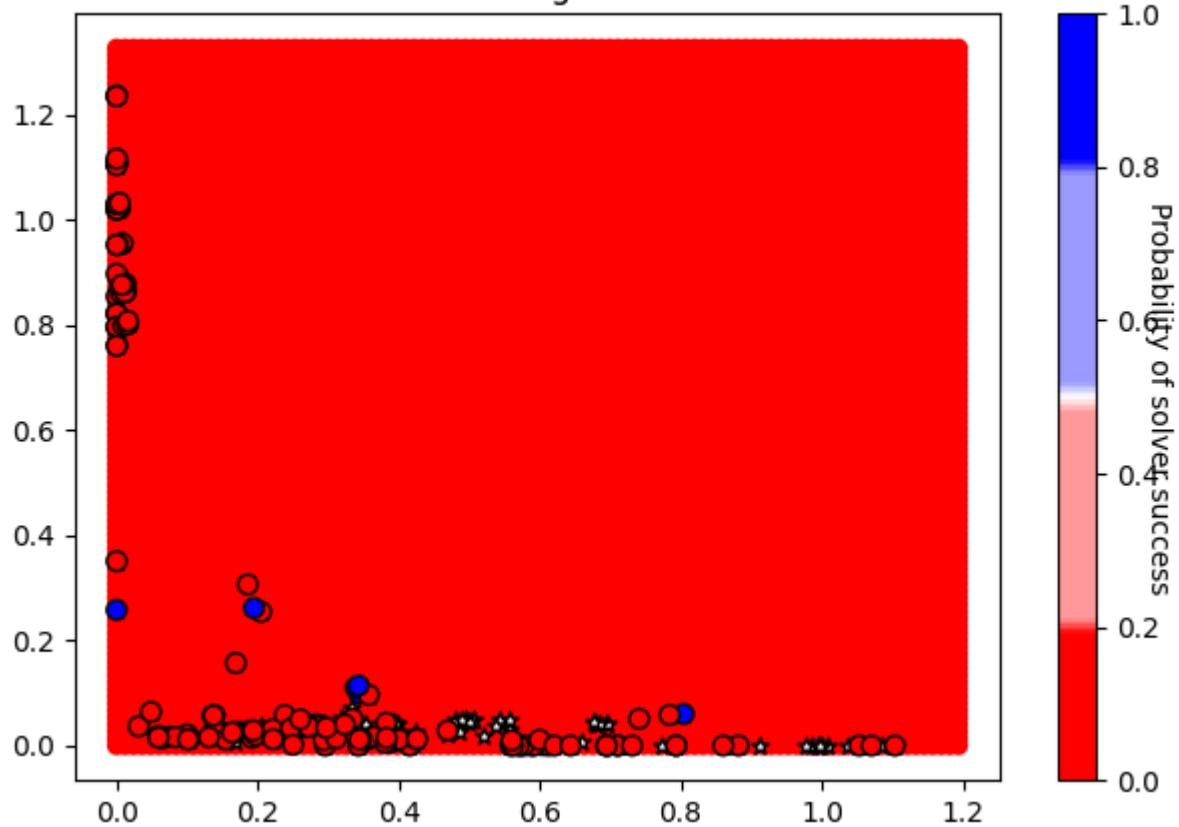
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



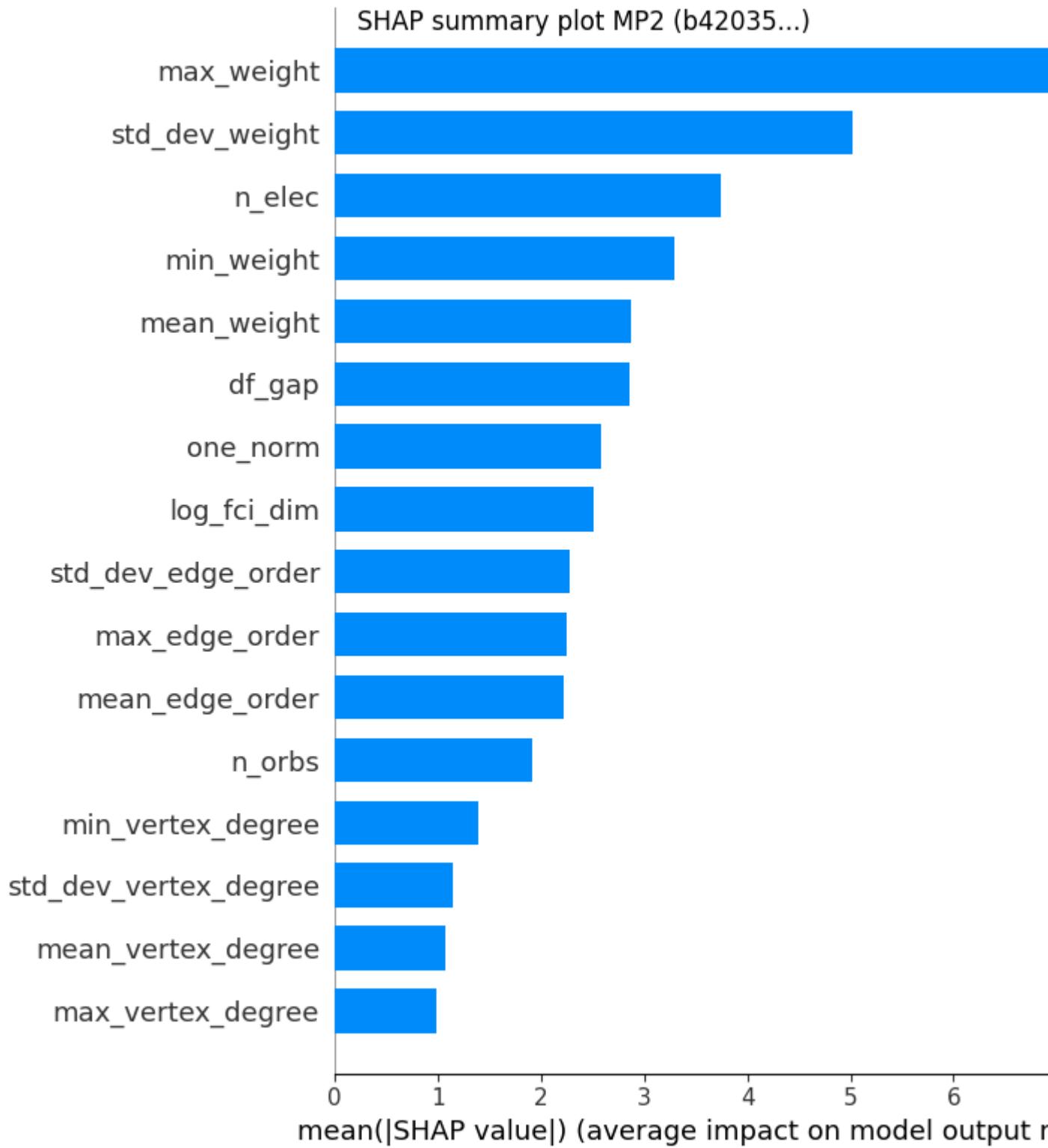
Solver MP2 (b42035...)
Embedding: PCA



Solver MP2 (b42035...)
Embedding: NNMF



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

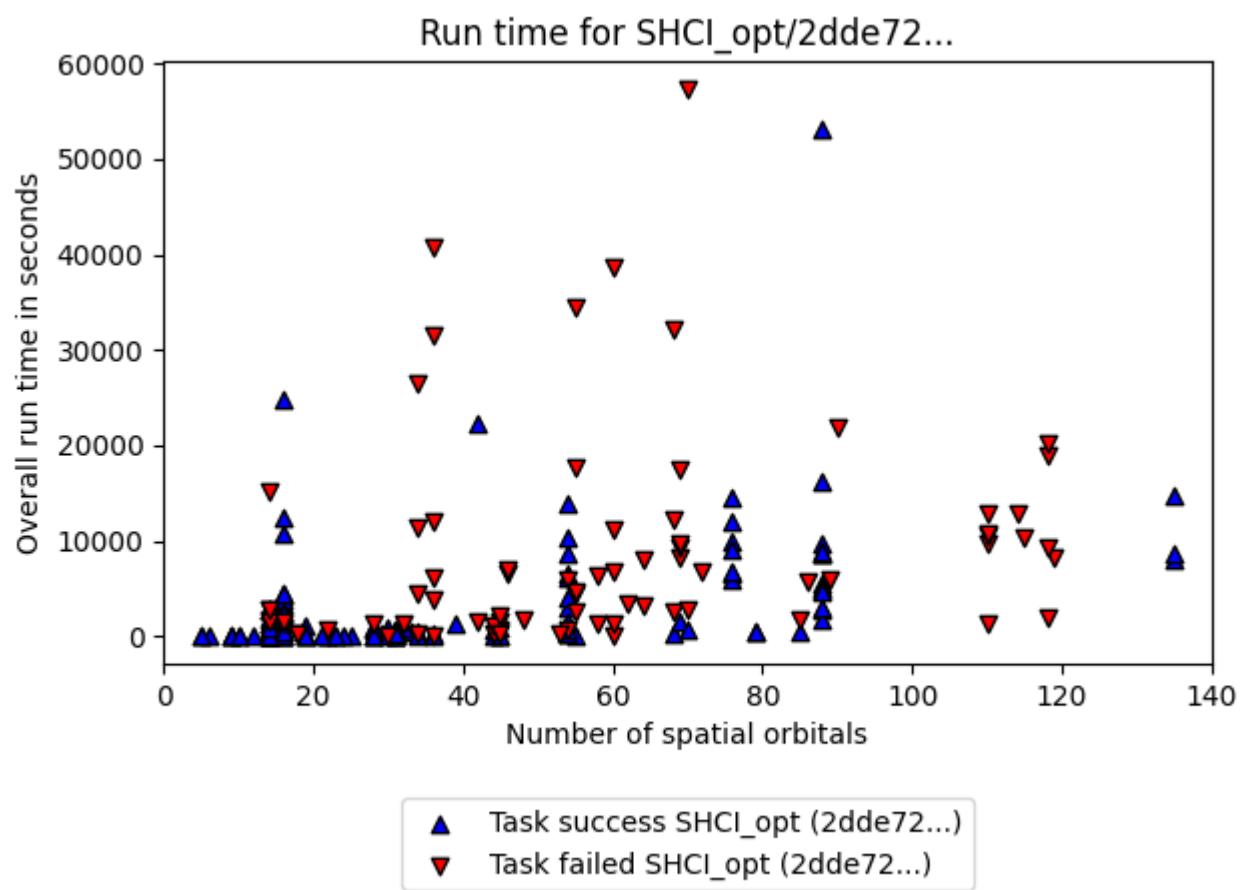


Solver SHCI_opt, 2dde727e-a881-44fa-aabf-bba6248e4baf

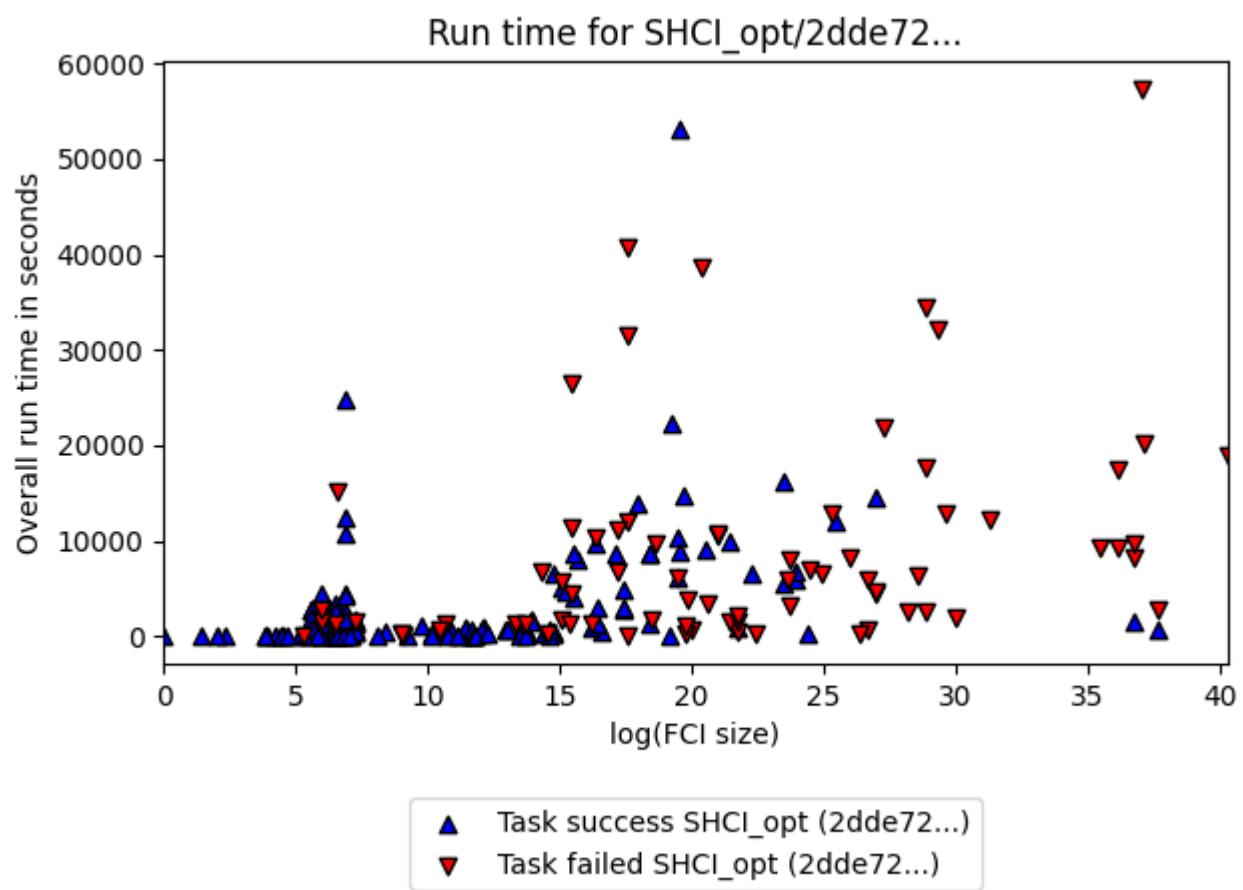
solver_uuid:2dde727e-a881-44fa-aabf-bba6248e4baf

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: 819c2f9e-f6ee-4174-9a30-304068b6902b
creation.timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 66
number_of_problem_instances_solved: 37
number_of_tasks: 228
number_of_tasks_attempted: 226
number_of_tasks_solved: 148
number_of_tasks_solved_within_run_time_limit: 226
number_of_tasks_solved_within_accuracy_threshold: 148
max_run_time_of_attempted_tasks: 57334.2
sum_of_run_time_of_attempted_tasks: 1100317.5919999995
solvability_ratio: 1.0
comments: solvability ratio based on PCA embedding.
f1_score: [0.8333333333333334, 0.9931972789115646]
ml.metrics_calculator_version: 1



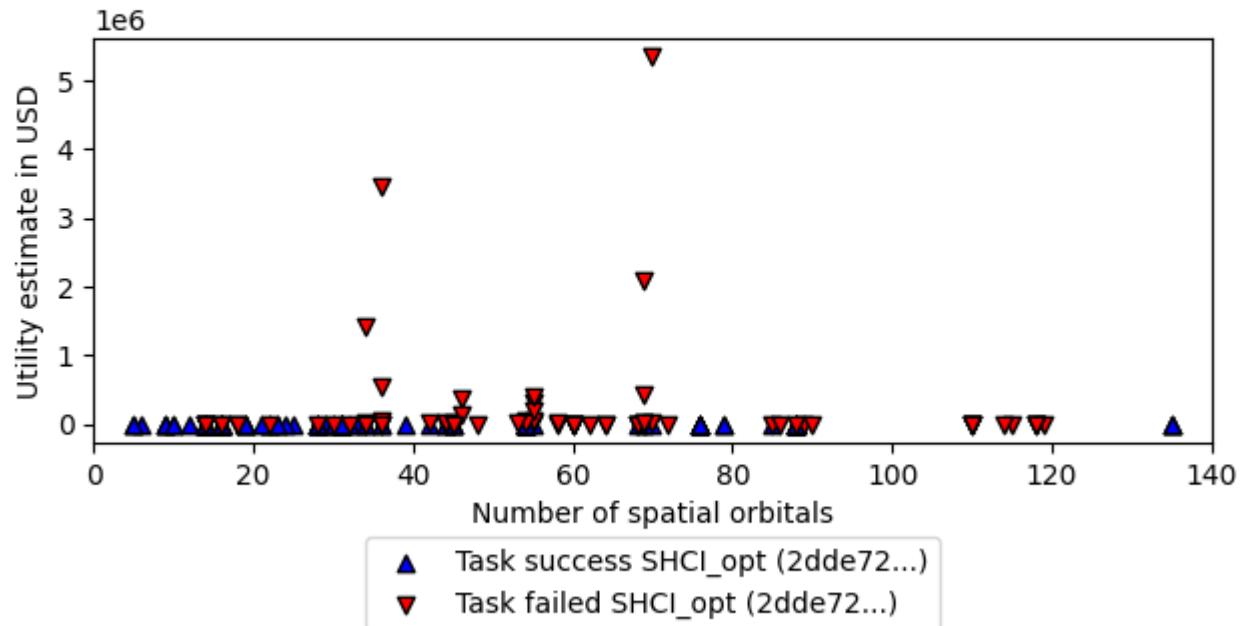
Note: plot only contains attempted tasks.



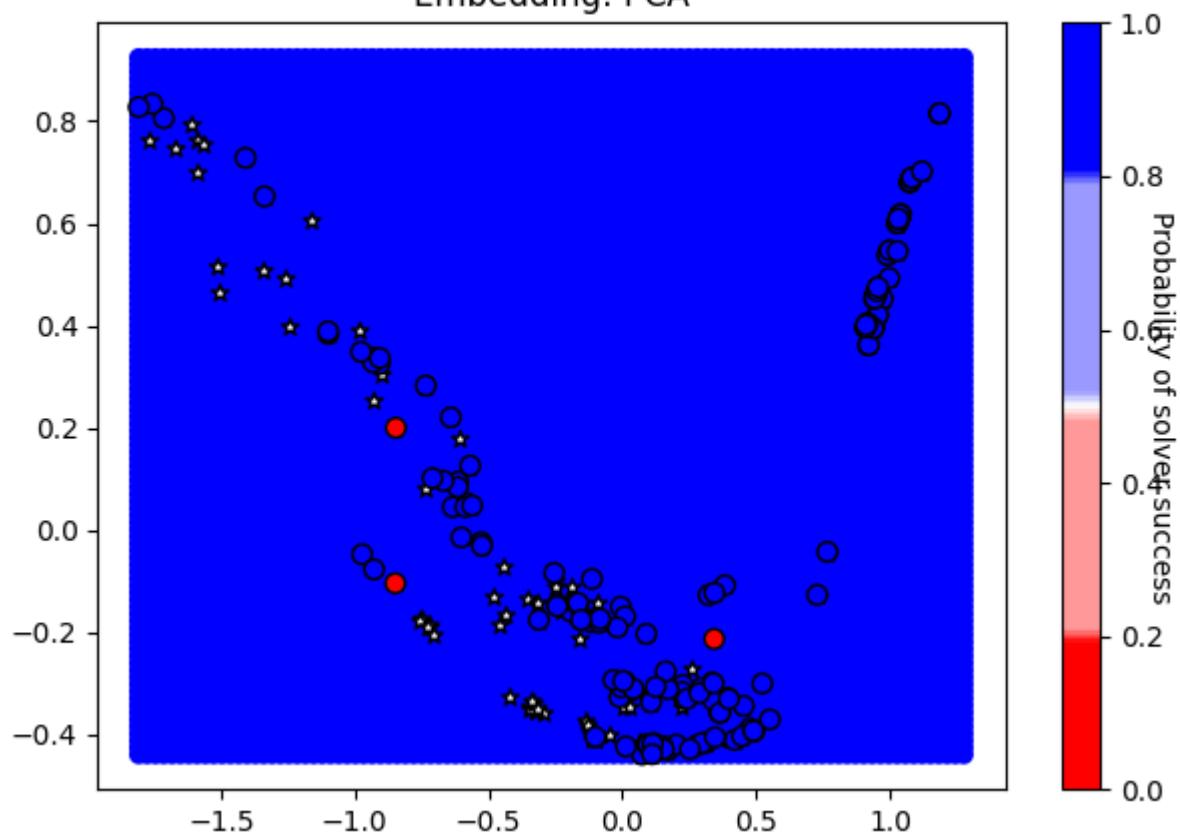
Note: plot only contains attempted tasks.

Utility capture from SHCI_opt/2dde72...

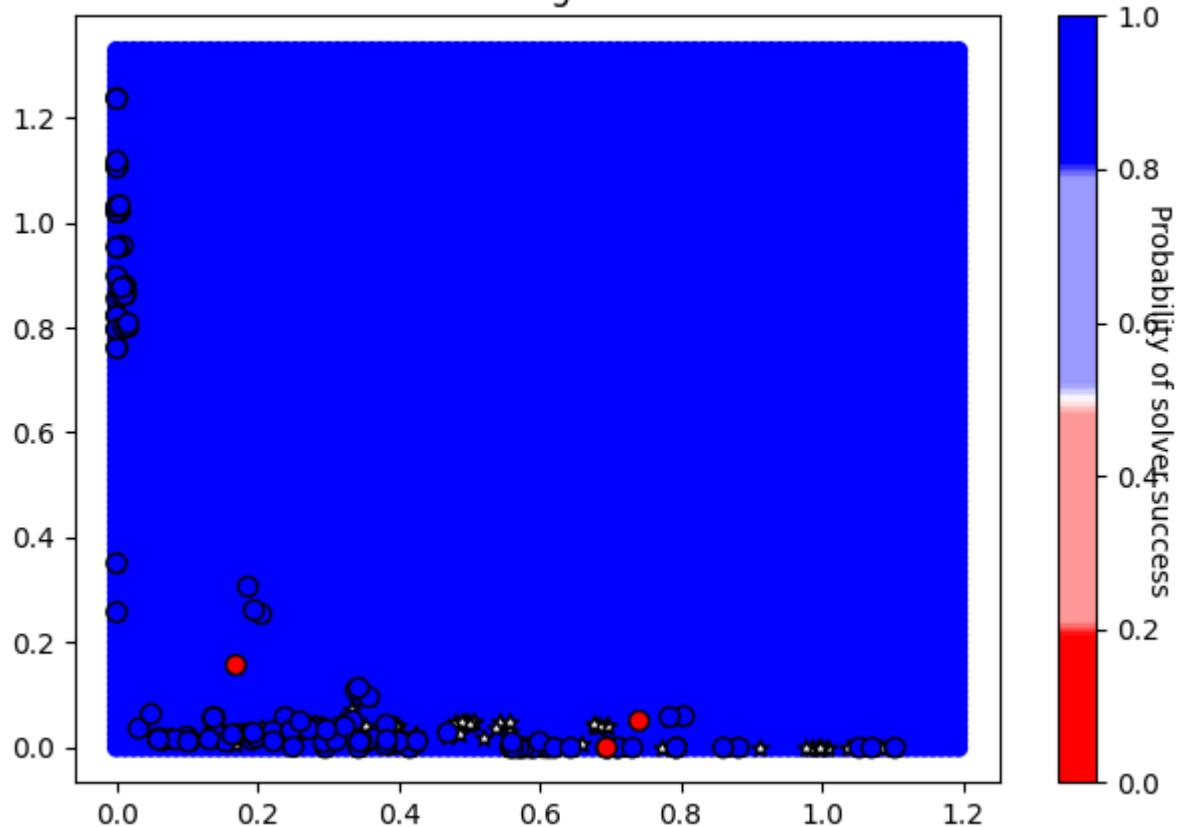
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



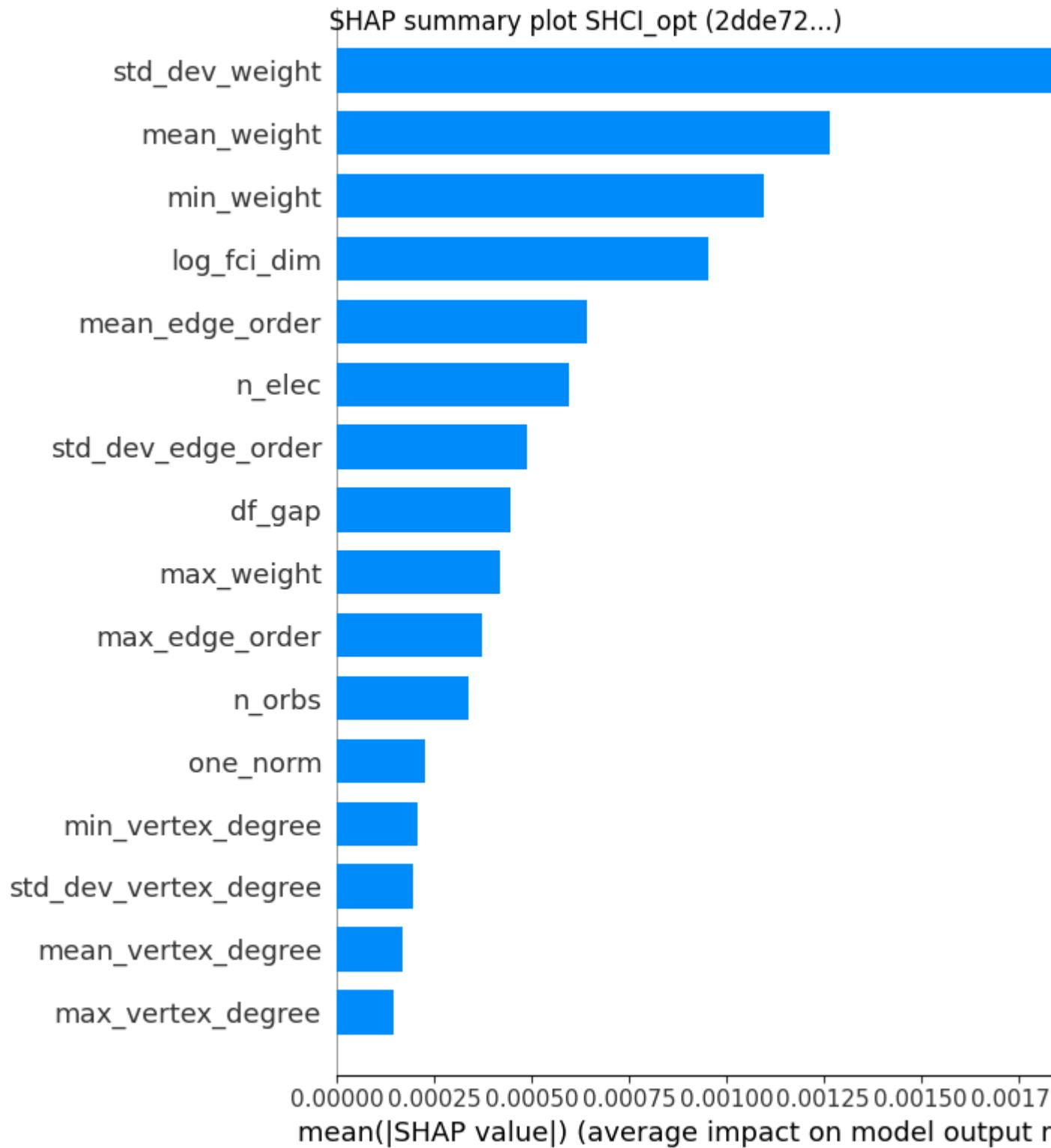
Solver SHCI_opt (2dde72...)
Embedding: PCA



Solver SHCI_opt (2ddee72...)
Embedding: NMF



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

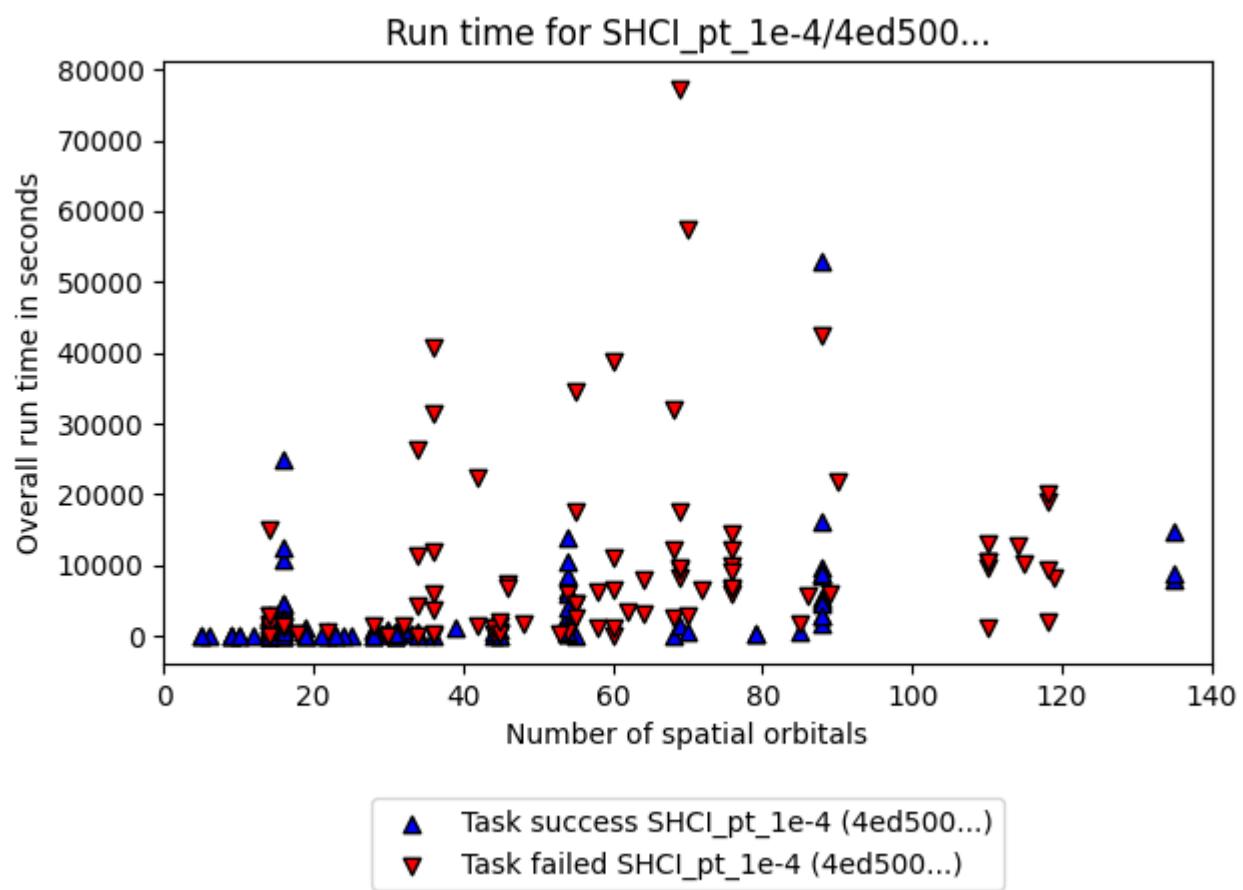


Solver SHCI_pt_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4

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

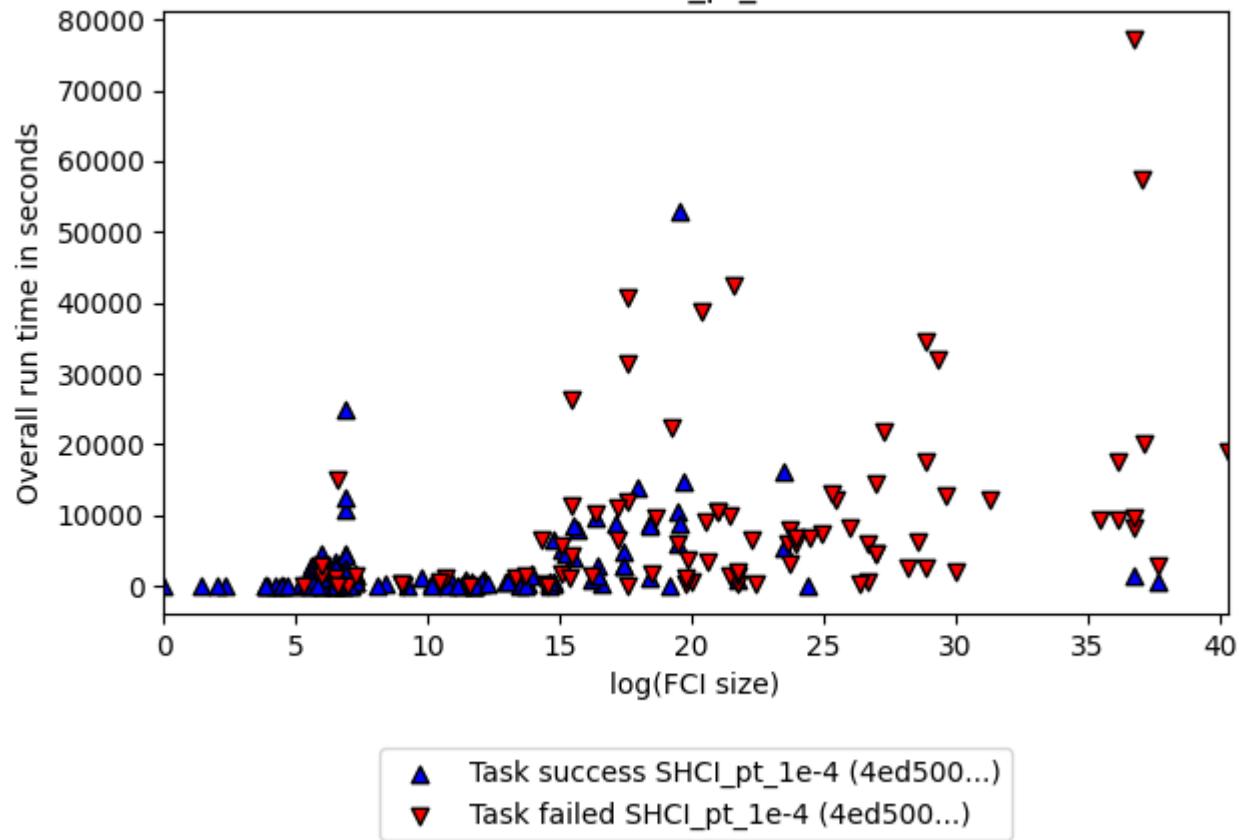
solver_short_name:SHCI_pt_1e-4

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: af24371d-13ea-4d50-a8a1-528966af7d0b
creation_timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 26
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 135
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 135
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 1.0
comments: solvability ratio based on PCA embedding.
f1_score: [0.7142857142857143, 0.9712230215827338]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

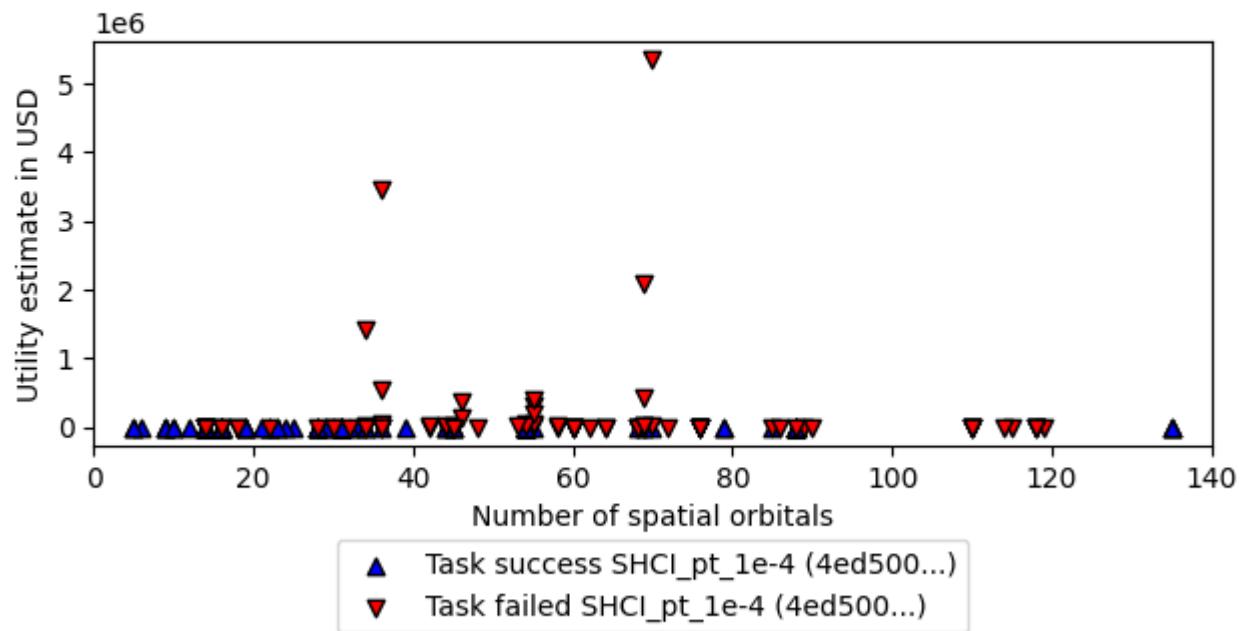
Run time for SHCI_pt_1e-4/4ed500...



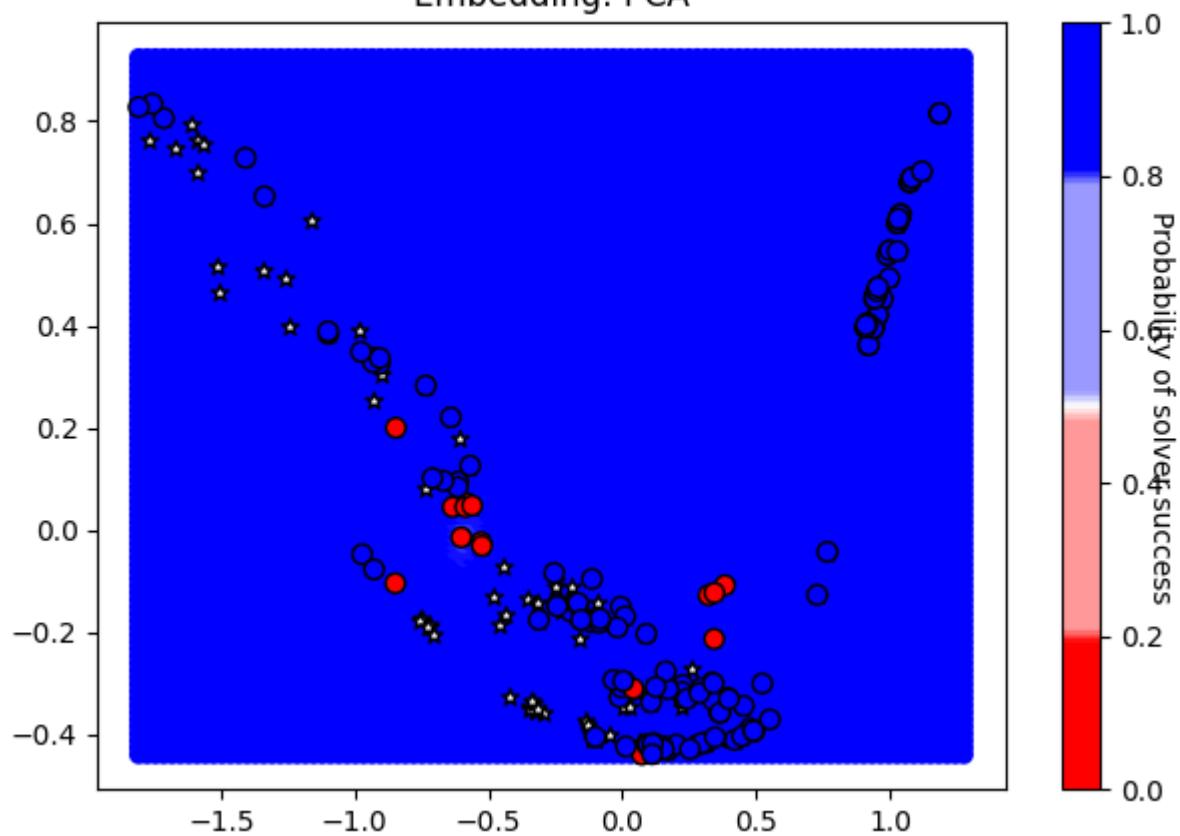
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_1e-4/4ed500...

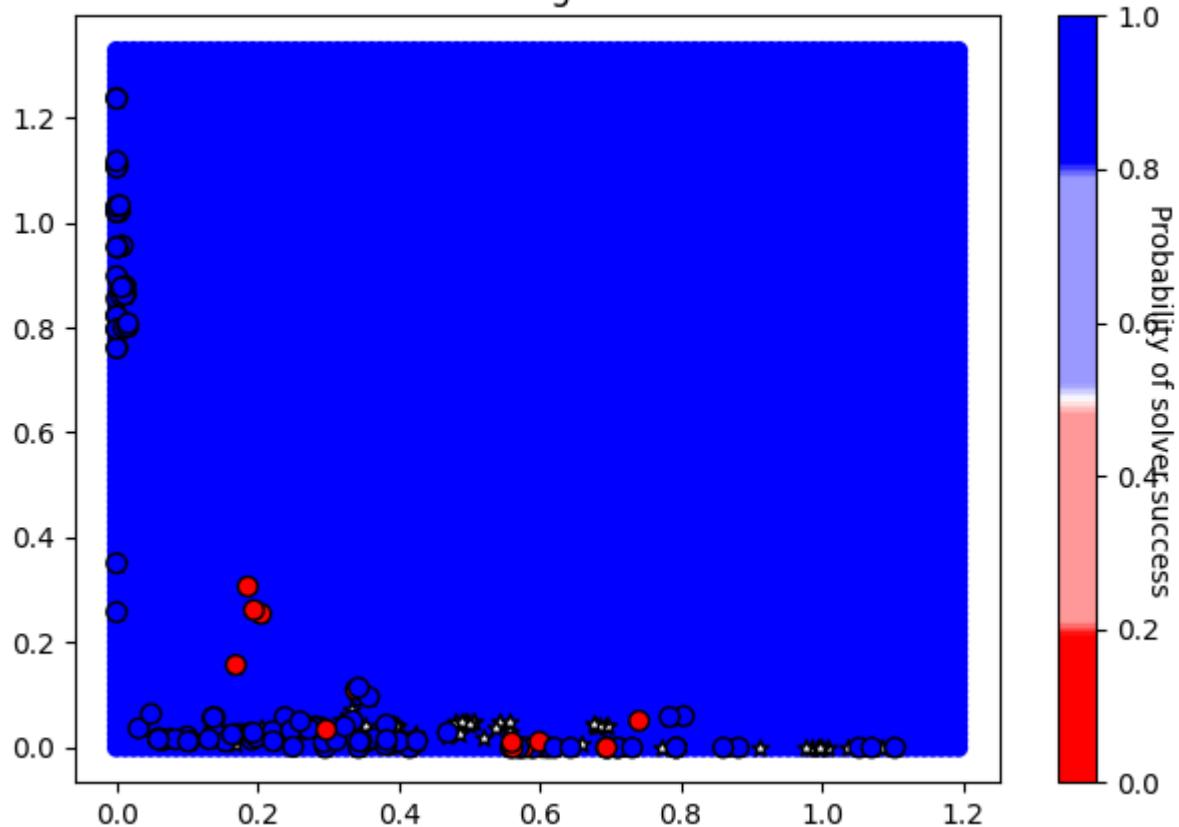
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



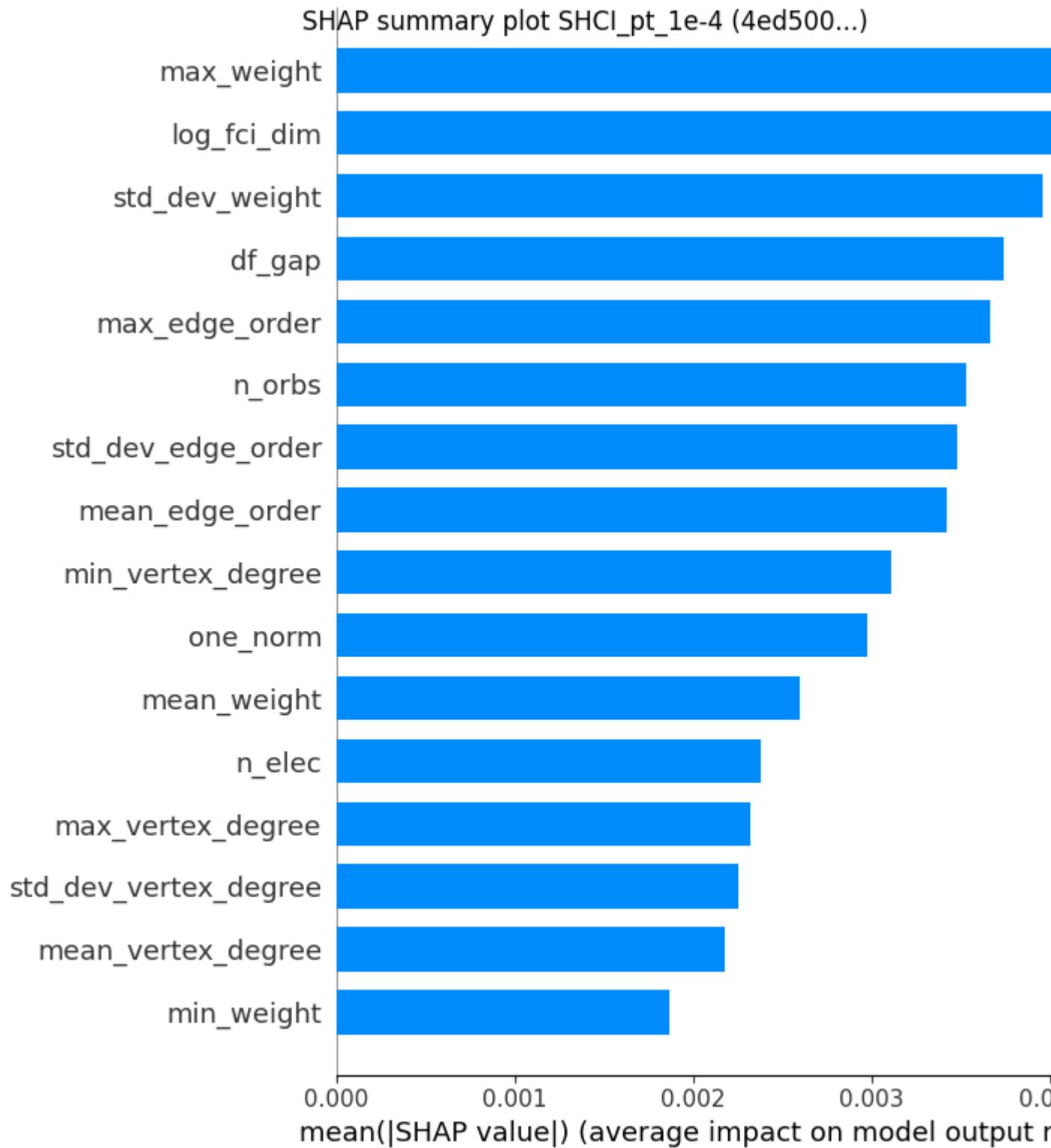
Solver SHCI_pt_1e-4 (4ed500...)
Embedding: PCA



Solver SHCI_pt_1e-4 (4ed500...)
Embedding: NMF



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

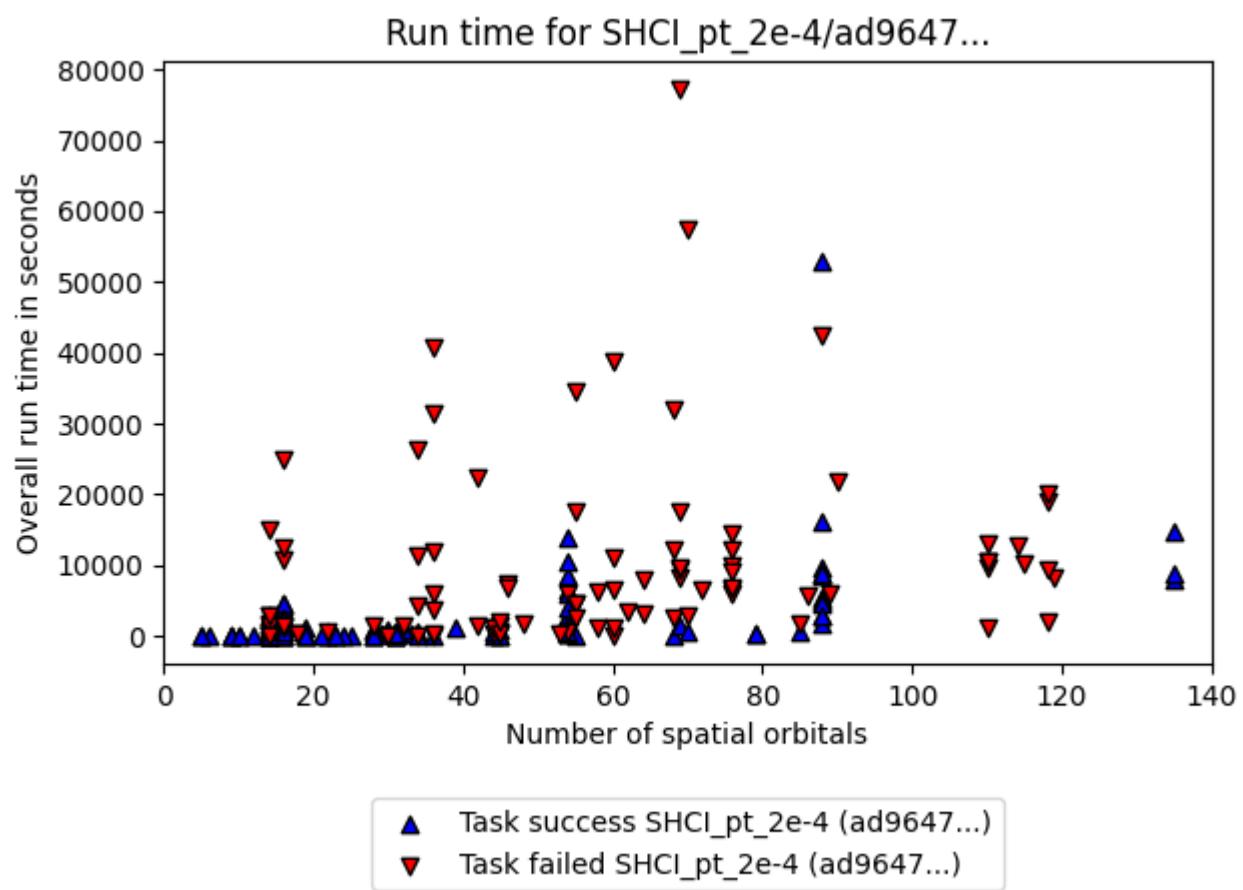


Solver SHCI_pt_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb

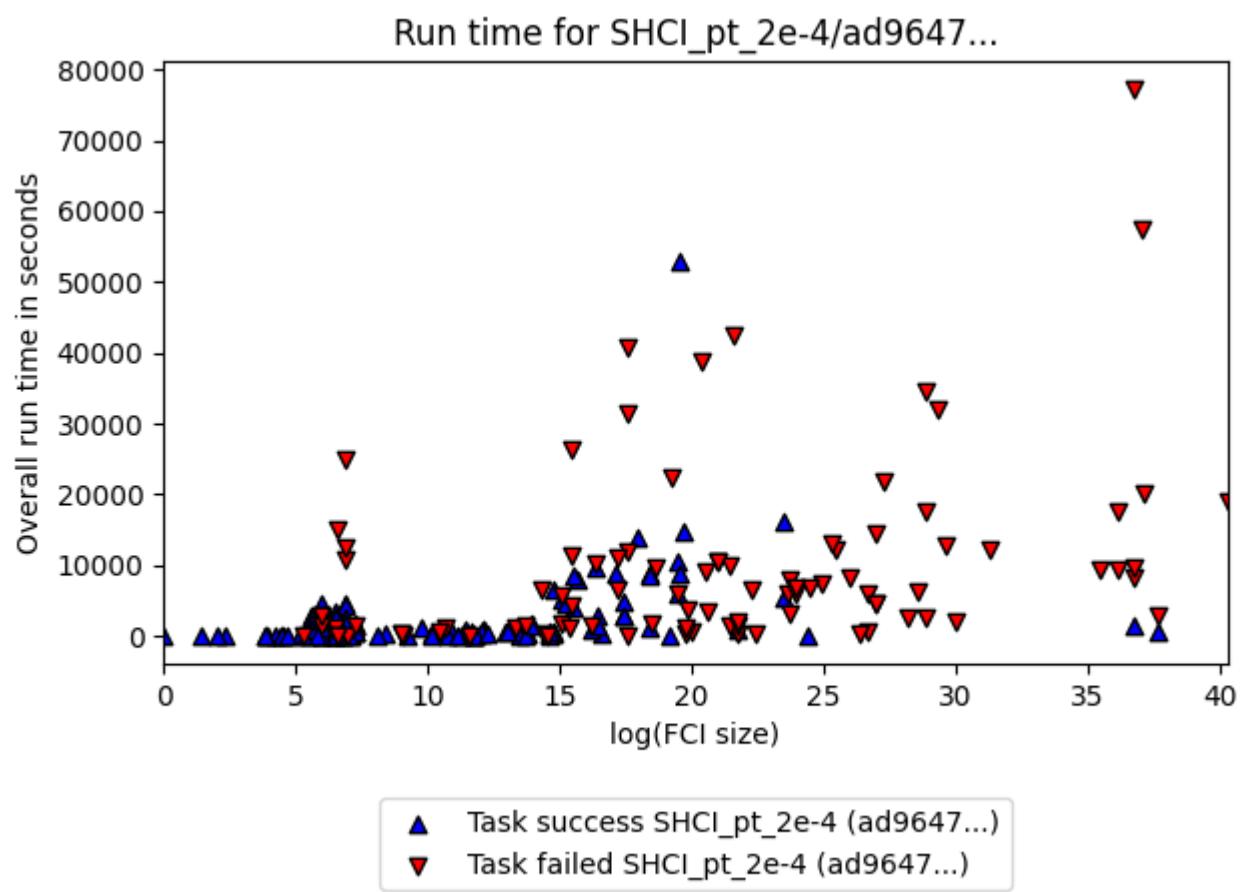
solver_uuid:ad964781-302e-4728-a26d-39918e0a6cdb

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: c9424a23-c810-4bc1-8f85-7f383fe7e76c
creation.timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 26
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 132
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 132
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 1.0
comments: solvability ratio based on PCA embedding.
f1_score: [0.8936170212765957, 0.9806949806949807]
ml.metrics_calculator_version: 1



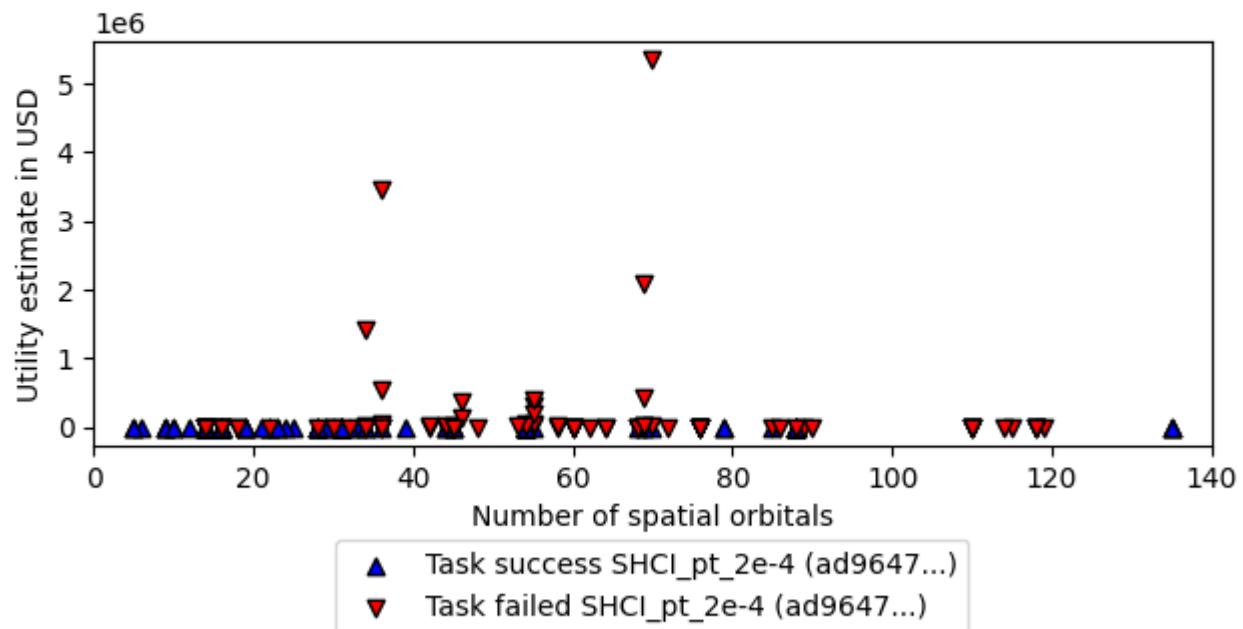
Note: plot only contains attempted tasks.



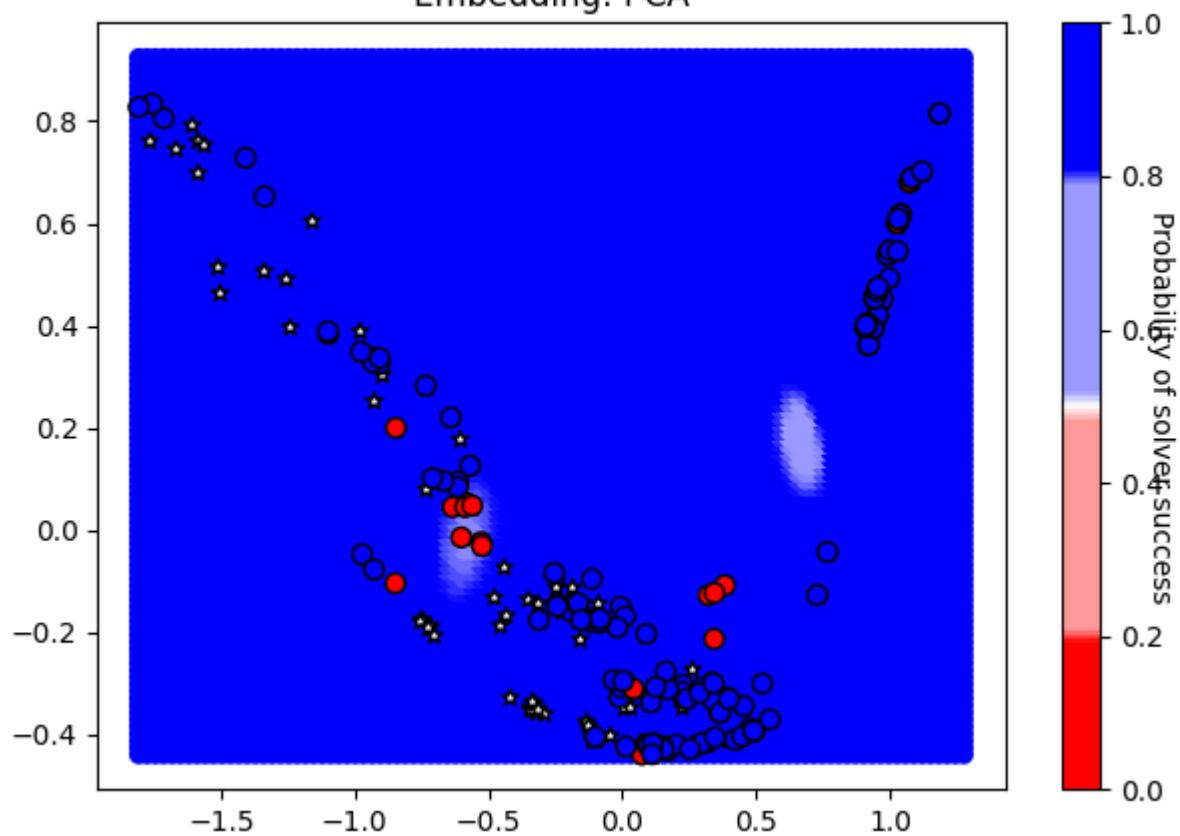
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-4/ad9647...

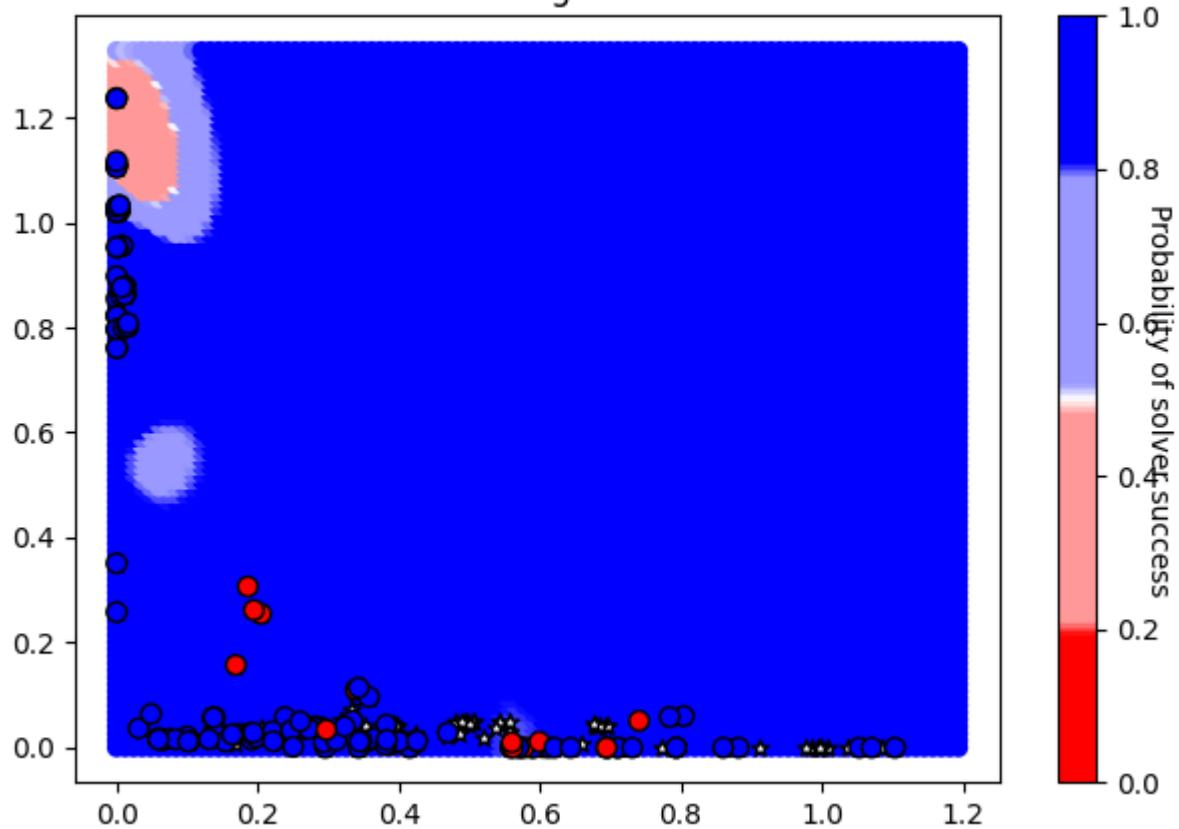
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



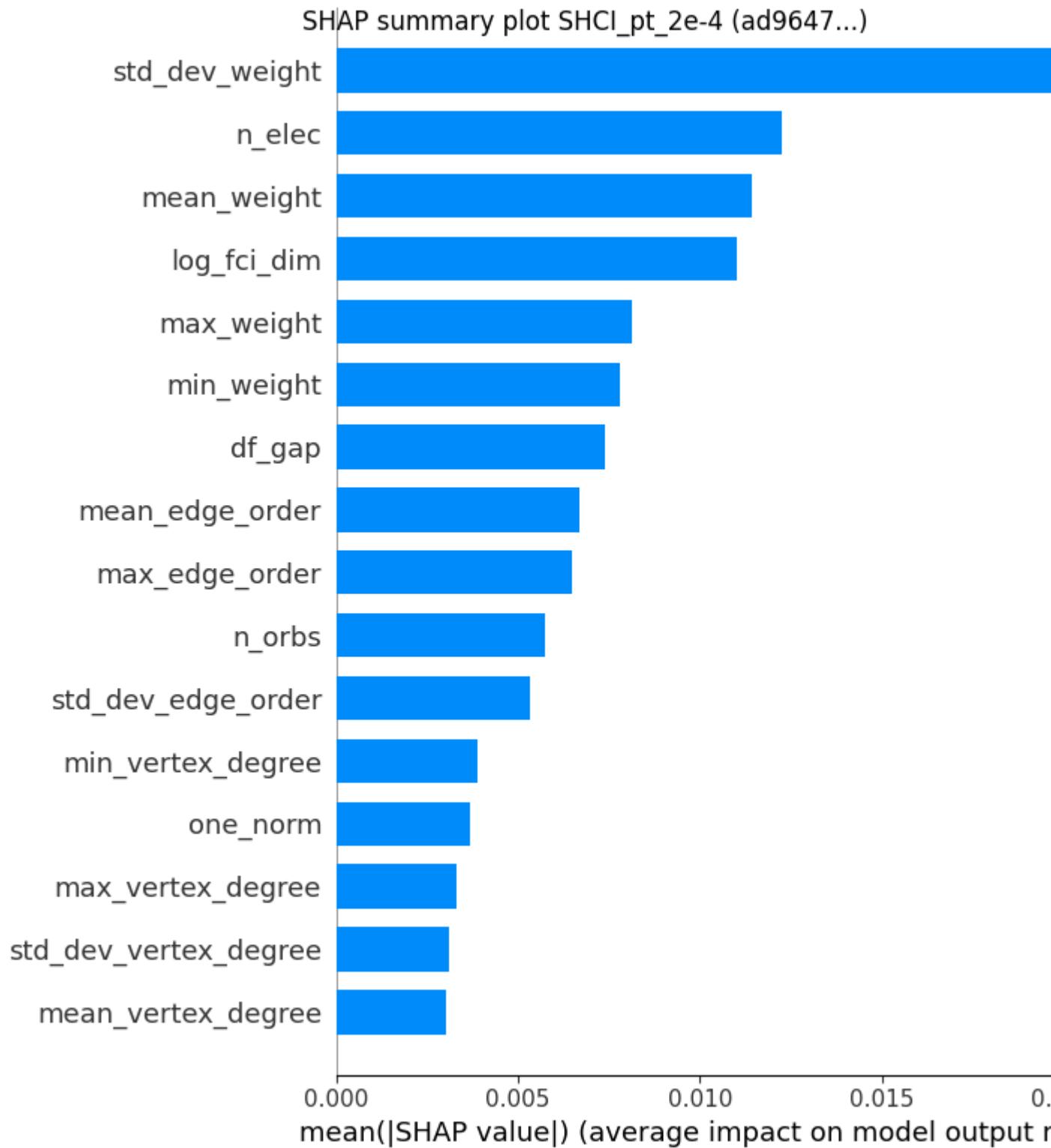
Solver SHCI_pt_2e-4 (ad9647...)
Embedding: PCA



Solver SHCI_pt_2e-4 (ad9647...)
Embedding: NMF



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

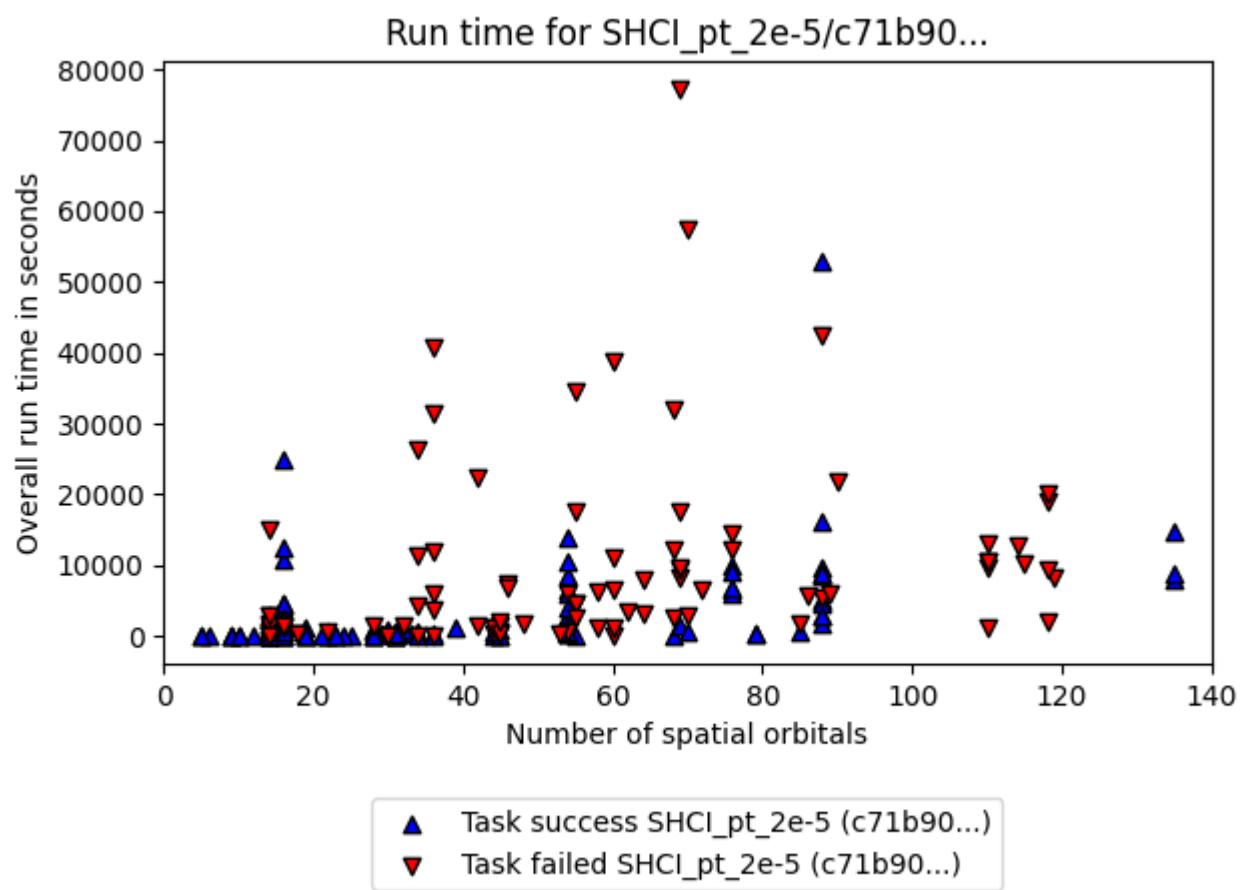


Solver SHCI_pt_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6

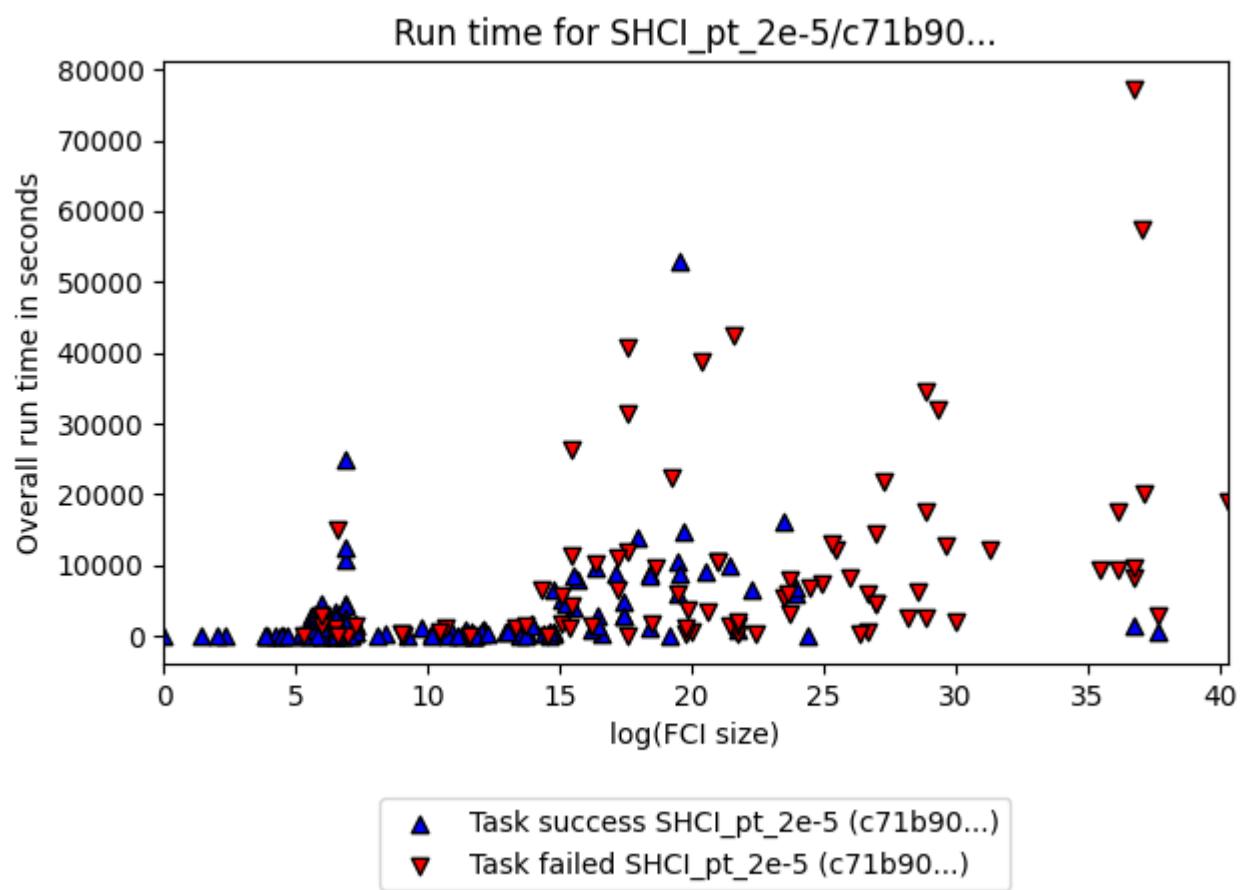
solver_uuid:c71b90bd-3250-4c0c-b4e7-fc9878f141f6

solver_short_name:SHCI_pt_2e-5

compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-5 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: b3f79610-07f1-429b-89c4-71233339c172
creation.timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 30
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 140
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 140
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 0.9317
comments: solvability ratio based on PCA embedding.
f1_score: [0.7647058823529411, 0.9705882352941176]
ml.metrics_calculator_version: 1



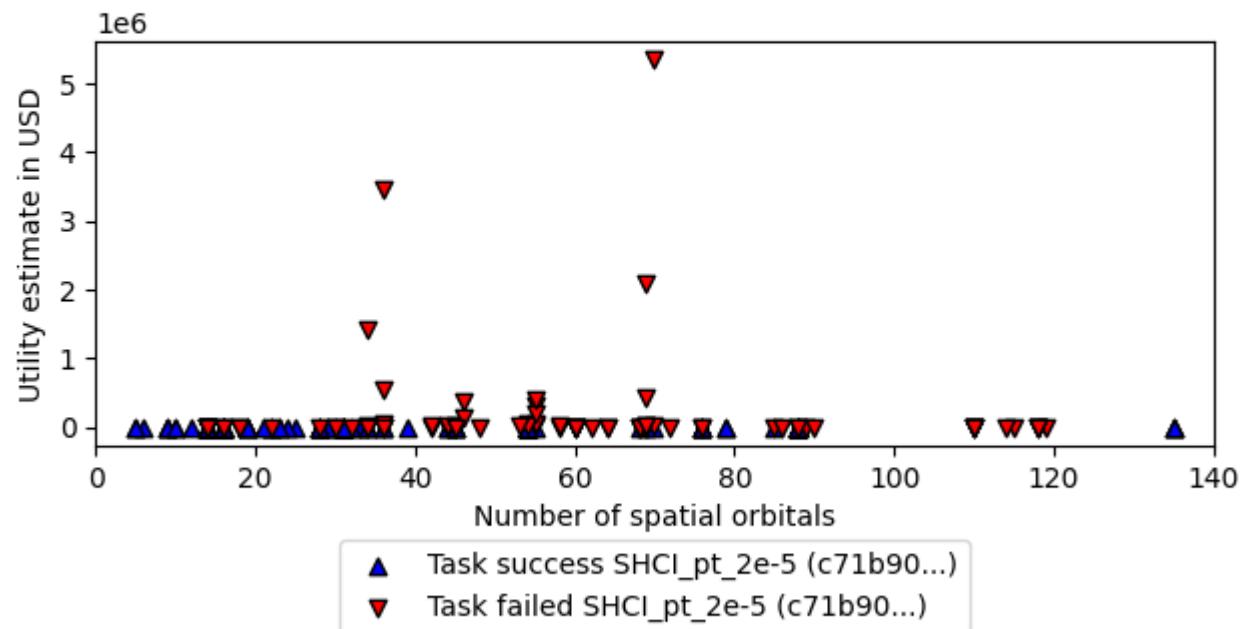
Note: plot only contains attempted tasks.



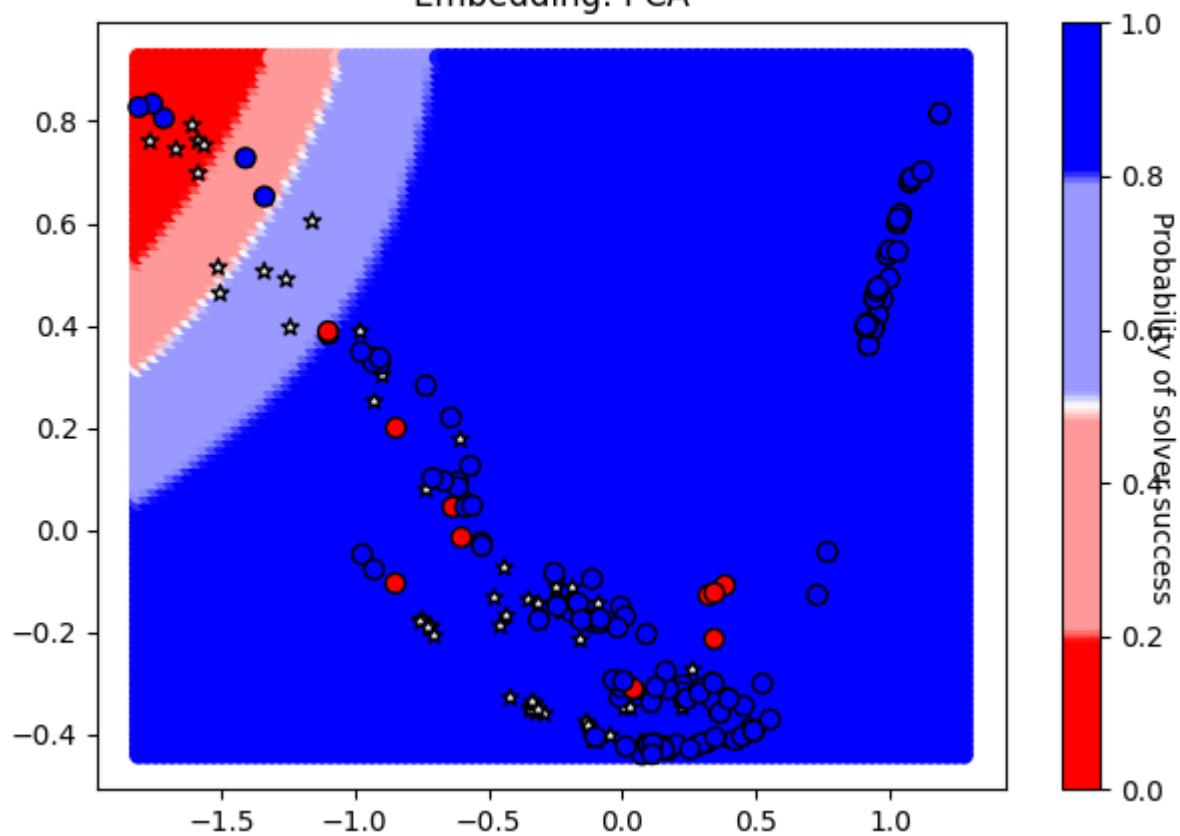
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-5/c71b90...

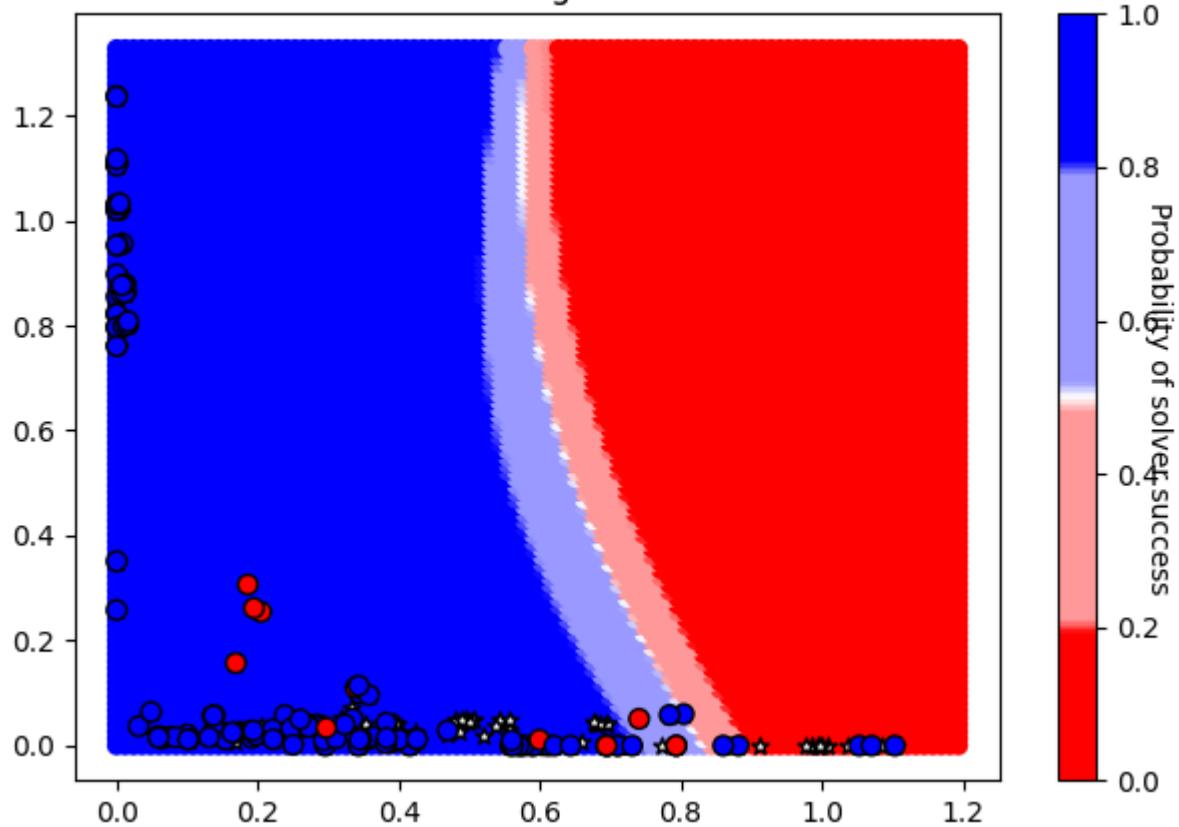
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



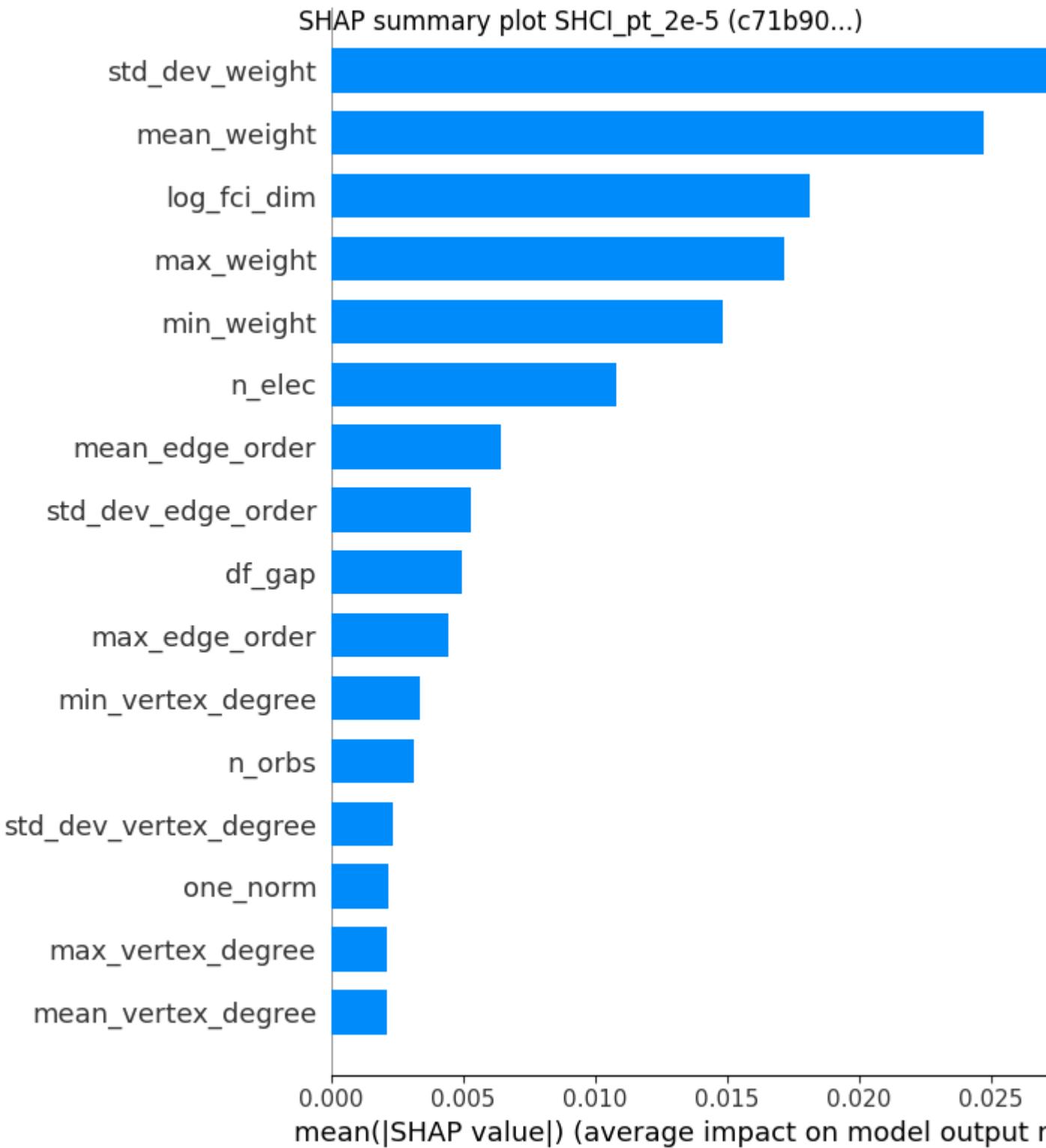
Solver SHCI_pt_2e-5 (c71b90...)
Embedding: PCA



Solver SHCI_pt_2e-5 (c71b90...)
Embedding: NMF



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

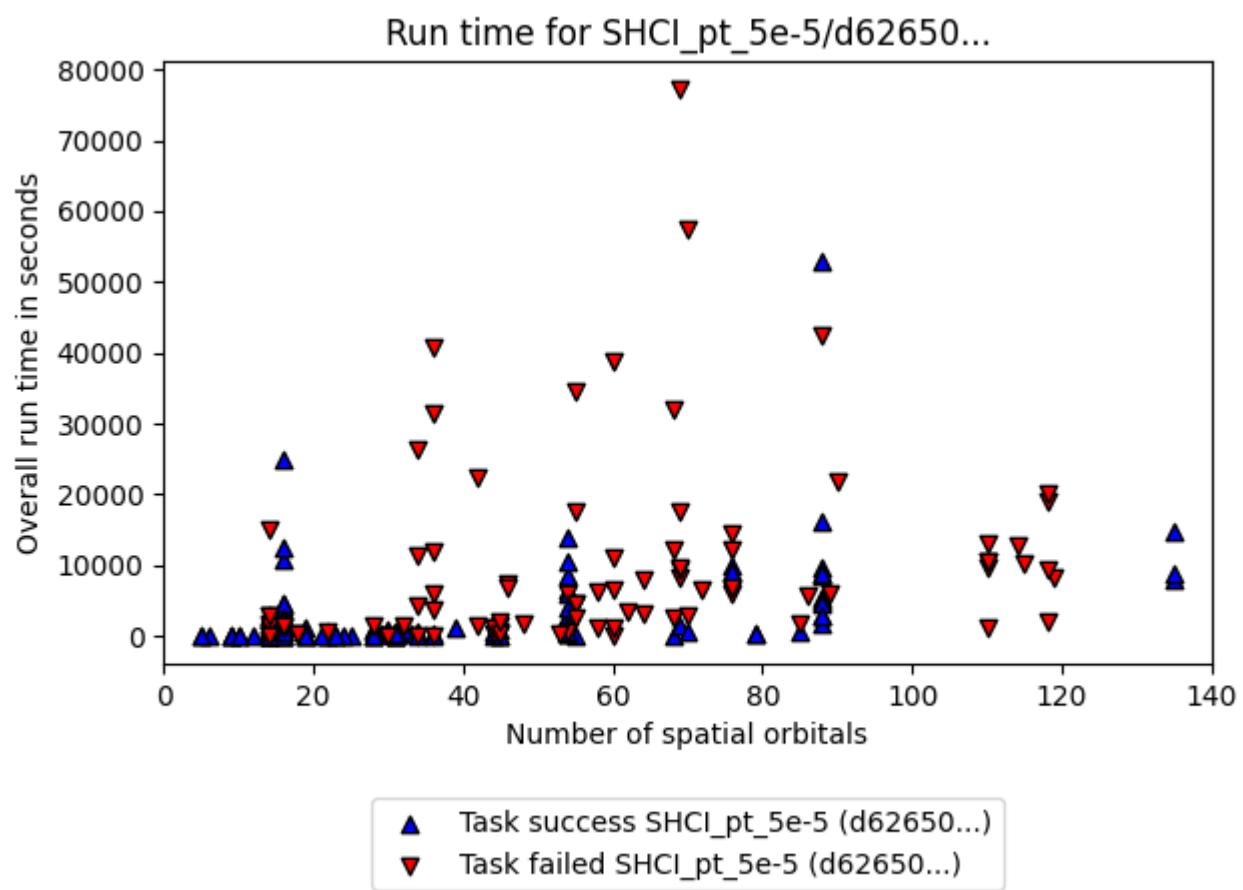


Solver SHCI_pt_5e-5, d626506c-7aae-4ad6-802a-b29af5f2bb93

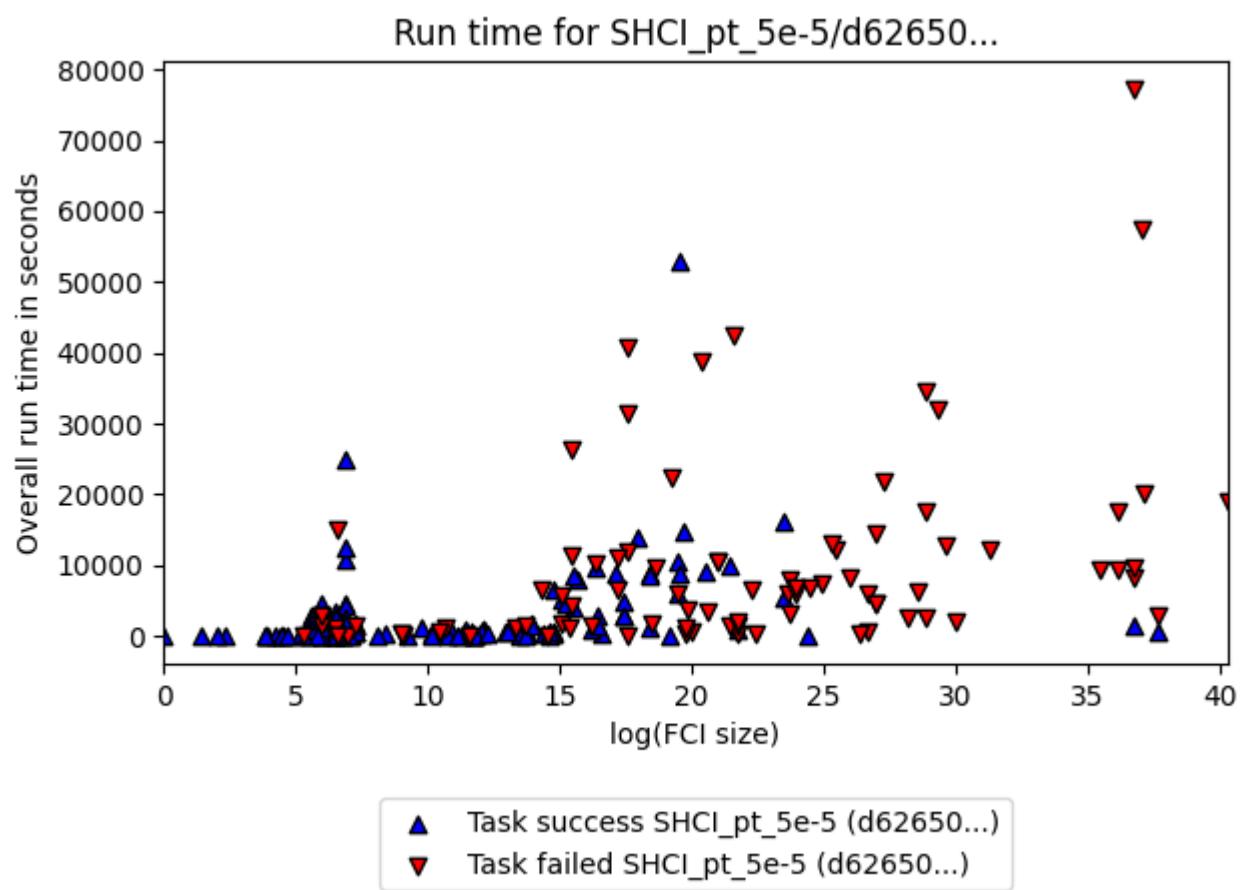
solver_uuid:d626506c-7aae-4ad6-802a-b29af5f2bb93

solver_short_name:SHCI_pt_5e-5

compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 5e-5 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: a80dcd6c-68c1-49e4-b8f3-6031f0d1a982
creation.timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 28
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 138
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 138
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 1.0
comments: solvability ratio based on PCA embedding.
f1_score: [0.9375, 0.9927007299270073]
ml.metrics_calculator_version: 1



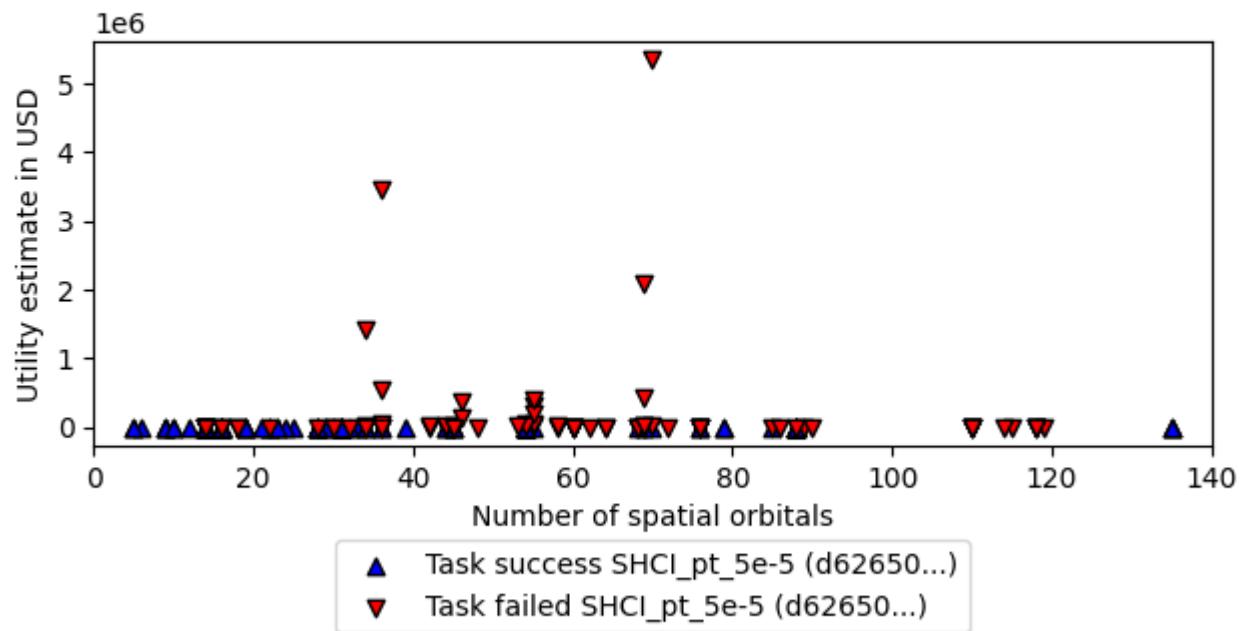
Note: plot only contains attempted tasks.



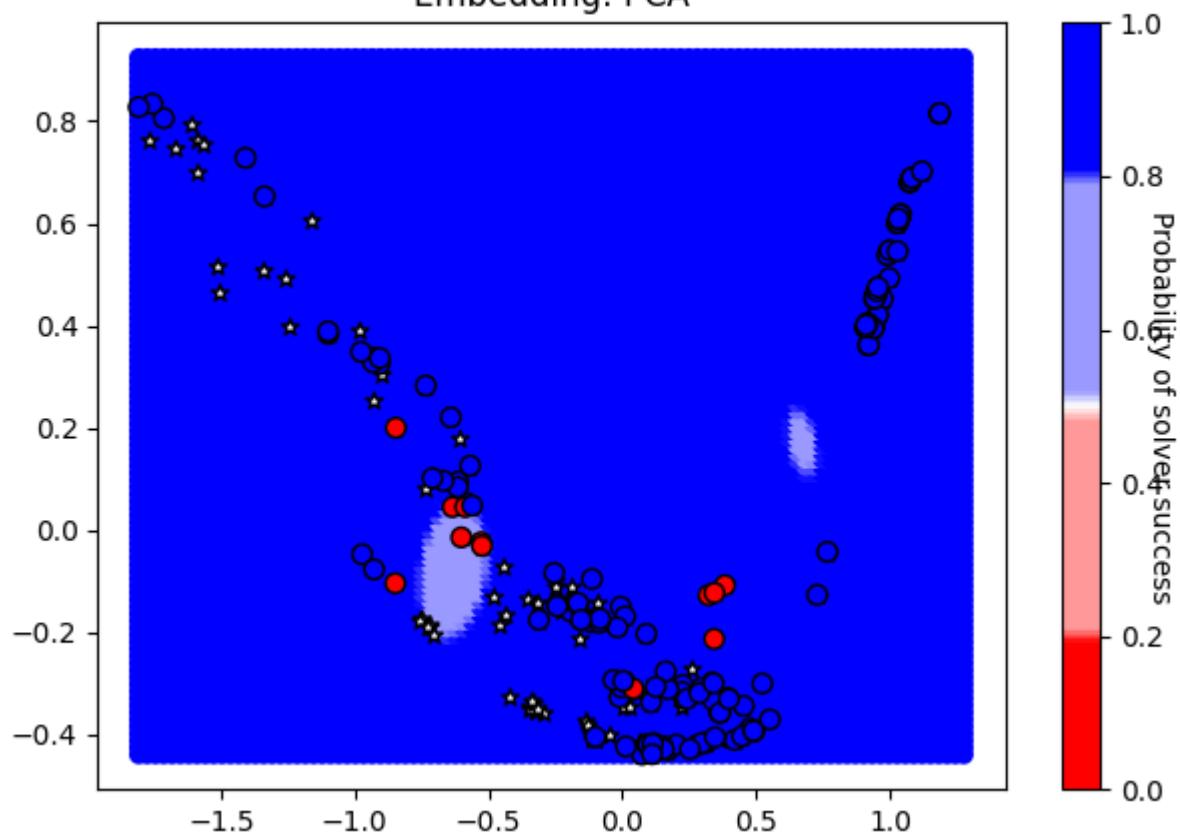
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_5e-5/d62650...

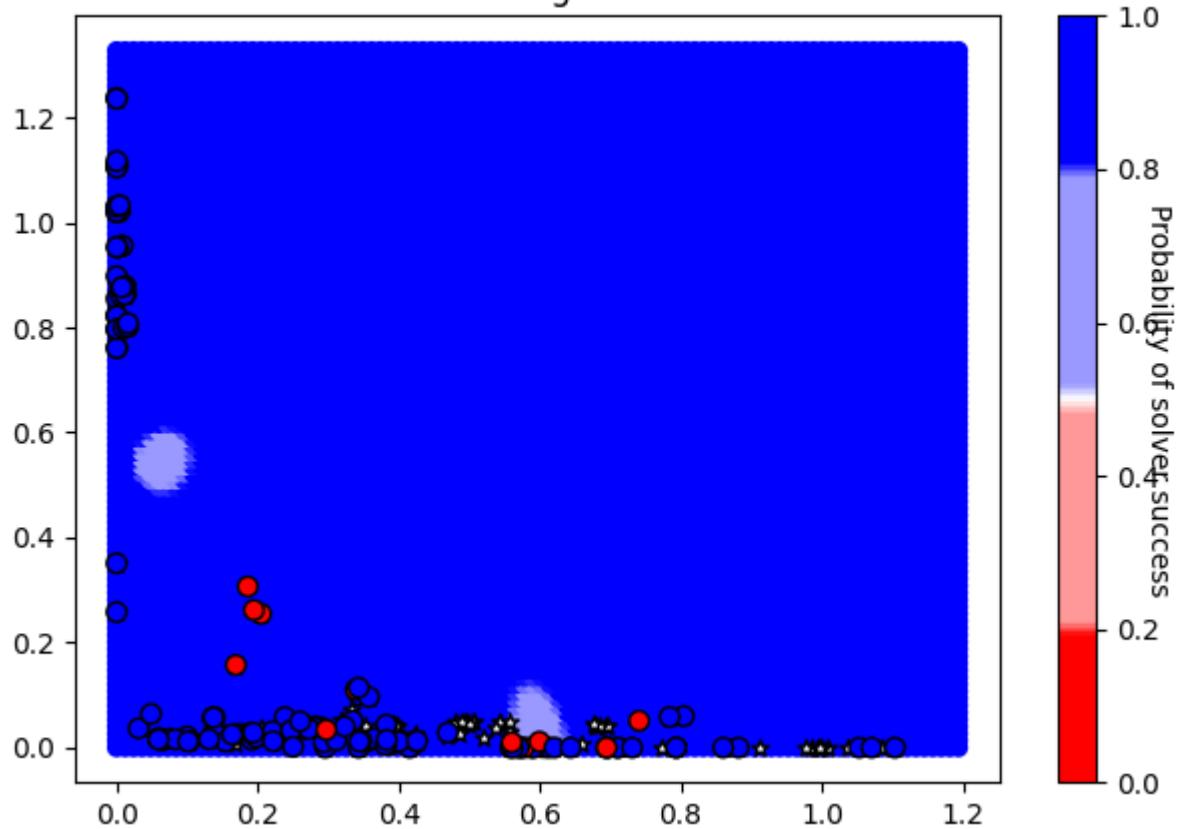
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



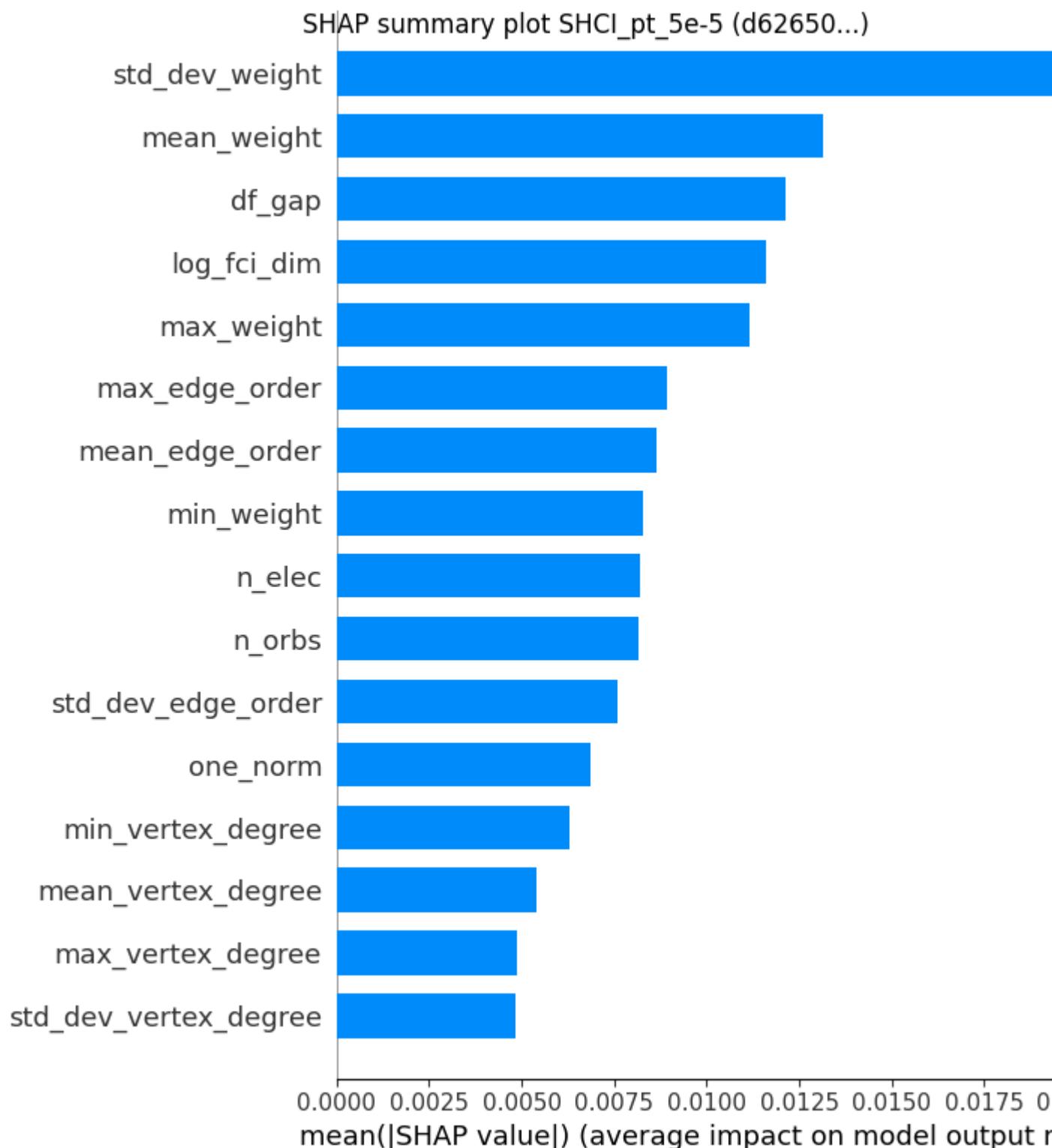
Solver SHCI_pt_5e-5 (d62650...)
Embedding: PCA



Solver SHCI_pt_5e-5 (d62650...)
Embedding: NMF



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

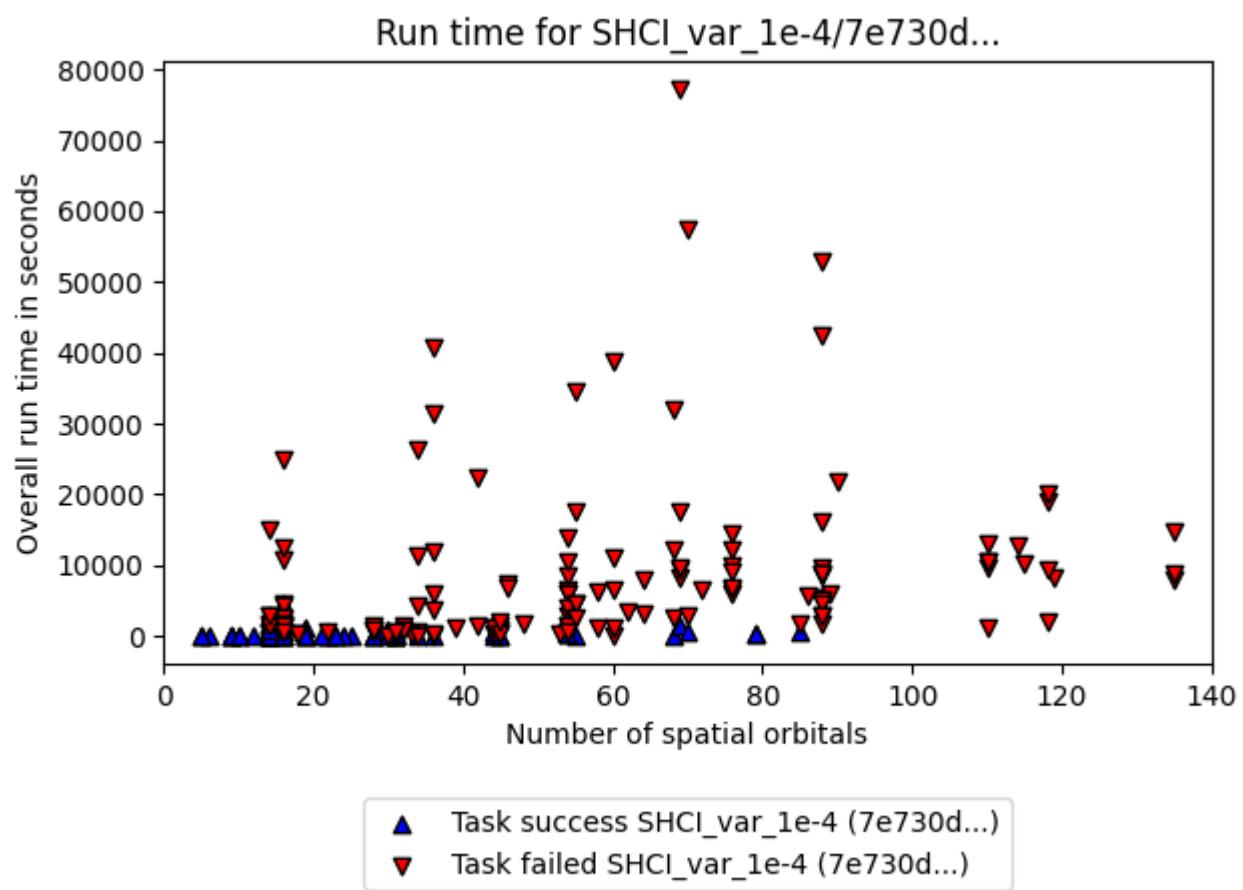


Solver SHCI_var_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54

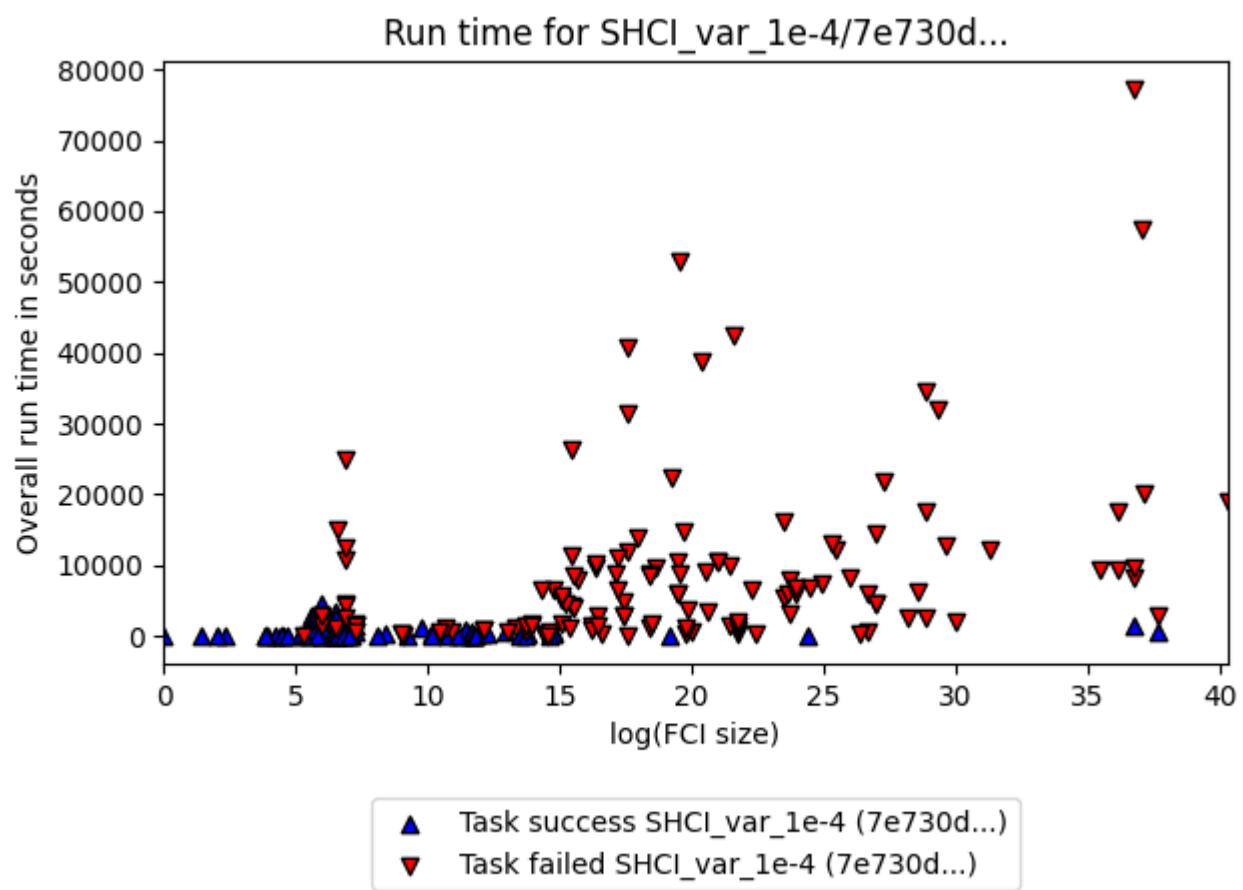
solver_uuid:7e730dfb-57ee-480b-a8a1-4b73f5f07c54

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: be2723ac-28b2-477f-bb6e-038cbb15b607
creation.timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 17
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 91
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 91
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 0.6562
comments: solvability ratio based on PCA embedding.
f1_score: [0.9838709677419355, 0.989010989010989]
ml.metrics_calculator_version: 1



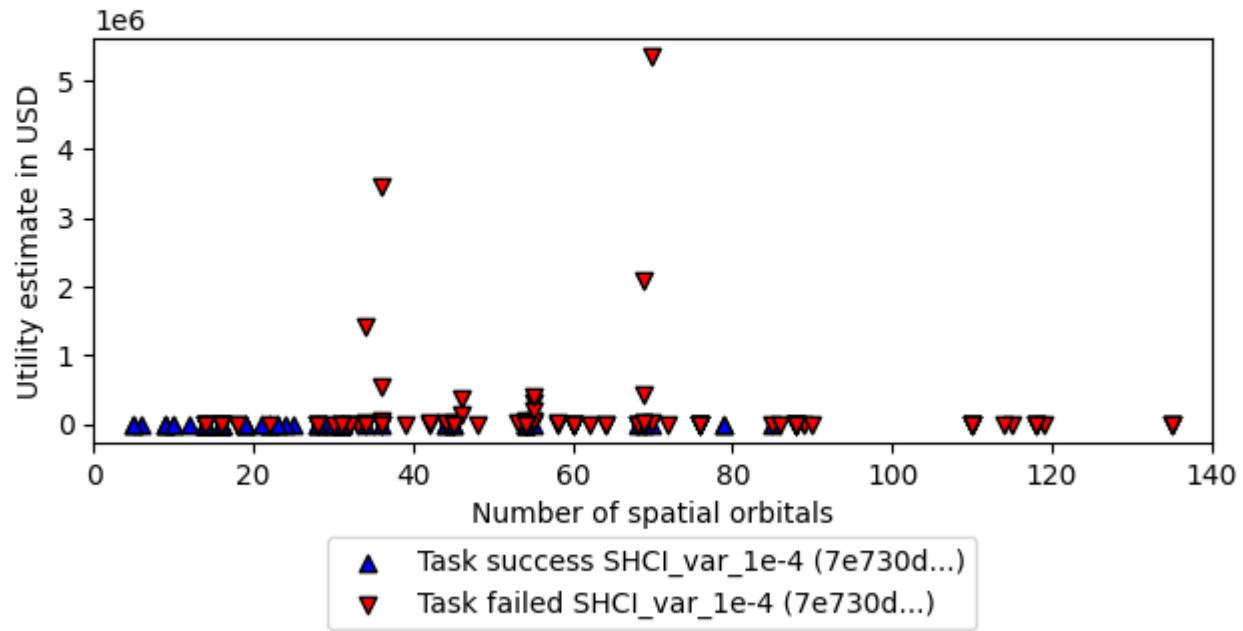
Note: plot only contains attempted tasks.



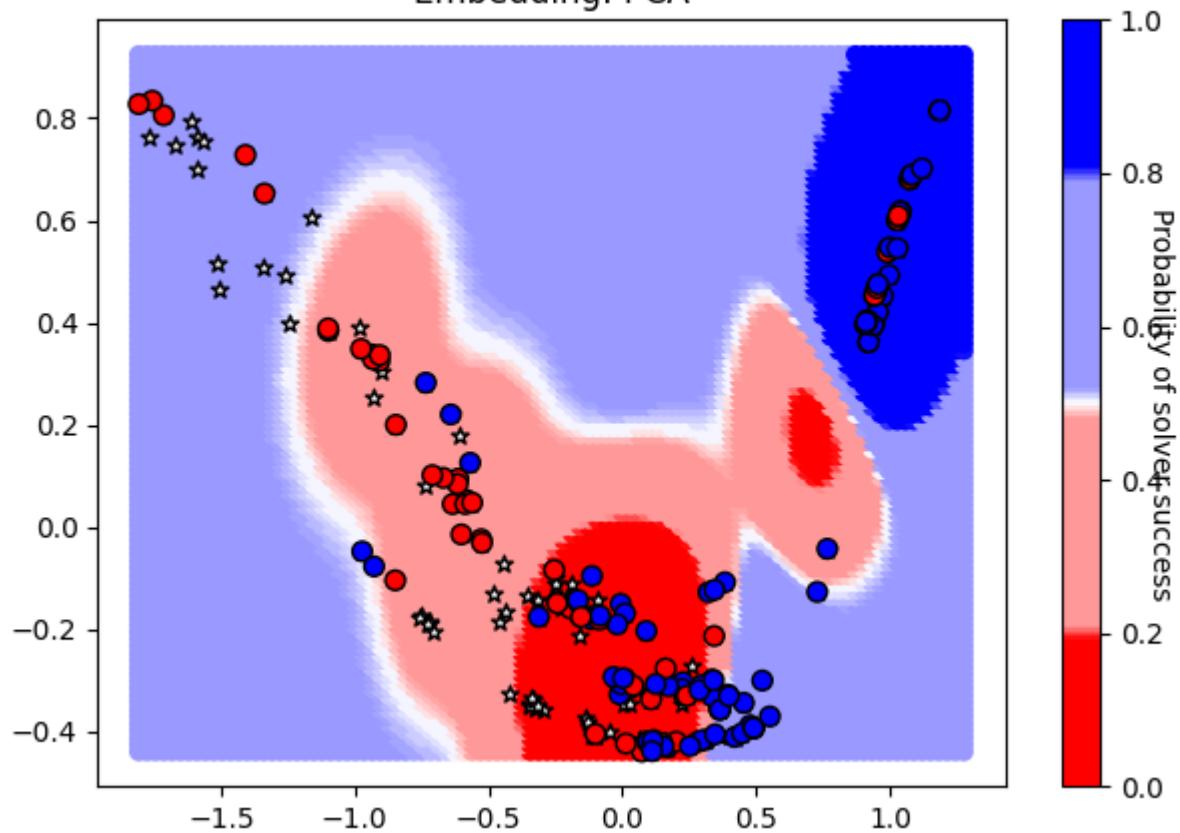
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_1e-4/7e730d...

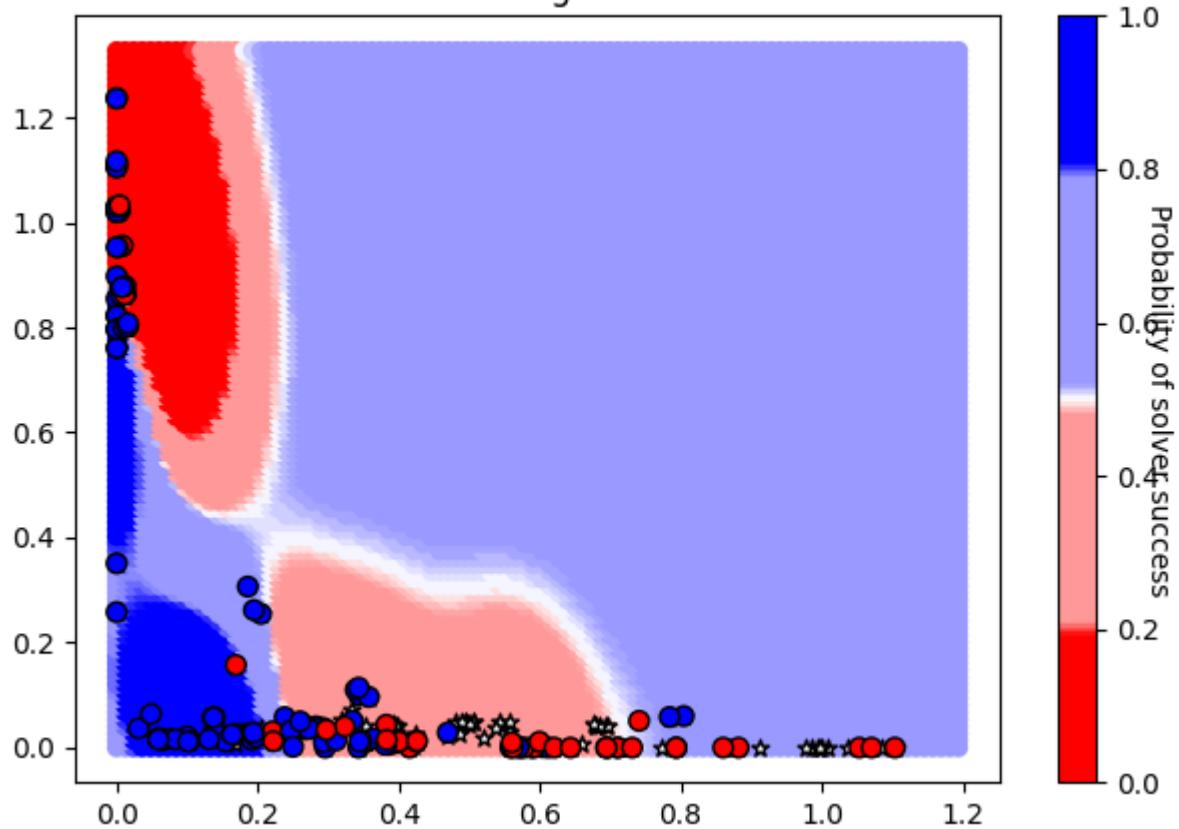
(captured: \$1.0e+02/1.5e+07, approximately 6.8e-04%)



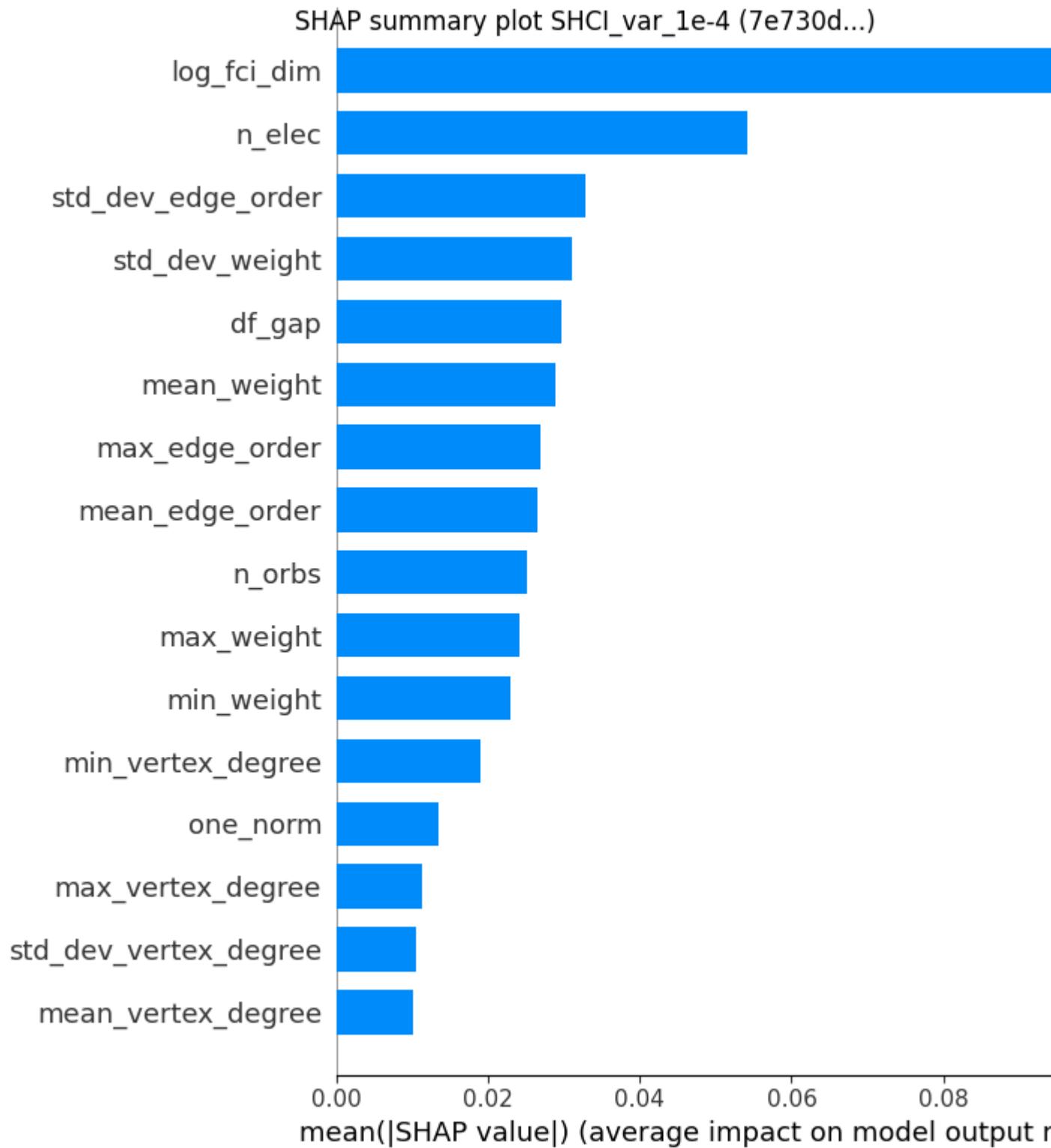
Solver SHCI_var_1e-4 (7e730d...)
Embedding: PCA



Solver SHCI_var_1e-4 (7e730d...)
Embedding: NMF



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

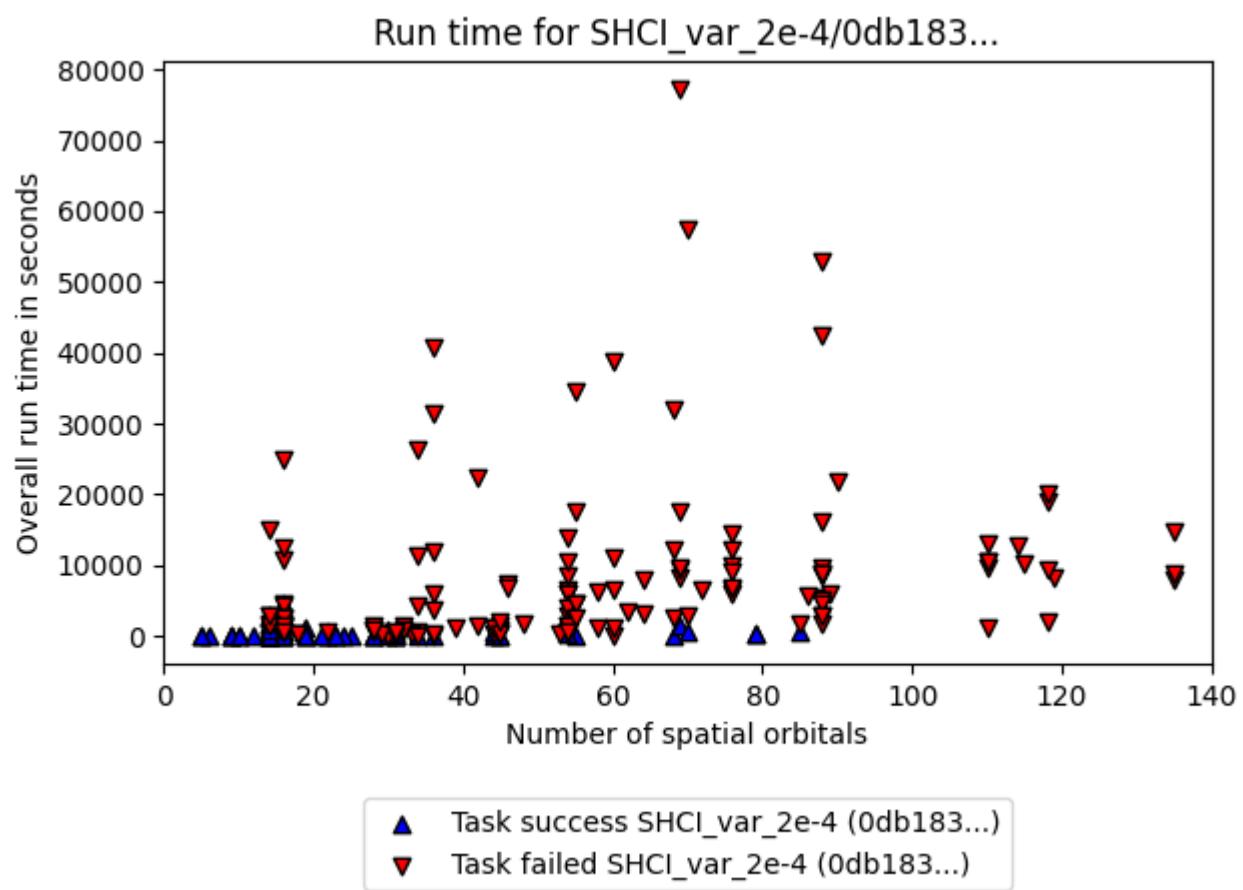


Solver SHCI_var_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a

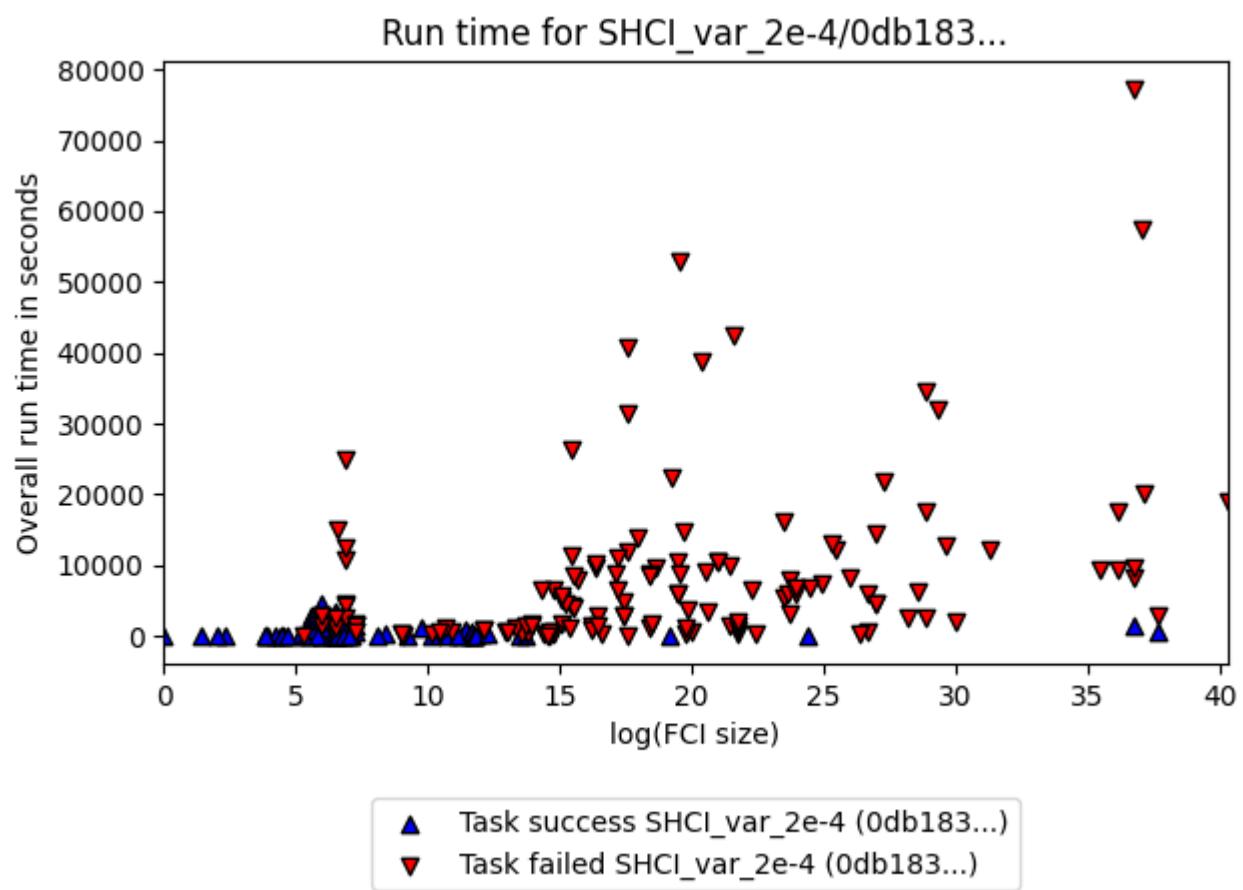
solver_uuid:0db183e3-a86d-491b-9125-599556e37c7a

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: 55d8b672-34e8-4e7d-8757-47221d6a5f54
creation.timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 17
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 83
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 83
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 0.8125
comments: solvability ratio based on PCA embedding.
f1_score: [0.9928057553956835, 0.9940119760479041]
ml.metrics_calculator_version: 1



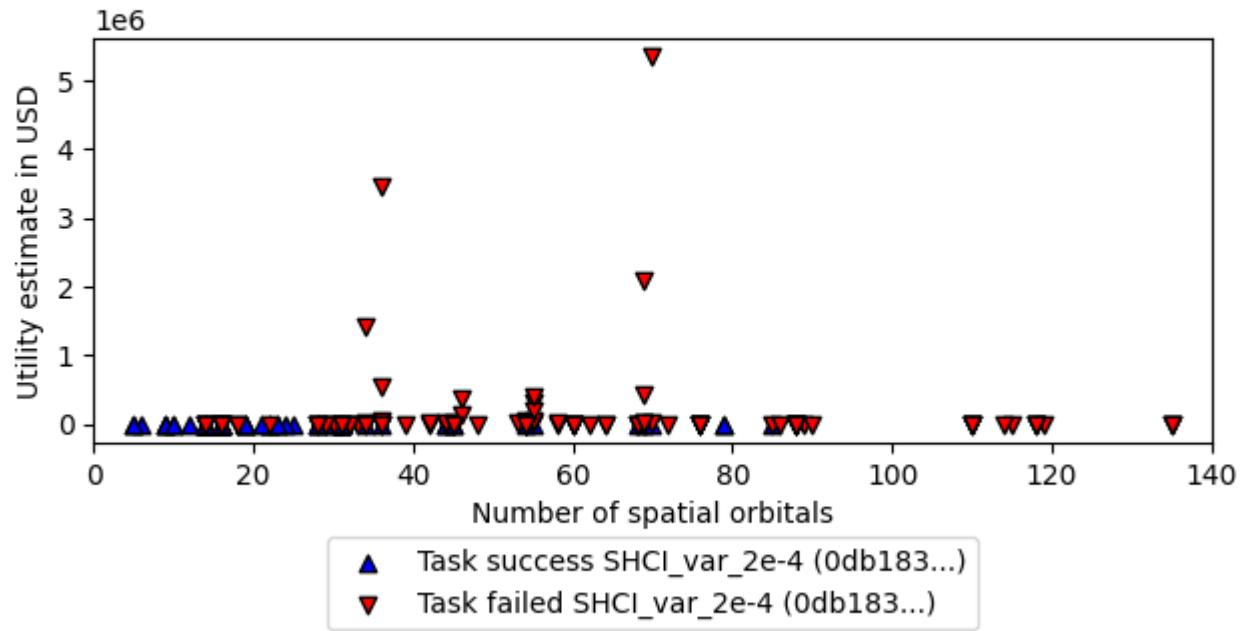
Note: plot only contains attempted tasks.



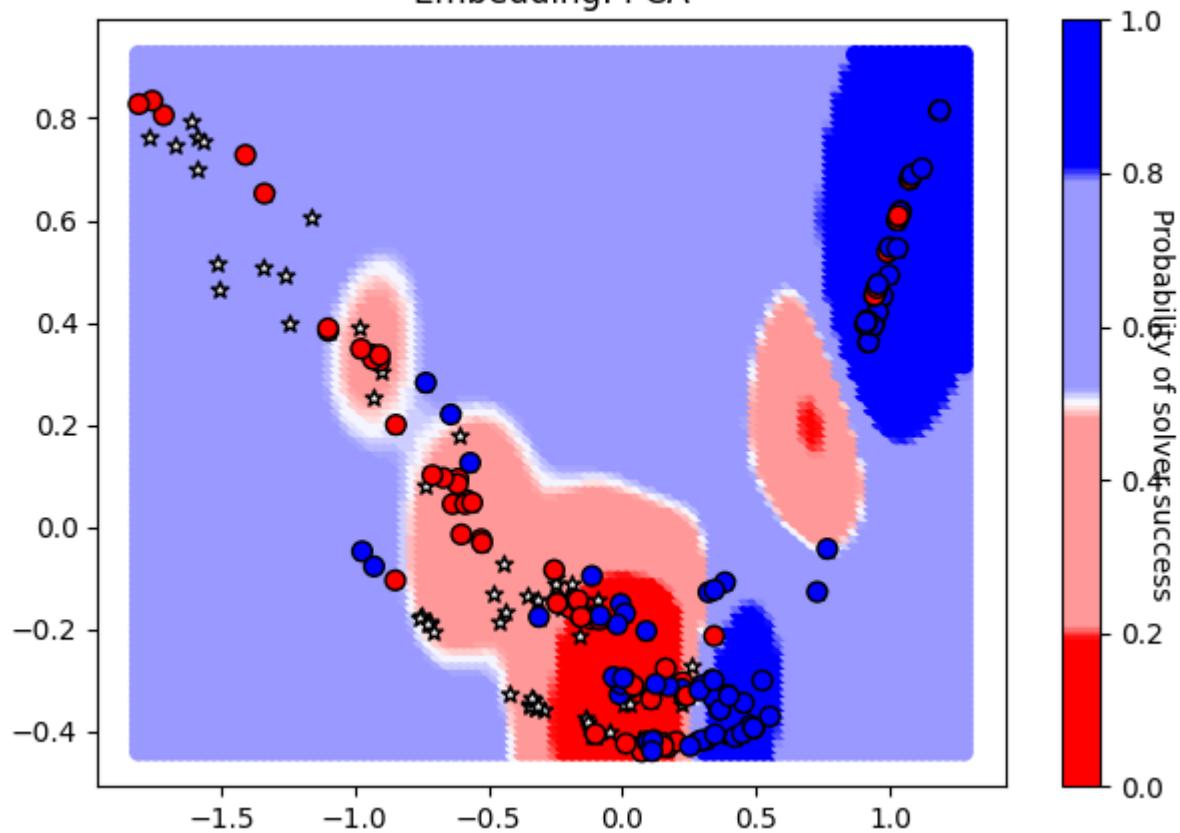
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_2e-4/0db183...

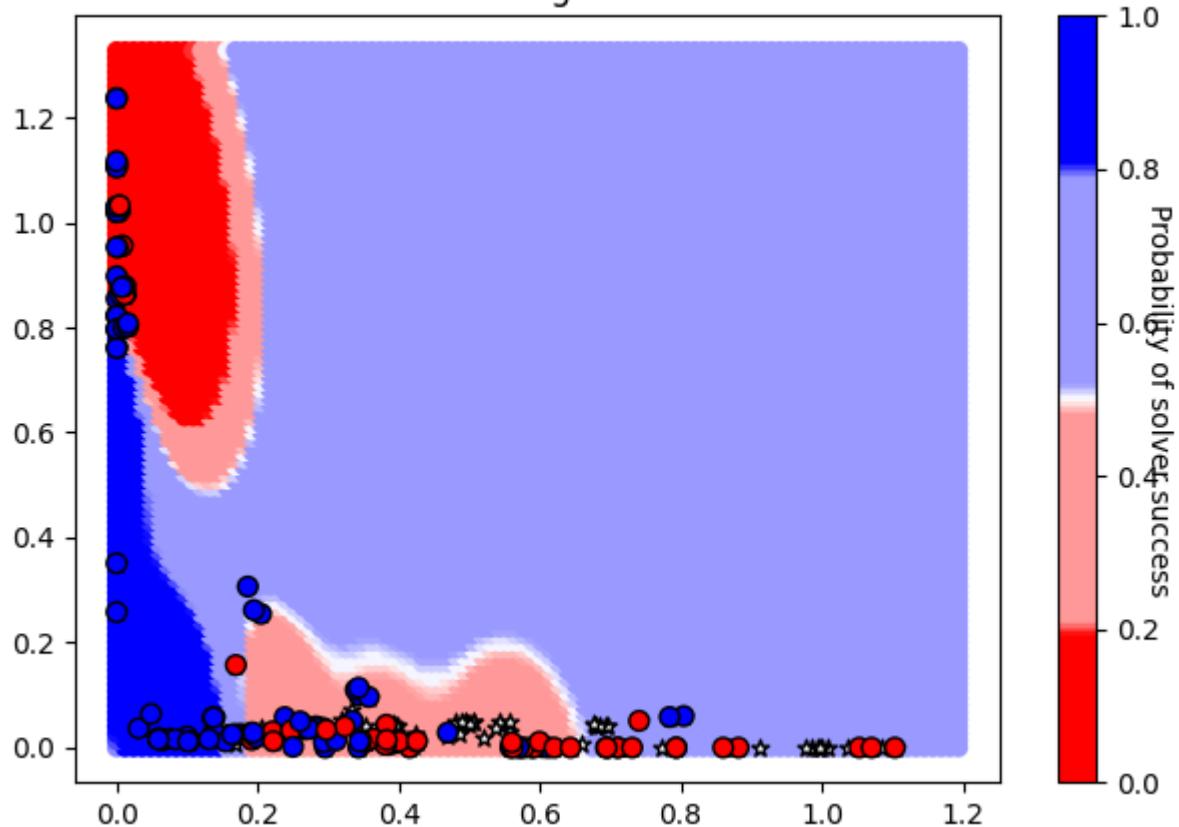
(captured: \$8.6e+01/1.5e+07, approximately 5.8e-04%)



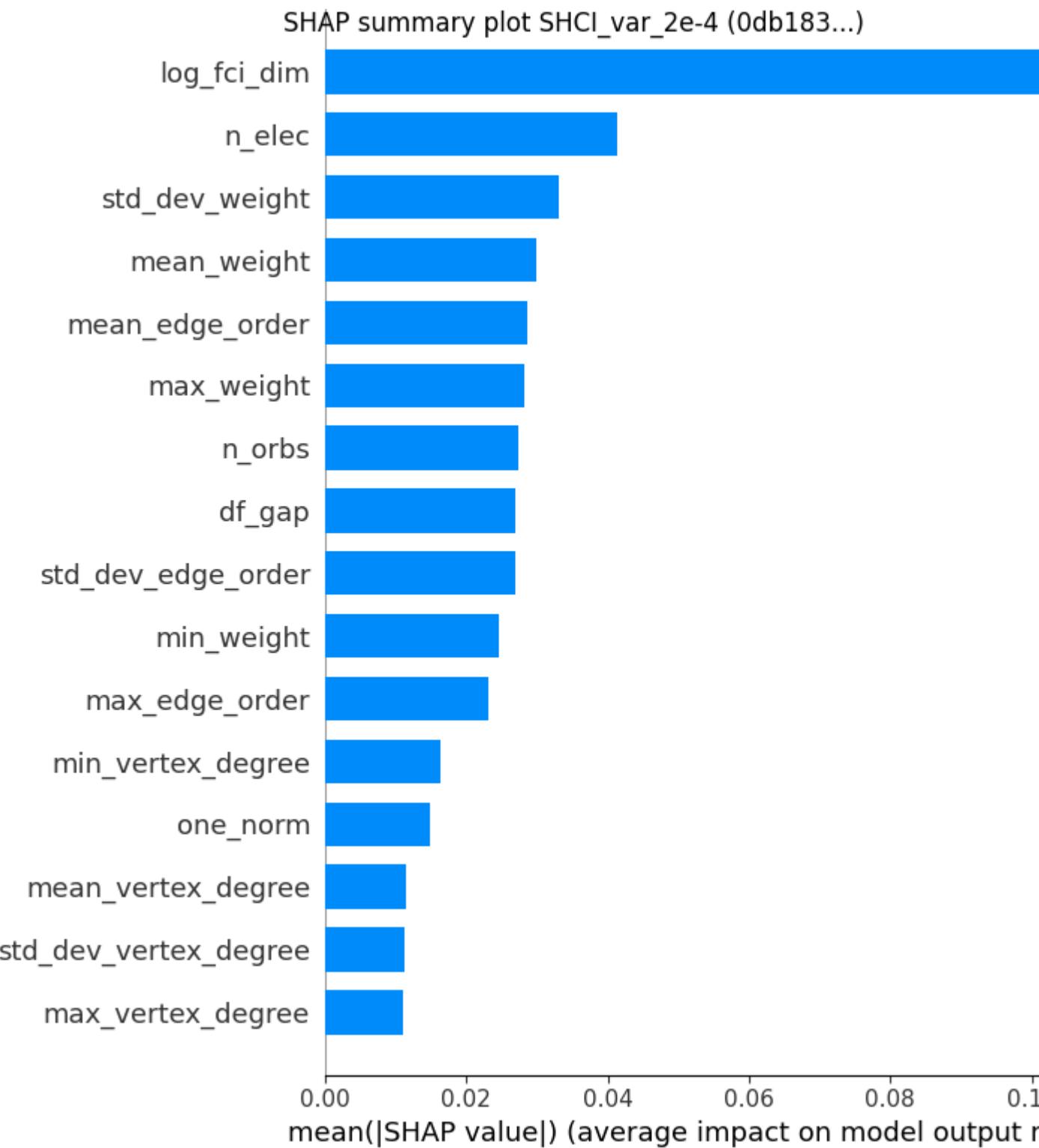
Solver SHCI_var_2e-4 (0db183...)
Embedding: PCA



Solver SHCI_var_2e-4 (0db183...)
Embedding: NMF



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

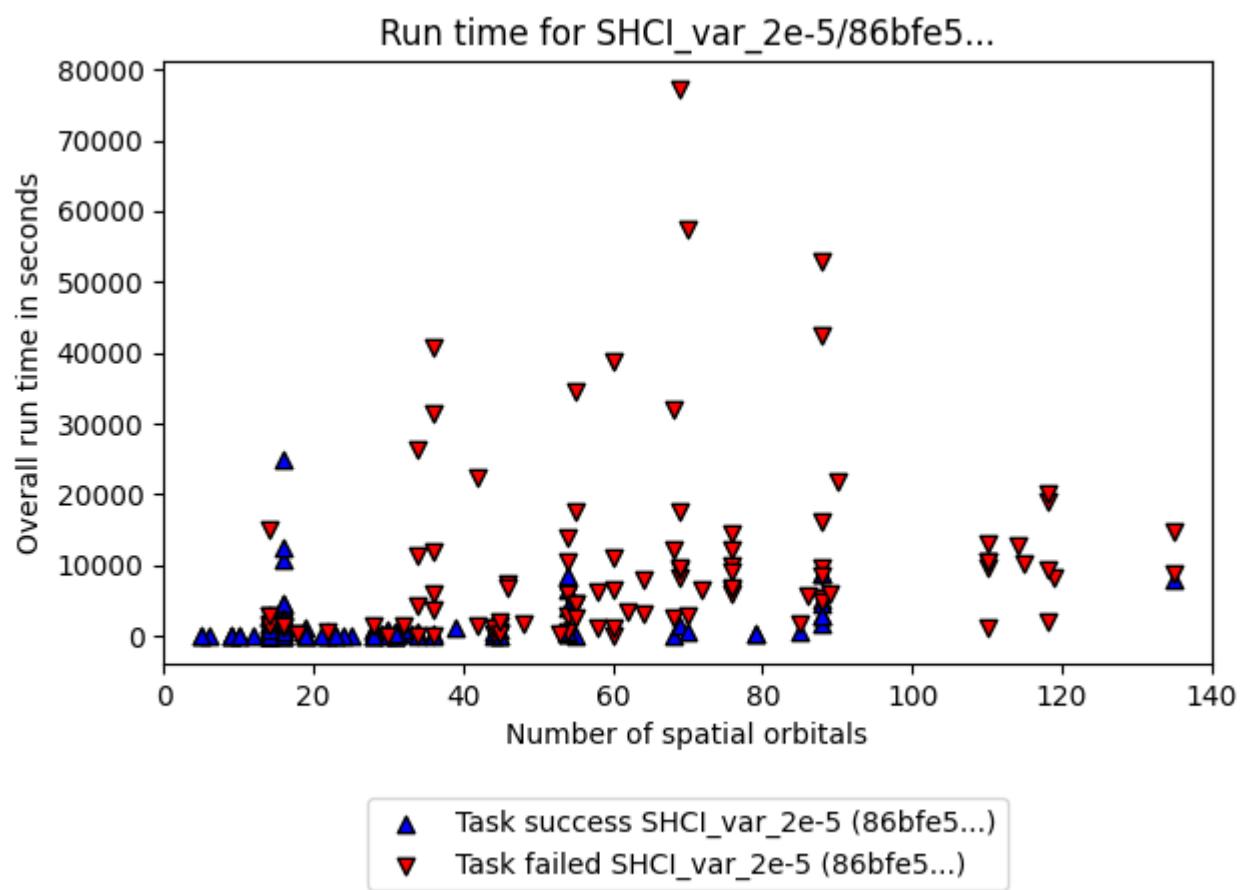


Solver SHCI_var_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688

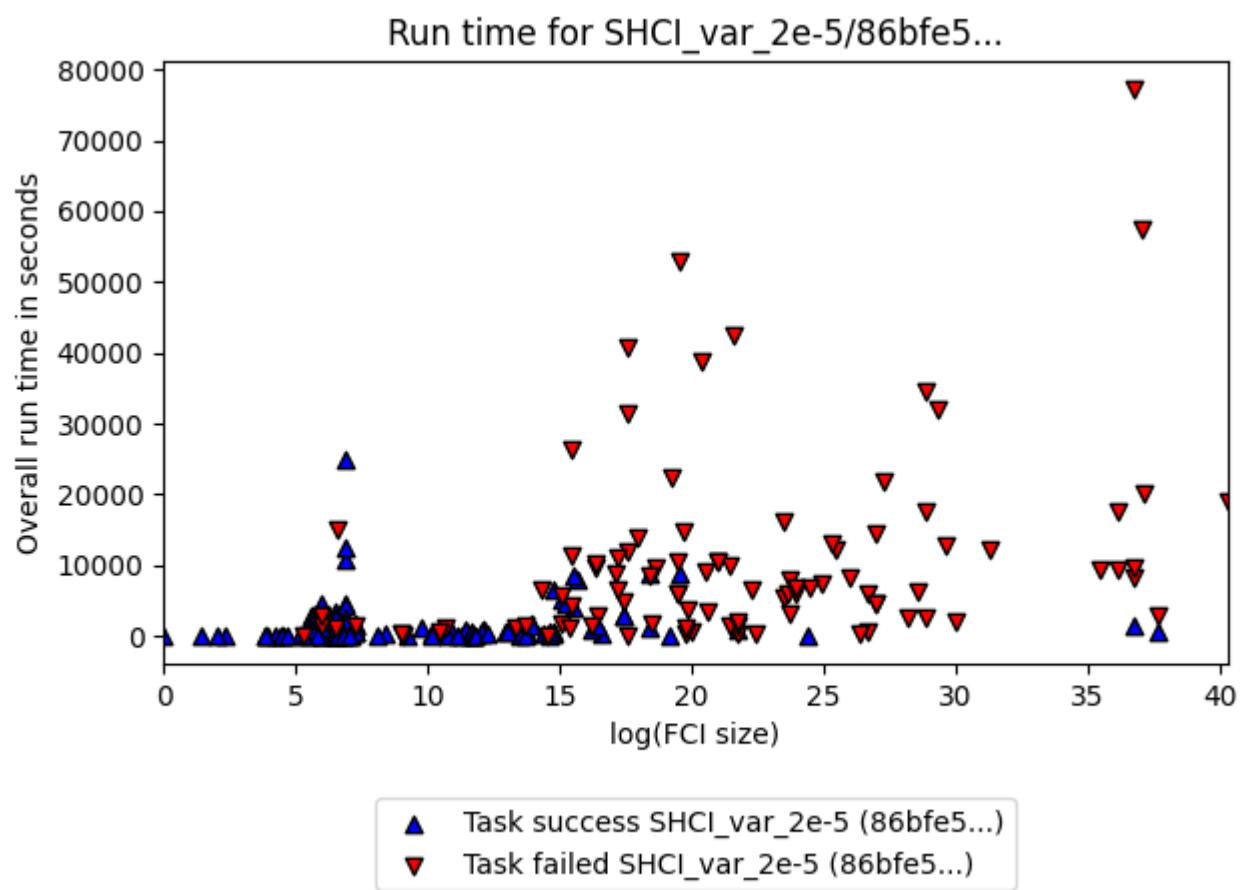
solver_uuid:86bfe50c-9342-4d54-bb68-abc8abd95688

solver_short_name:SHCI_var_2e-5

compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:SHCI with eps_var 2e-5
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: d3b49c36-b913-4059-9bad-a1bde21d75fb
creation_timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 22
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 128
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 128
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 0.6486
comments: solvability ratio based on PCA embedding.
f1_score: [0.88, 0.9765625]
ml_metrics_calculator_version: 1



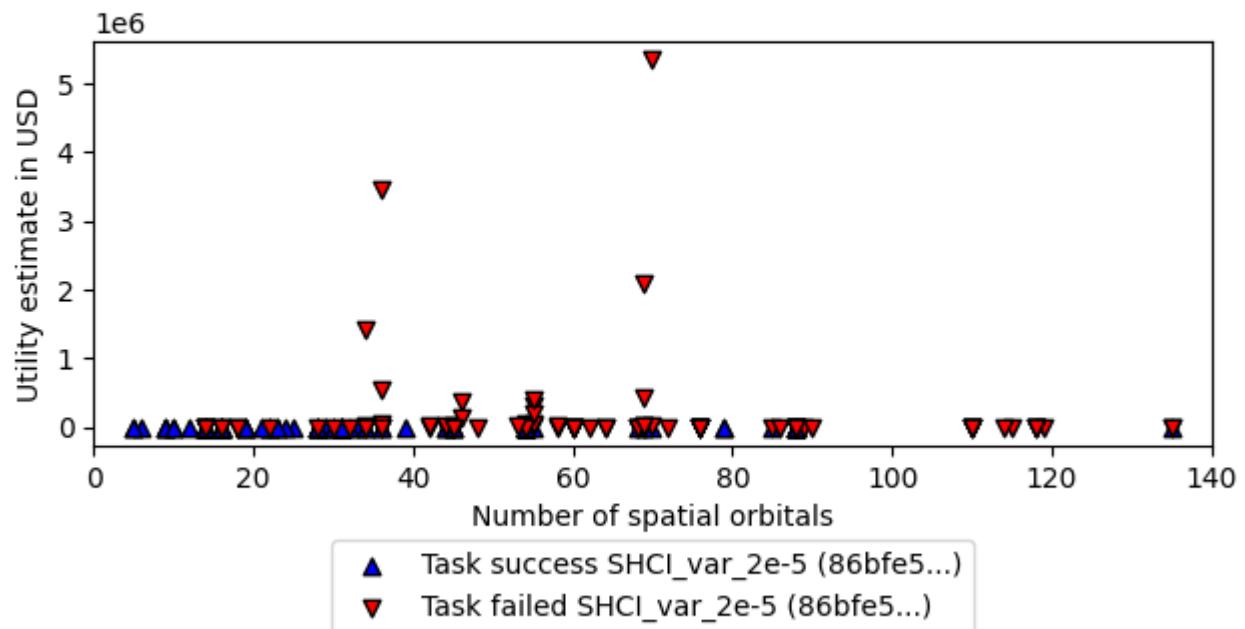
Note: plot only contains attempted tasks.



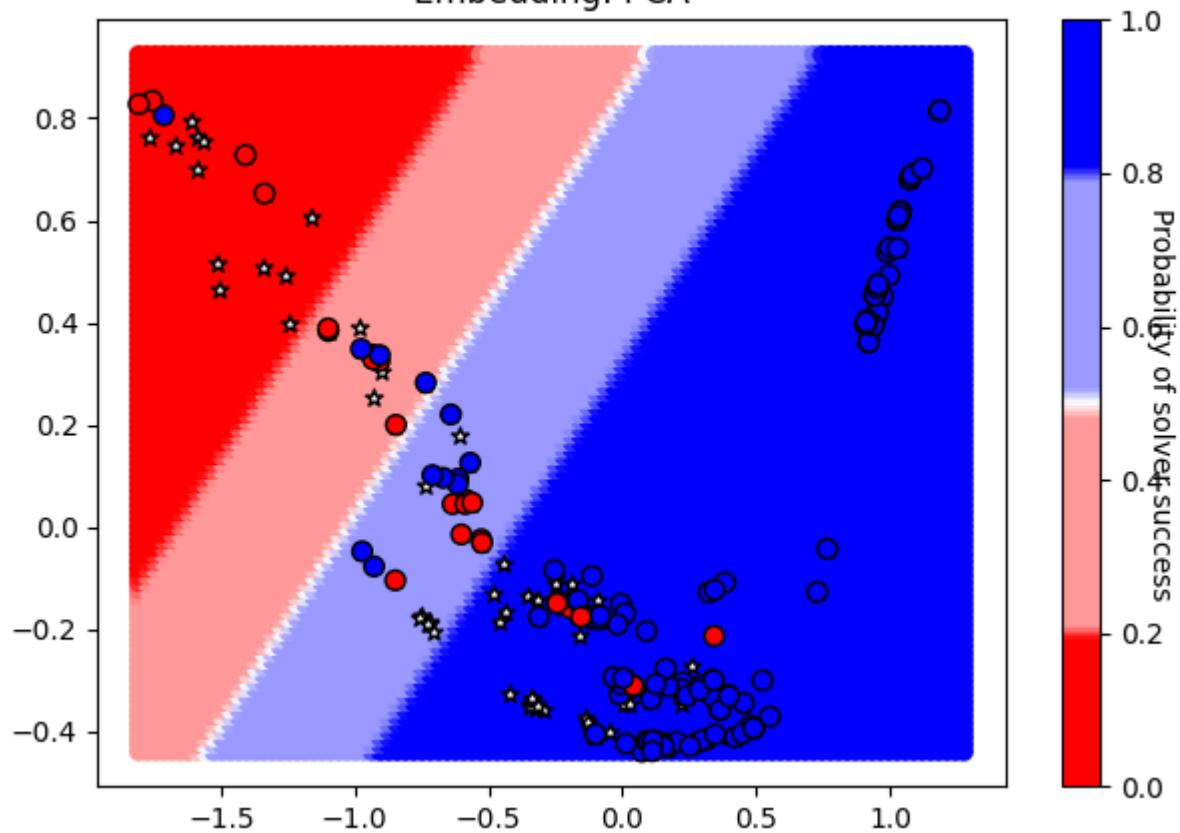
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_2e-5/86bfe5...

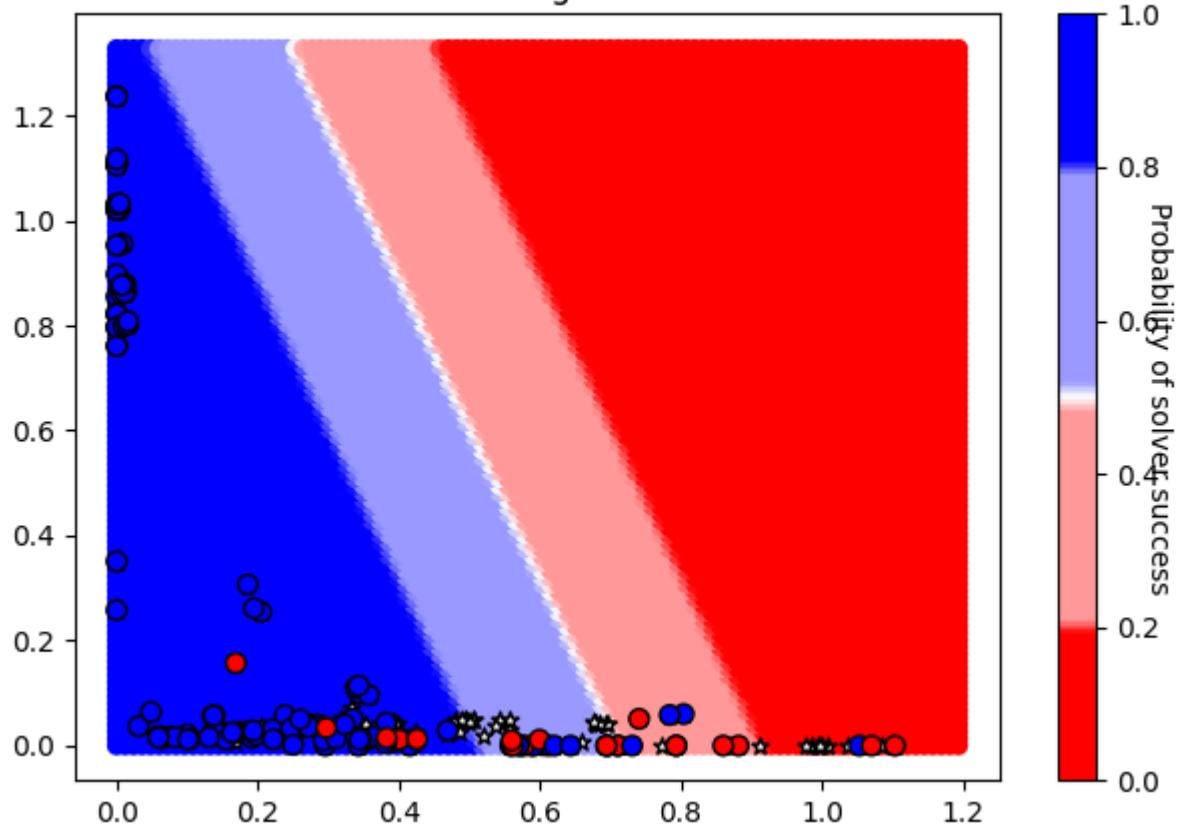
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



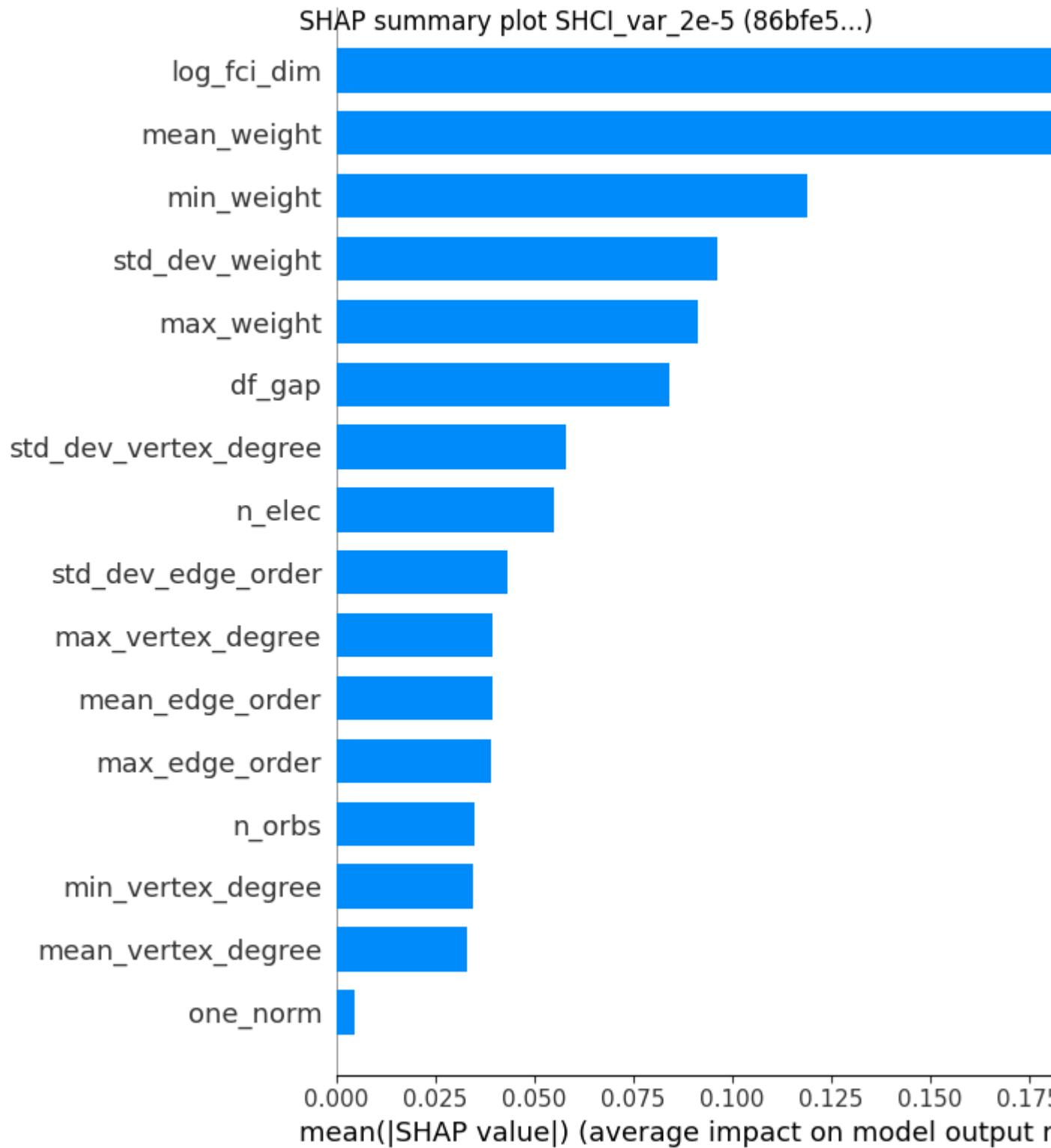
Solver SHCI_var_2e-5 (86bfe5...)
Embedding: PCA



Solver SHCI_var_2e-5 (86bfe5...)
Embedding: NMF



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

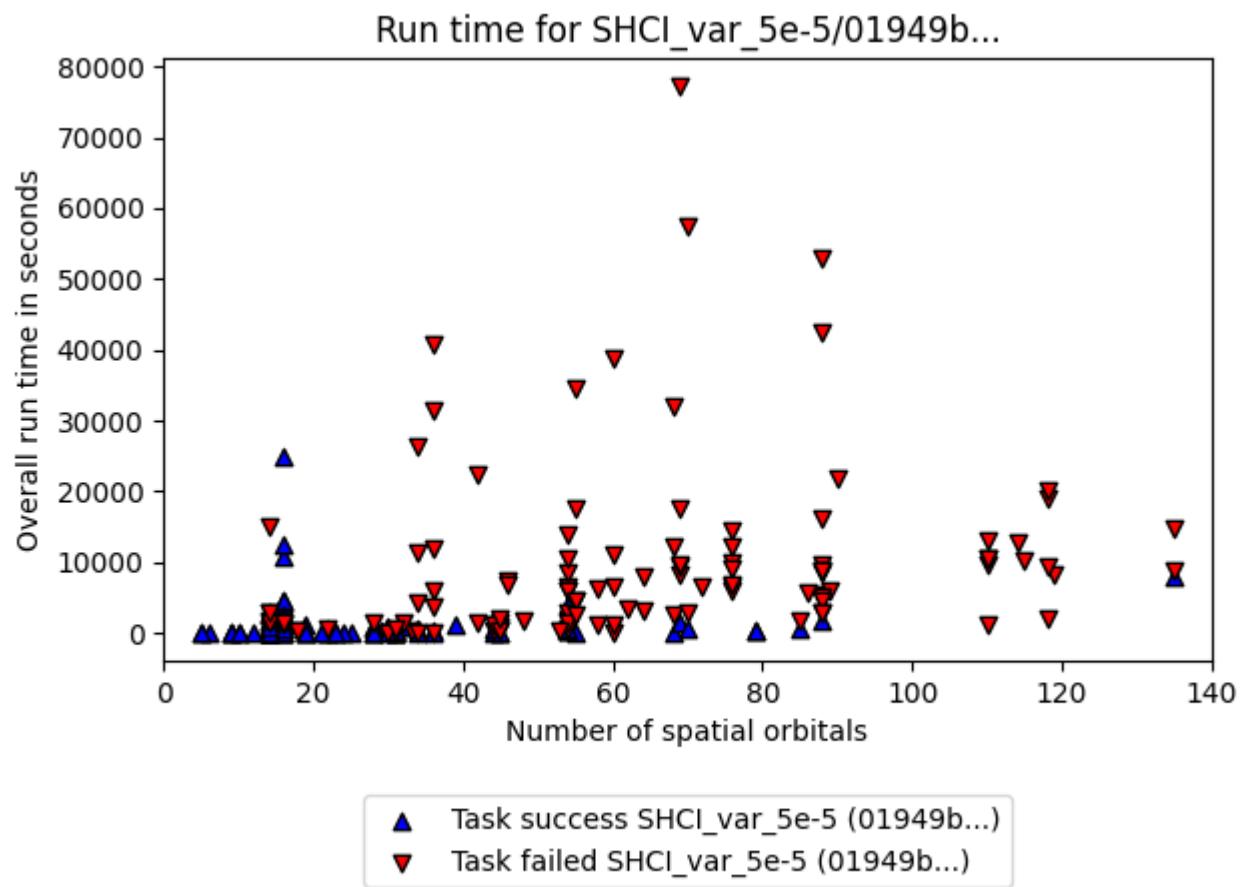


Solver SHCI_var_5e-5, 01949b95-c427-4693-9134-01f47f688c09

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

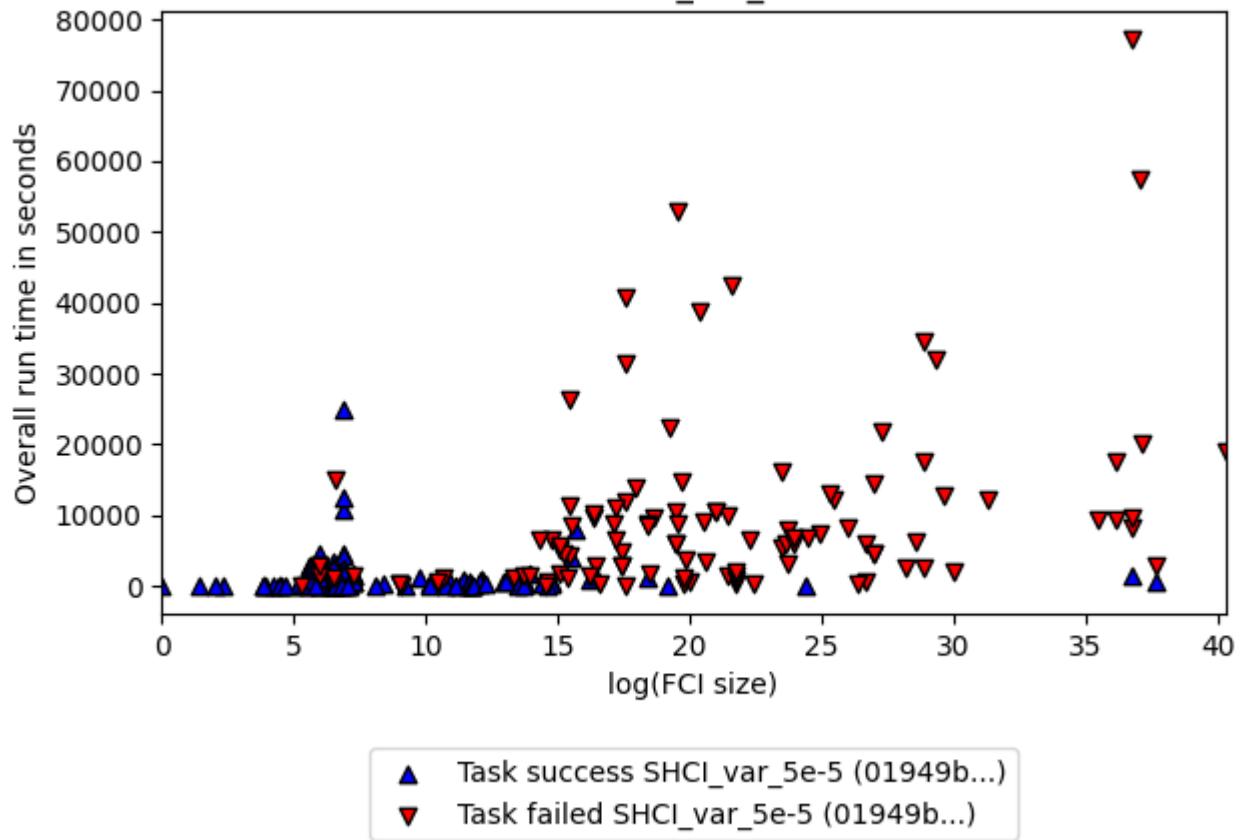
solver_short_name:SHCI_var_5e-5

compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:SHCI with eps_var 5e-5
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: 989dfca2-b618-4b4d-a845-2b1ed2de12f8
creation_timestamp: 2025-06-12T20:42:55.603395+00:00
number_of_problem_instances: 68
number_of_problem_instances_attempted: 68
number_of_problem_instances_solved: 18
number_of_tasks: 228
number_of_tasks_attempted: 228
number_of_tasks_solved: 115
number_of_tasks_solved_within_run_time_limit: 227
number_of_tasks_solved_within_accuracy_threshold: 115
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1220721.7950000002
solvability_ratio: 0.8749
comments: solvability ratio based on PCA embedding.
f1_score: [0.8395061728395061, 0.9422222222222222]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

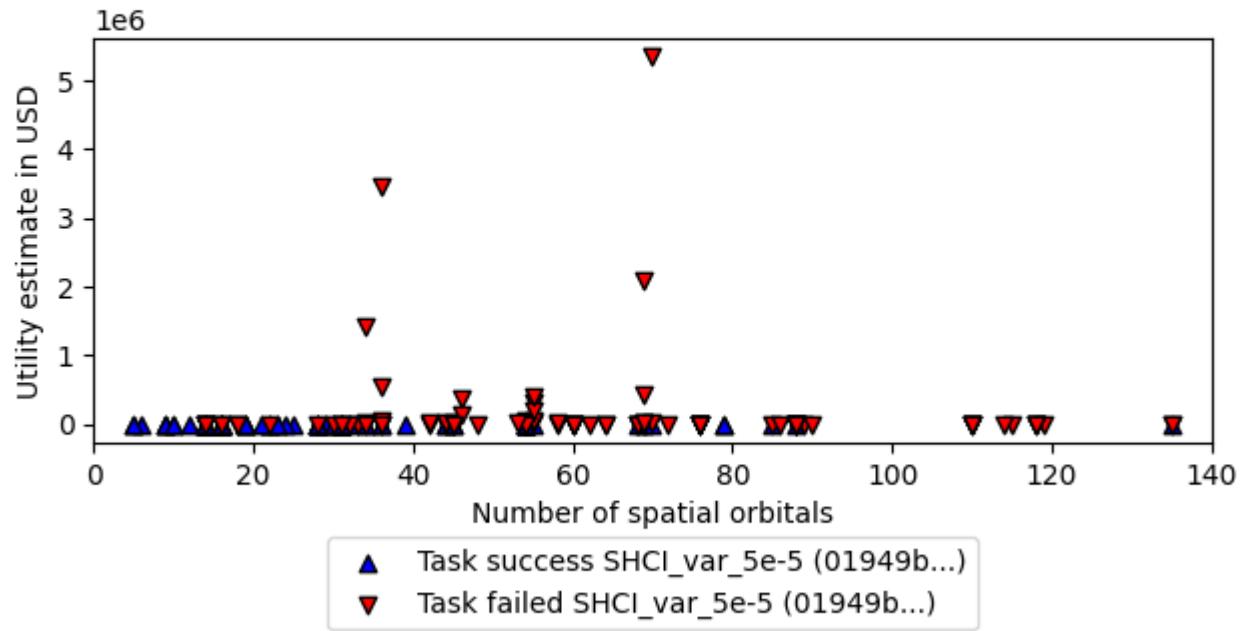
Run time for SHCI_var_5e-5/01949b...



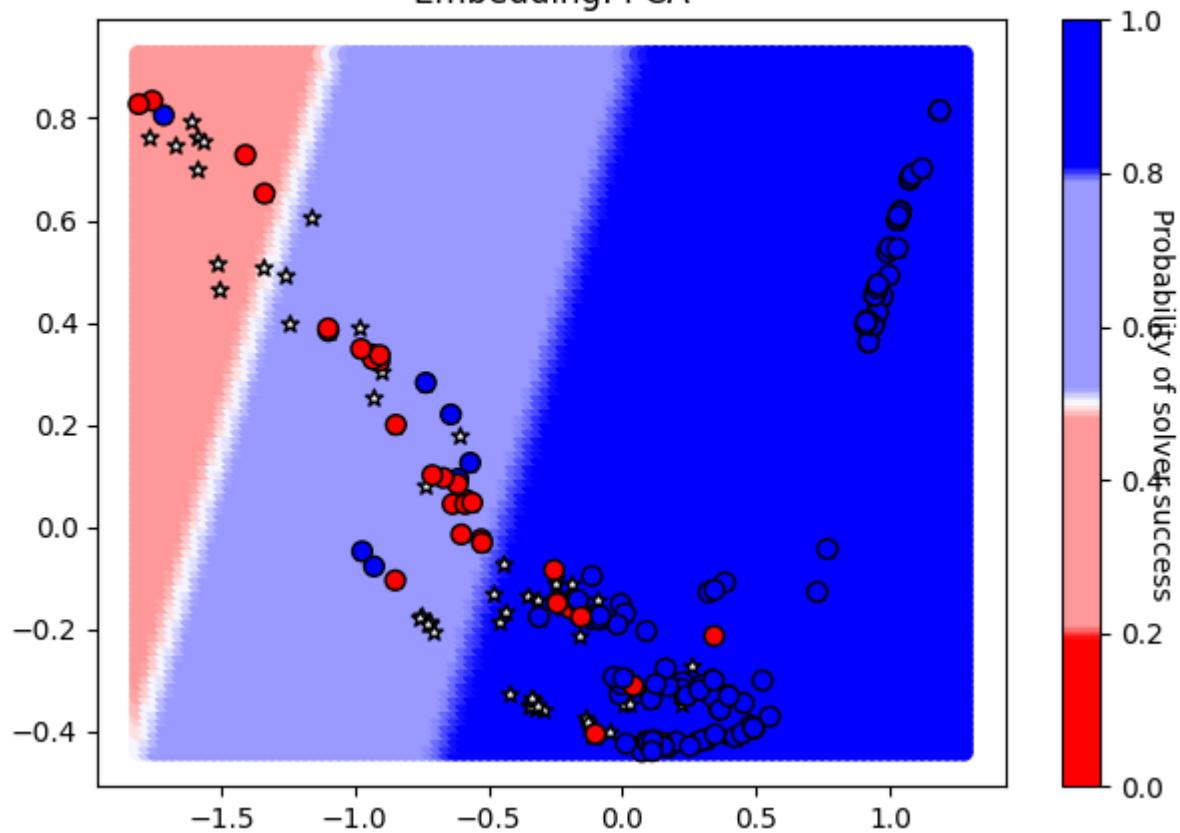
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_5e-5/01949b...

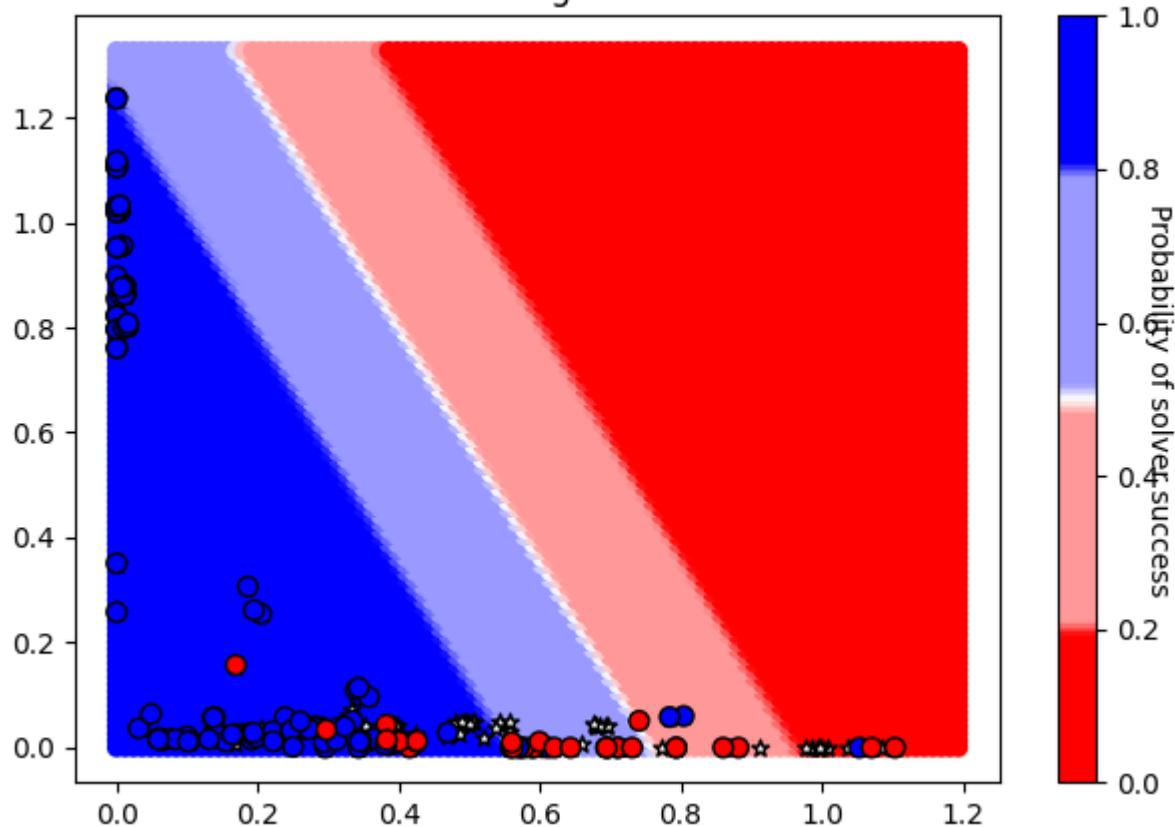
(captured: $\$4.5\text{e+}02/1.5\text{e+}07$, approximately $3.0\text{e-}03\%$)



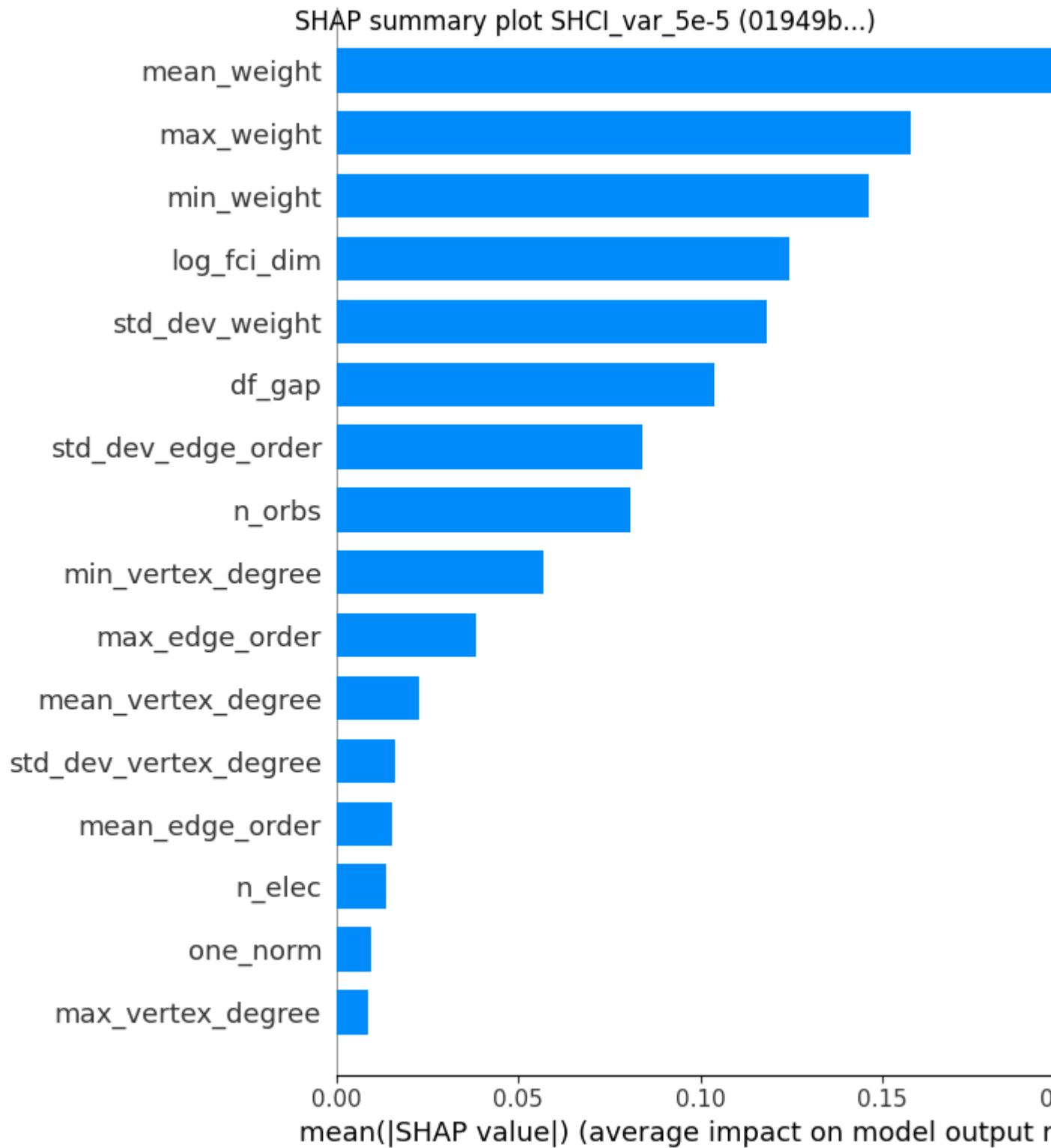
Solver SHCI_var_5e-5 (01949b...)
Embedding: PCA



Solver SHCI_var_5e-5 (01949b...)
Embedding: NMF



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



Solver THC_BLISS_QPE_1mHa, b8ed03bd-9c3e-4d07-80af-8f77f0e7c2ac

solver_uuid:b8ed03bd-9c3e-4d07-80af-8f77f0e7c2ac

solver_short_name:THC_BLISS_QPE_1mHa

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': "", 'algorithm_parameters': {'overlap_csv': 'overlaps.csv'}, 'description': 'Tensor Hypercontraction + BLock Invariant Symmetry Shift (BLISS) QPE resource estimates for 1mHa accuracy (more stringent than benchmark-requested 1.59 mHa accuracy) based on methodology in arXiv:2406.06335v2, which is a modified form of the method in arXiv: 2501.06165. 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 this DMRG runtime is not included in the classical compute costs.'}

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': '3.12.2'}, {'software_name': 'JAX', 'software_version': '0.4.31'}, {'software_name': 'benchq', 'software_version': '0.1.dev153+g3d429cb.d20250508'}]

logical_resource_estimate_solution_uuid:f8ca6f38-884b-40da-b8e8-093f31a15aac

quantum_hardware_details:{'quantum_hardware_description': 'Superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494. Used with THC+BLISS.', 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.001, 'cycle_time_microseconds': 1}}

logical_resource_estimate_solver_uuid:12fbca08-3df3-4f3e-b7fd-c535b6b44b1c

performance_metrics_uuid: 0f12e038-d6a0-43b7-b756-b1046bb61b4a

creation_timestamp: 2025-06-12T20:42:55.603395+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: 68780768267.04153

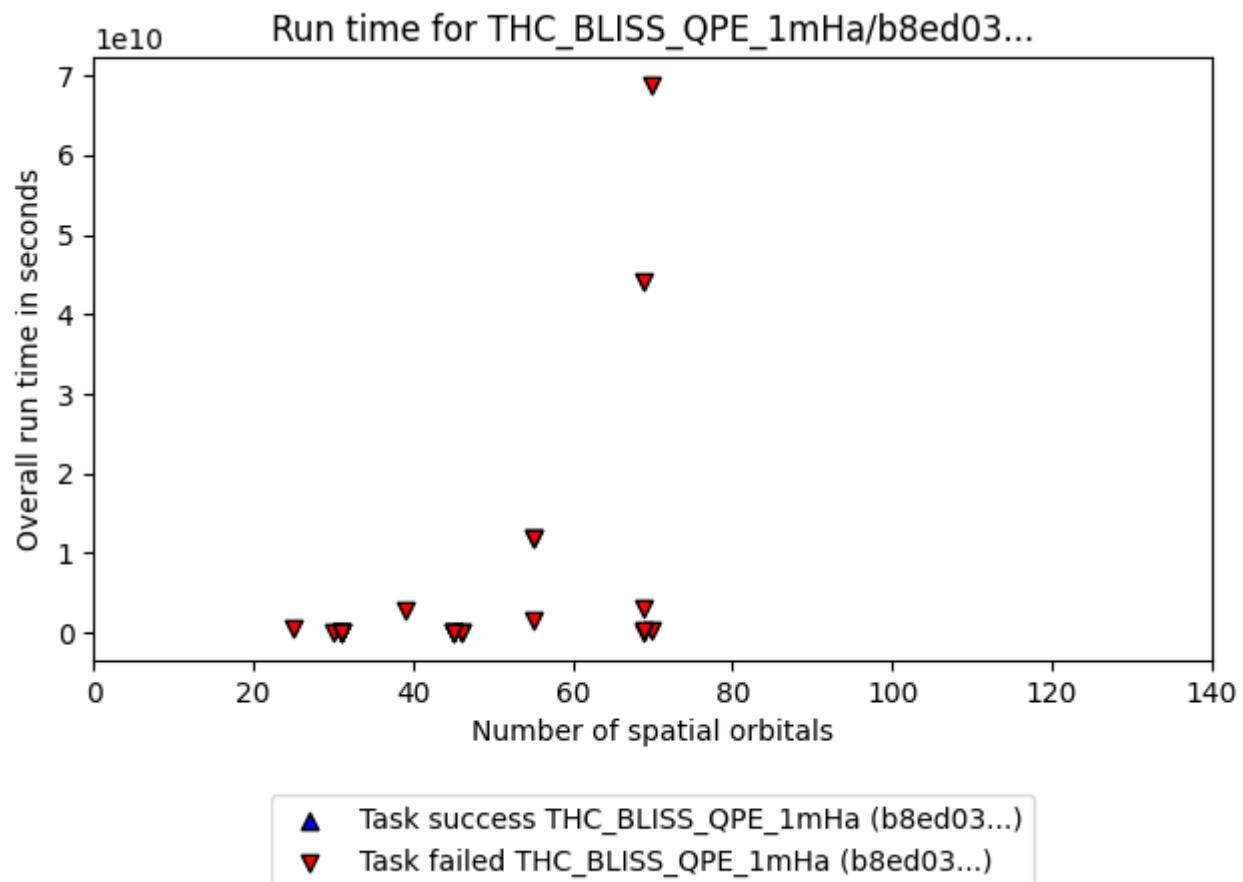
sum_of_run_time_of_attempted_tasks: 145936991321.73734

solvability_ratio: None

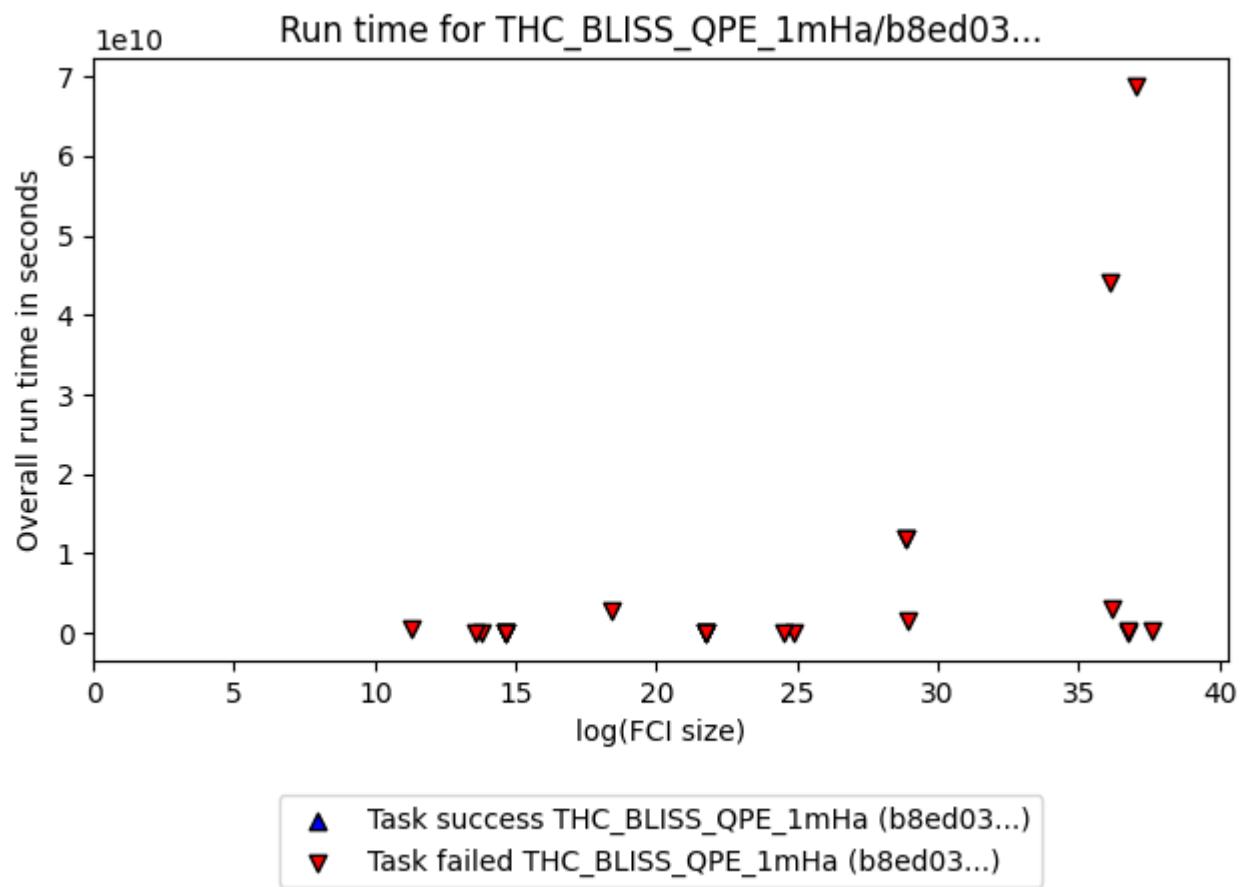
f1_score: None

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.



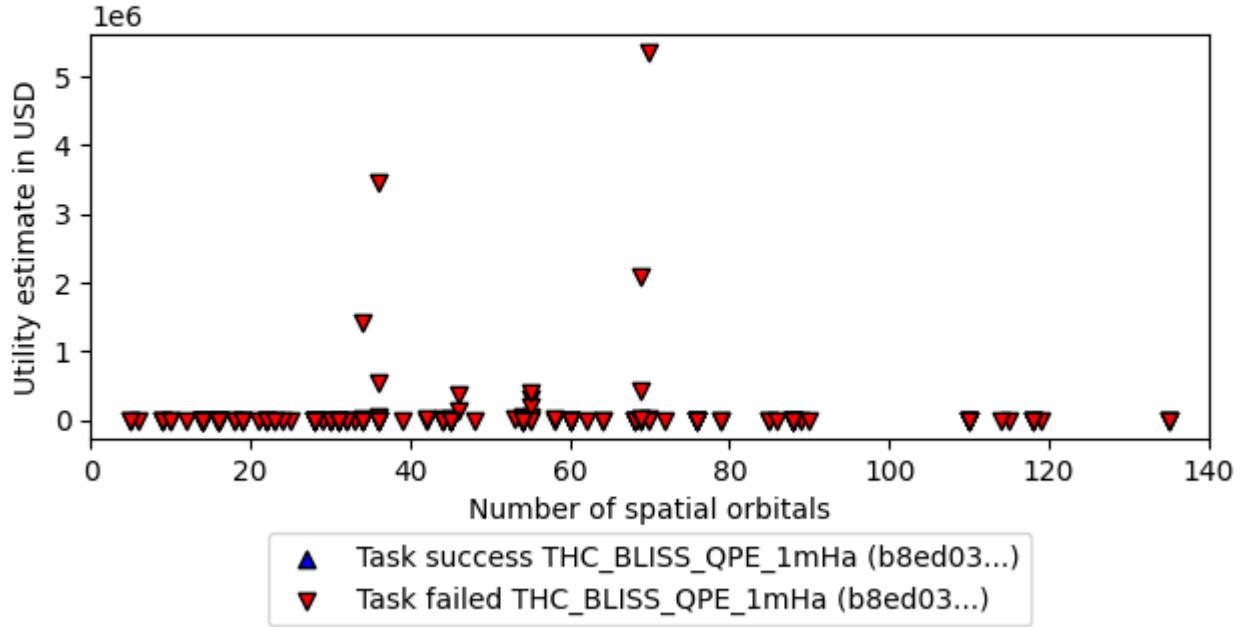
Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from THC_BLISS_QPE_1mHa/b8ed03...

(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

Solver THC_QPE_1mHa, 18c187af-3e5b-4e6c-87fd-73c26fd48a60

solver_uuid:18c187af-3e5b-4e6c-87fd-73c26fd48a60

solver_short_name:THC_QPE_1mHa

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Tensor Hypercontraction QPE resource estimates based on methodology of arXiv:2011.03494. 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'}, 'description': 'Tensor Hypercontraction QPE resource estimates for 1mHa accuracy (more stringent than benchmark-requested 1.59 mHa accuracy) based on methodology of arXiv:2011.03494. 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.'}

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': '3.12.2'}, {'software_name': 'JAX', 'software_version': '0.4.31'}, {'software_name': 'benchq', 'software_version': '0.1.dev153+g3d429cb.d20250508'}]

logical_resource_estimate_solution_uuid:c718bf66-8aa1-49e3-b26d-5d18168b6a98

quantum_hardware_details:{'quantum_hardware_description': 'Superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494. Used with THC.', 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.001, 'cycle_time_microseconds': 1}}

logical_resource_estimate_solver_uuid:d6f49cca-6f10-4de8-bc94-4c6fe4d23296

performance_metrics_uuid: cc1c4533-28d0-43d4-9f3e-9343f6db3f27

creation_timestamp: 2025-06-12T20:42:55.603395+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: 203781742944.55988

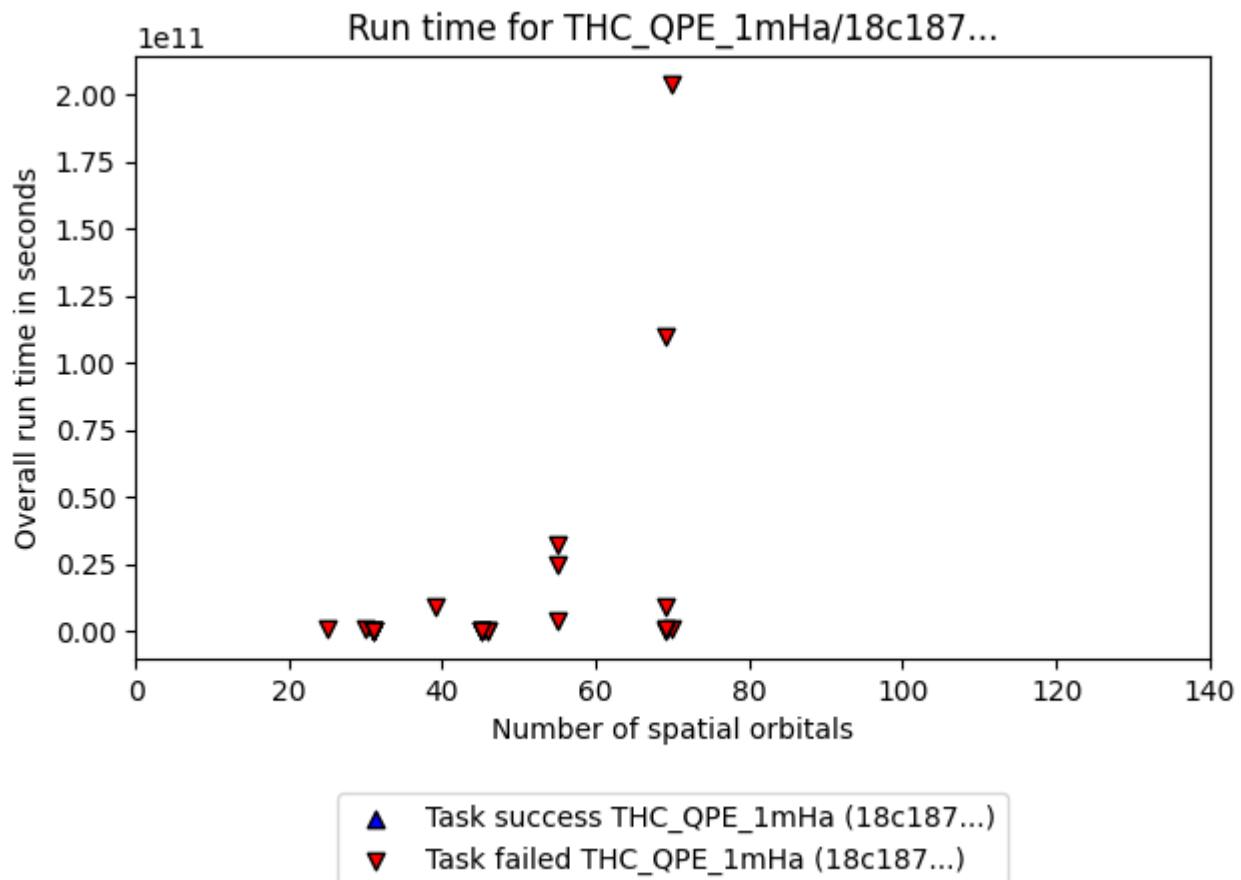
sum_of_run_time_of_attempted_tasks: 398497180382.5945

solvability_ratio: None

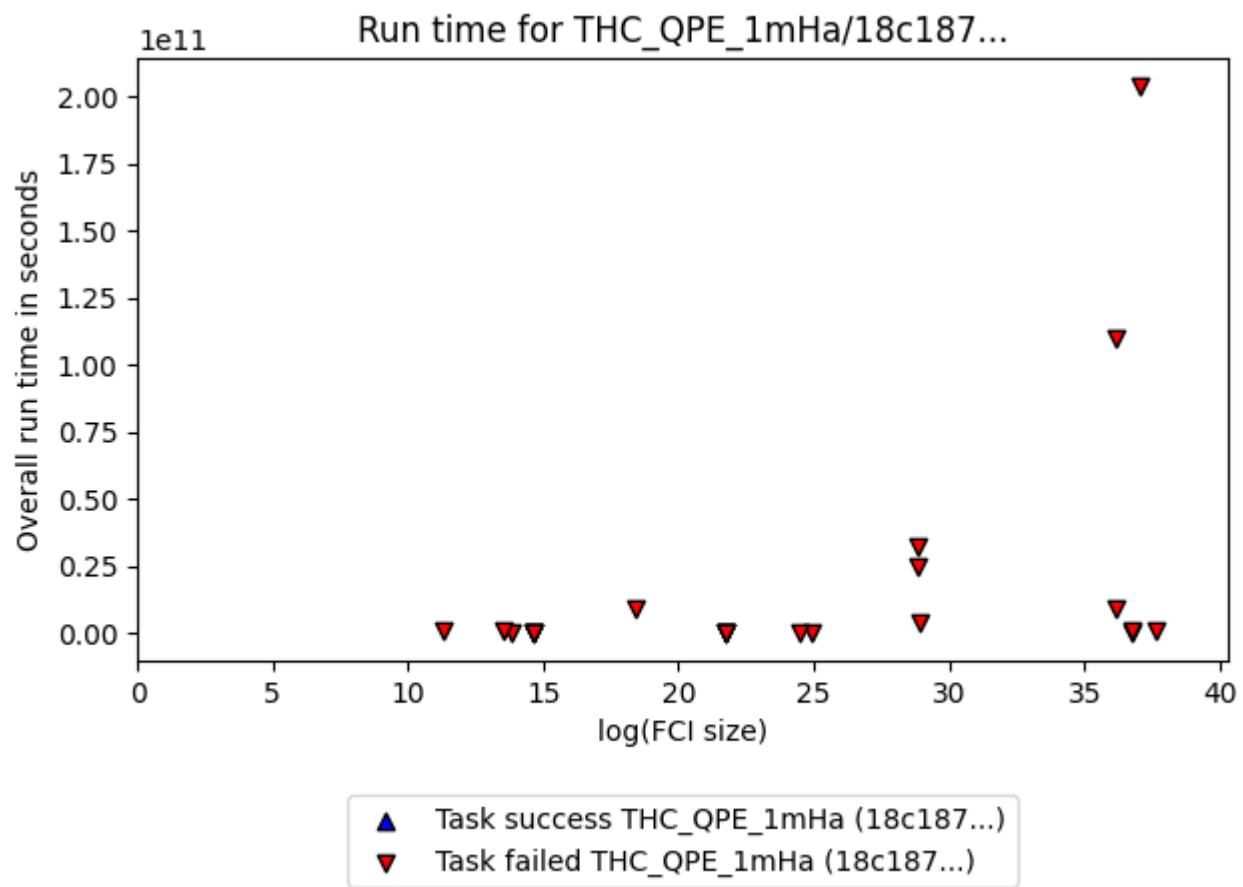
f1_score: None

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.

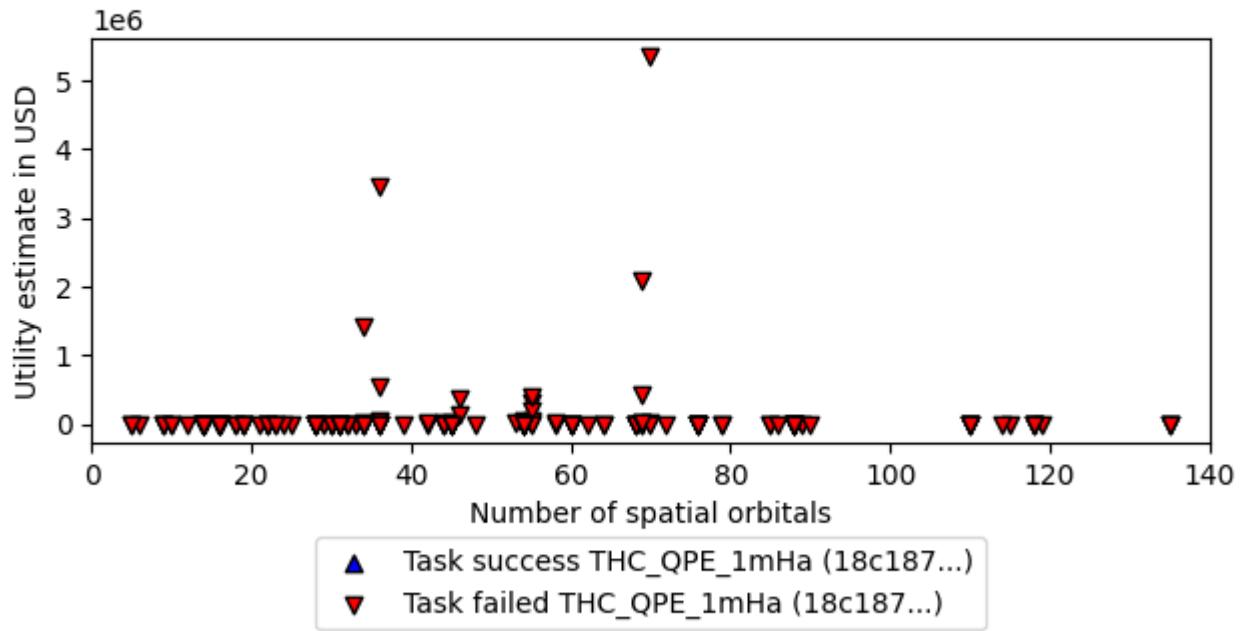


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from THC_QPE_1mHa/18c187...
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



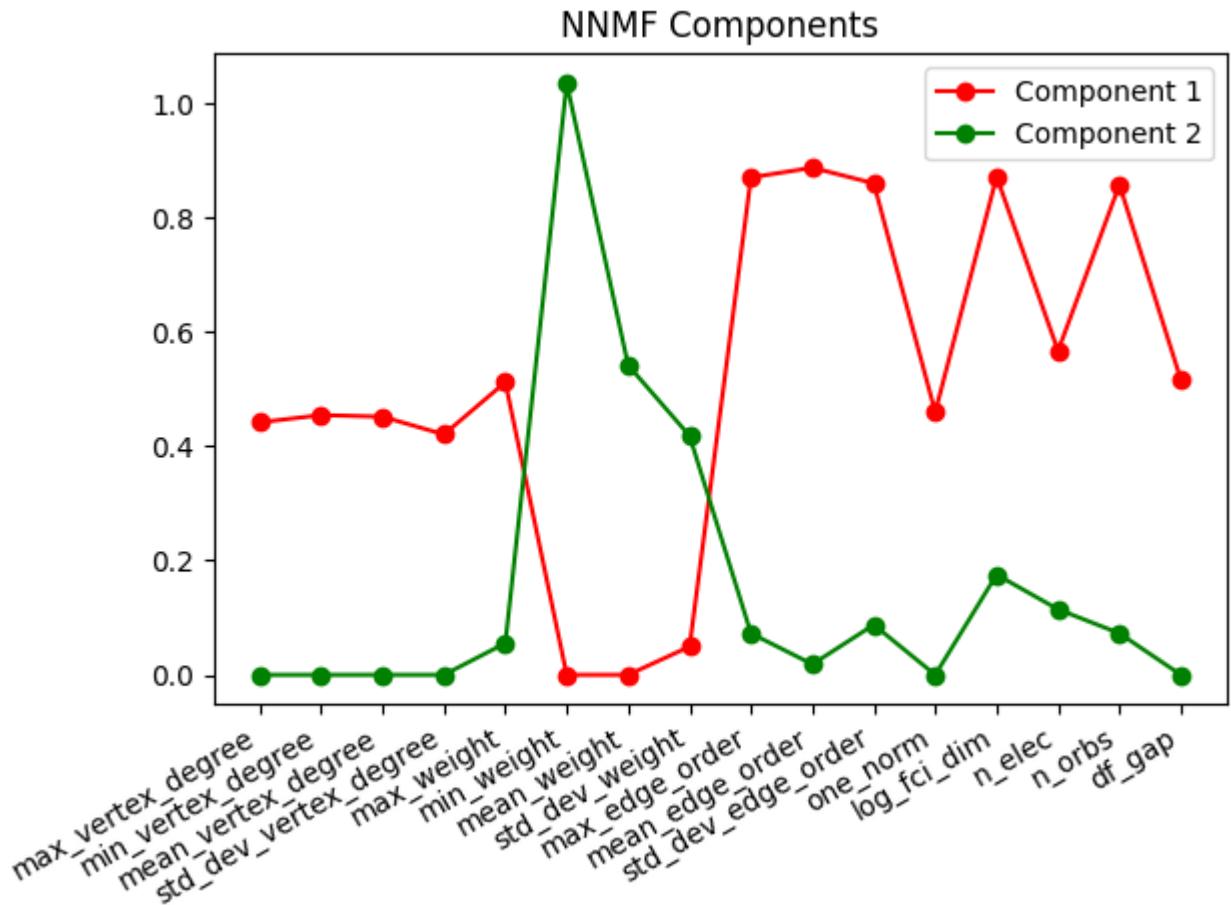
Solver PCA plot

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

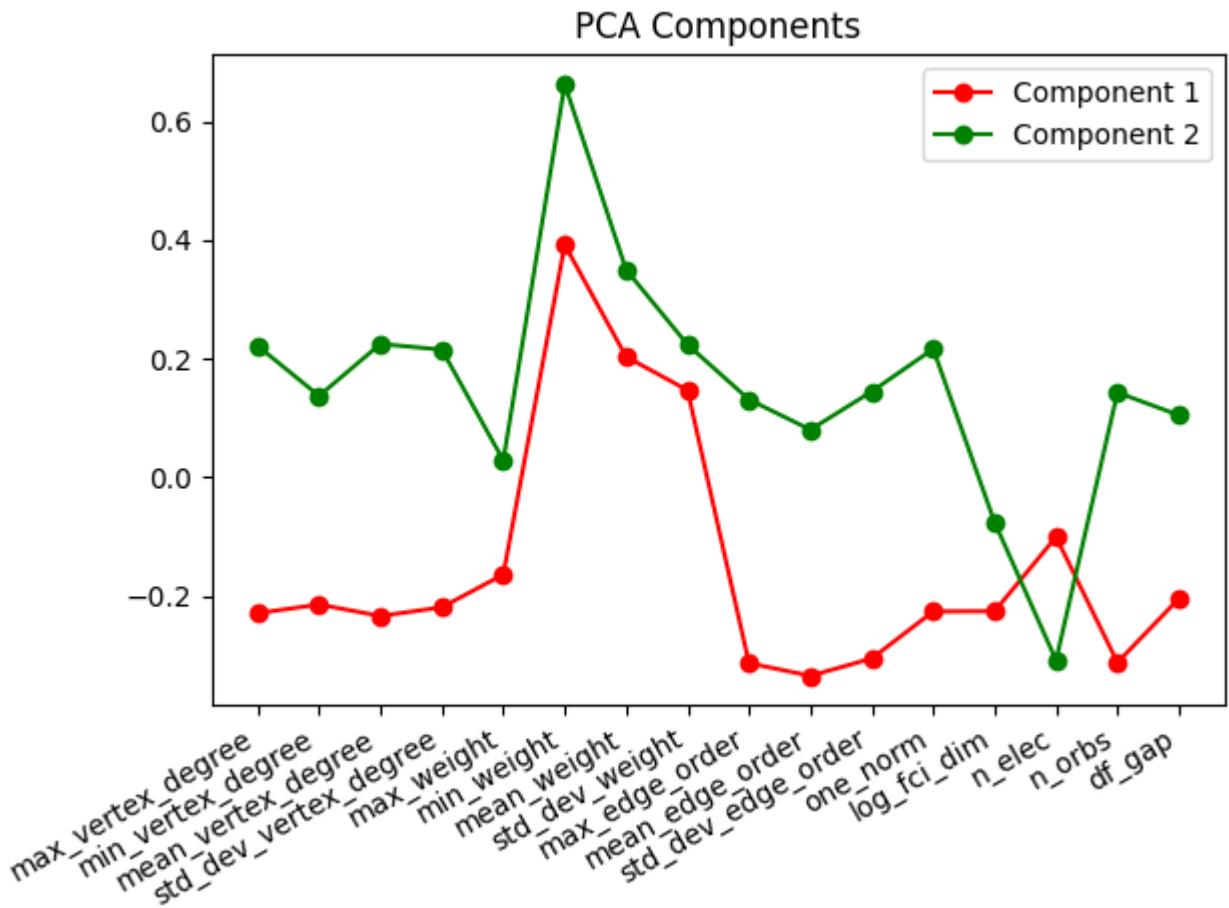
ML Feature Analysis



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.]

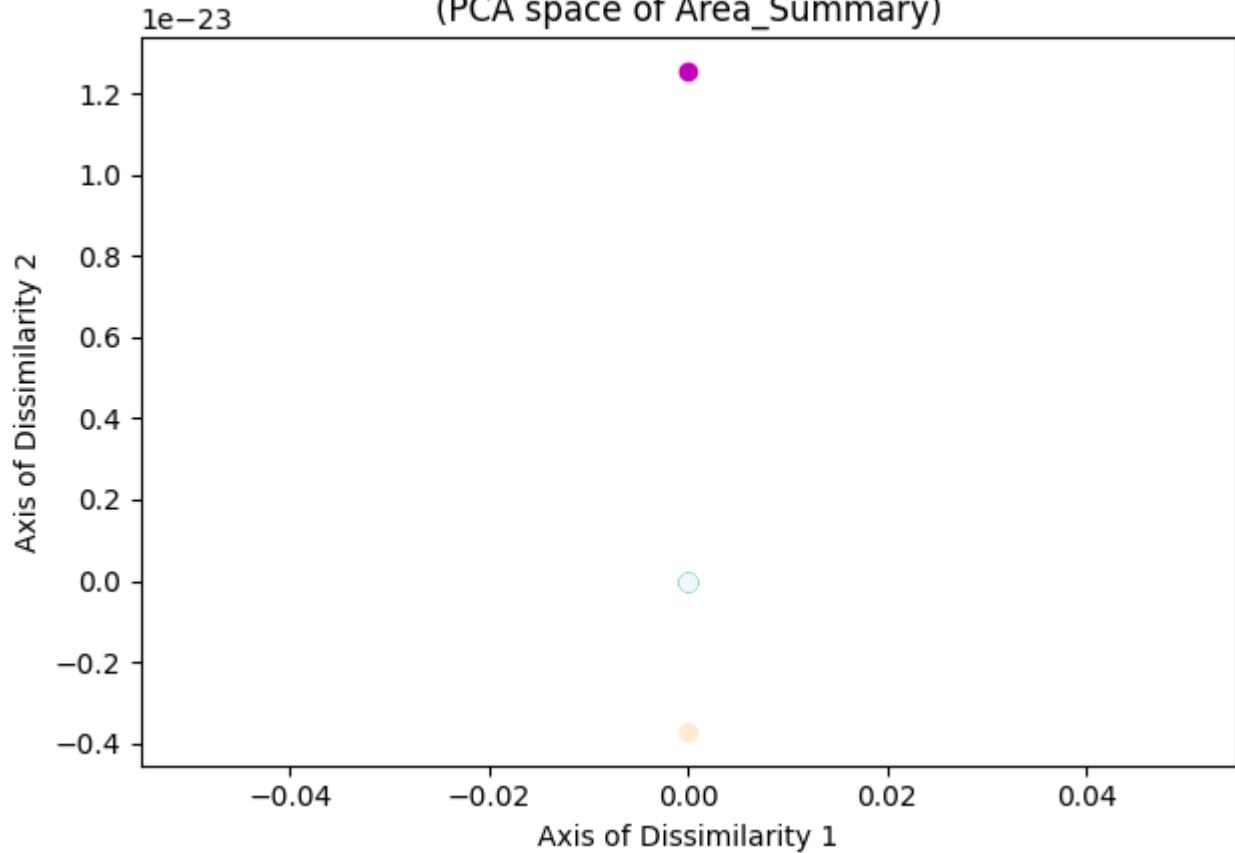


Features: ['max_vertex_degree', 'min_vertex_degree', 'mean_vertex_degree', 'std_dev_vertex_degree', 'max_weight', 'min_weight', 'mean_weight', 'std_dev_weight', 'max_edge_order', 'mean_edge_order', 'std_dev_edge_order', 'one_norm', 'log_fci_dim', 'n_elec', 'n_orbs', 'df_gap']

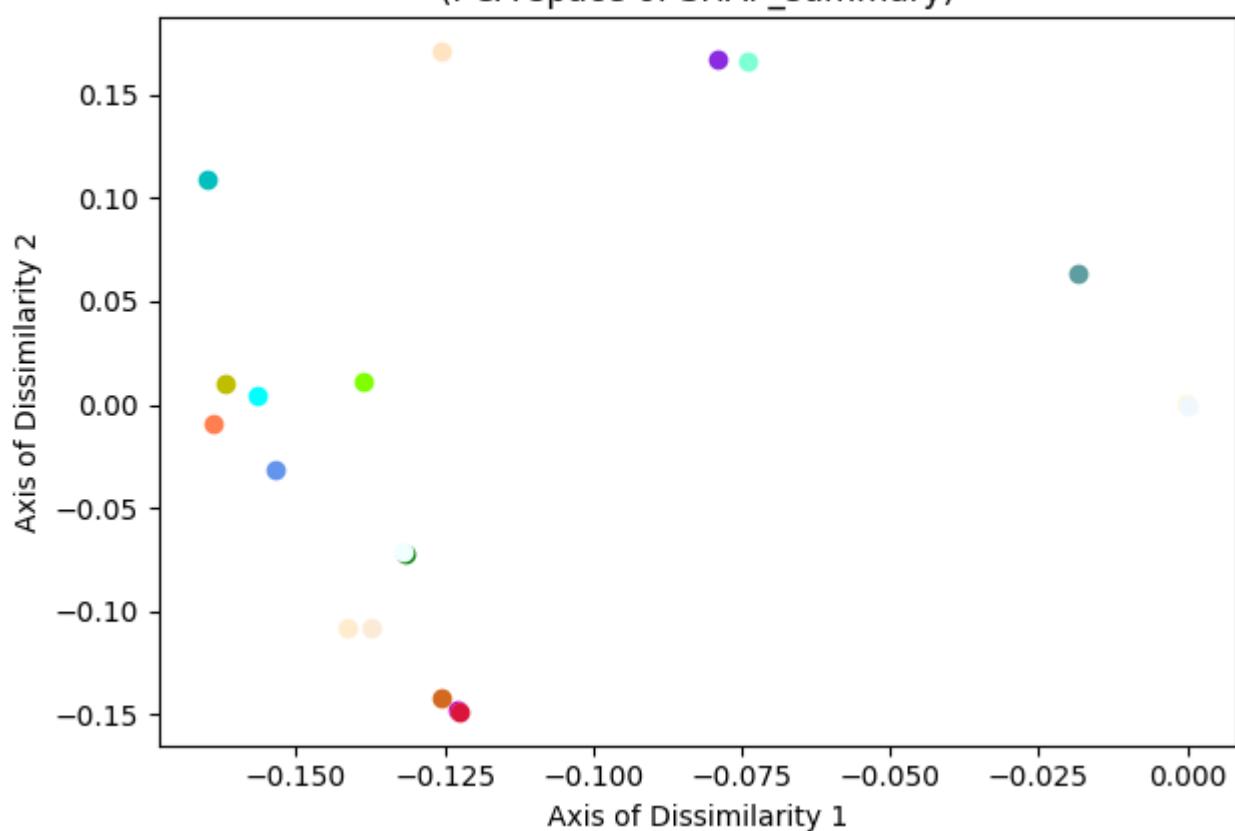
PCA Component 1: [-0.22922229 -0.21461603 -0.23398401 -0.21923522
 -0.16402432 0.39183587 0.20302013 0.14659357 -0.3134204 -0.33485059
 -0.30553226 -0.22630863 -0.2258685 -0.10070305 -0.31226268
 -0.20457232]

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]

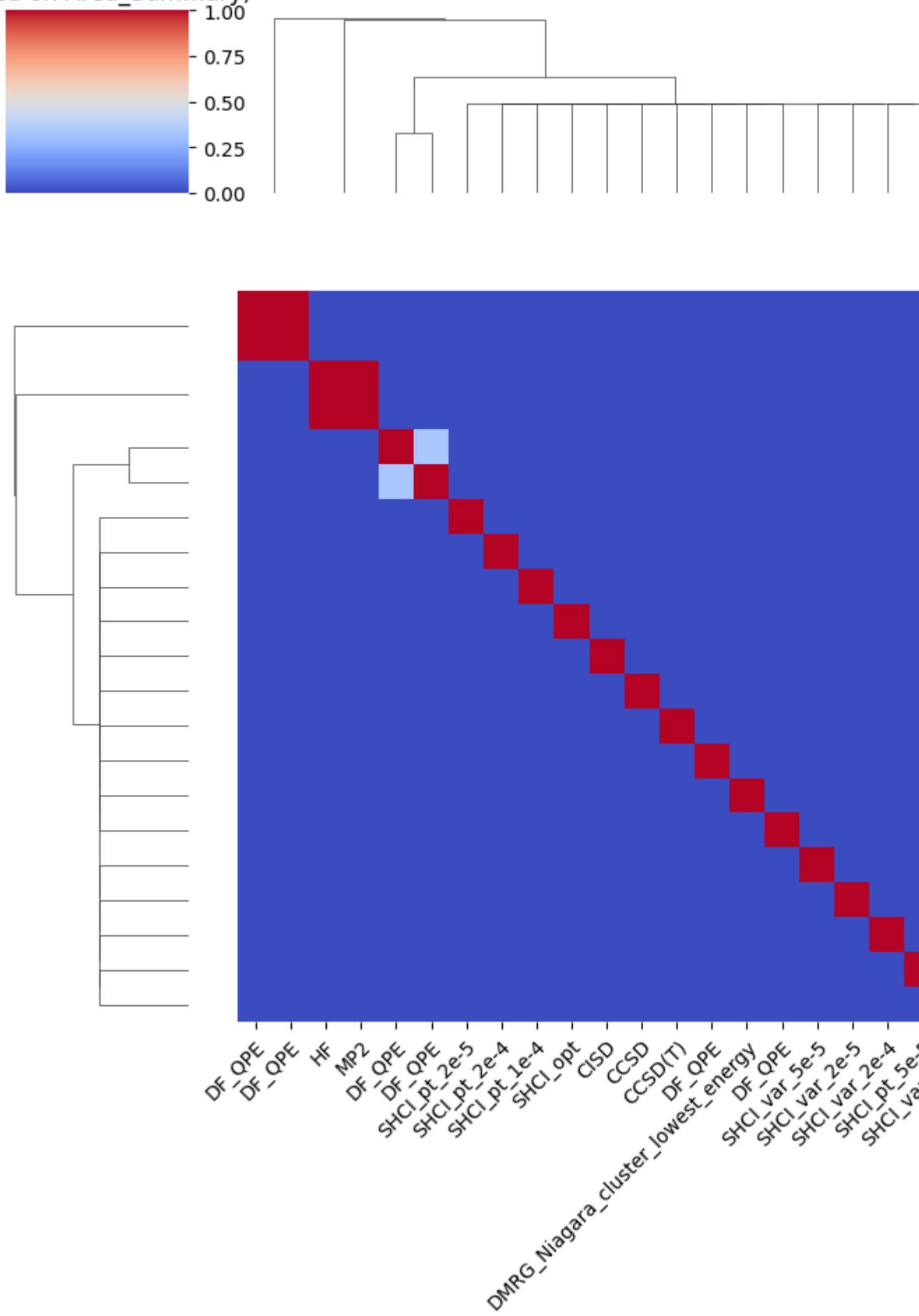
Solver points in PCA space
(PCA space of Area_Summary)



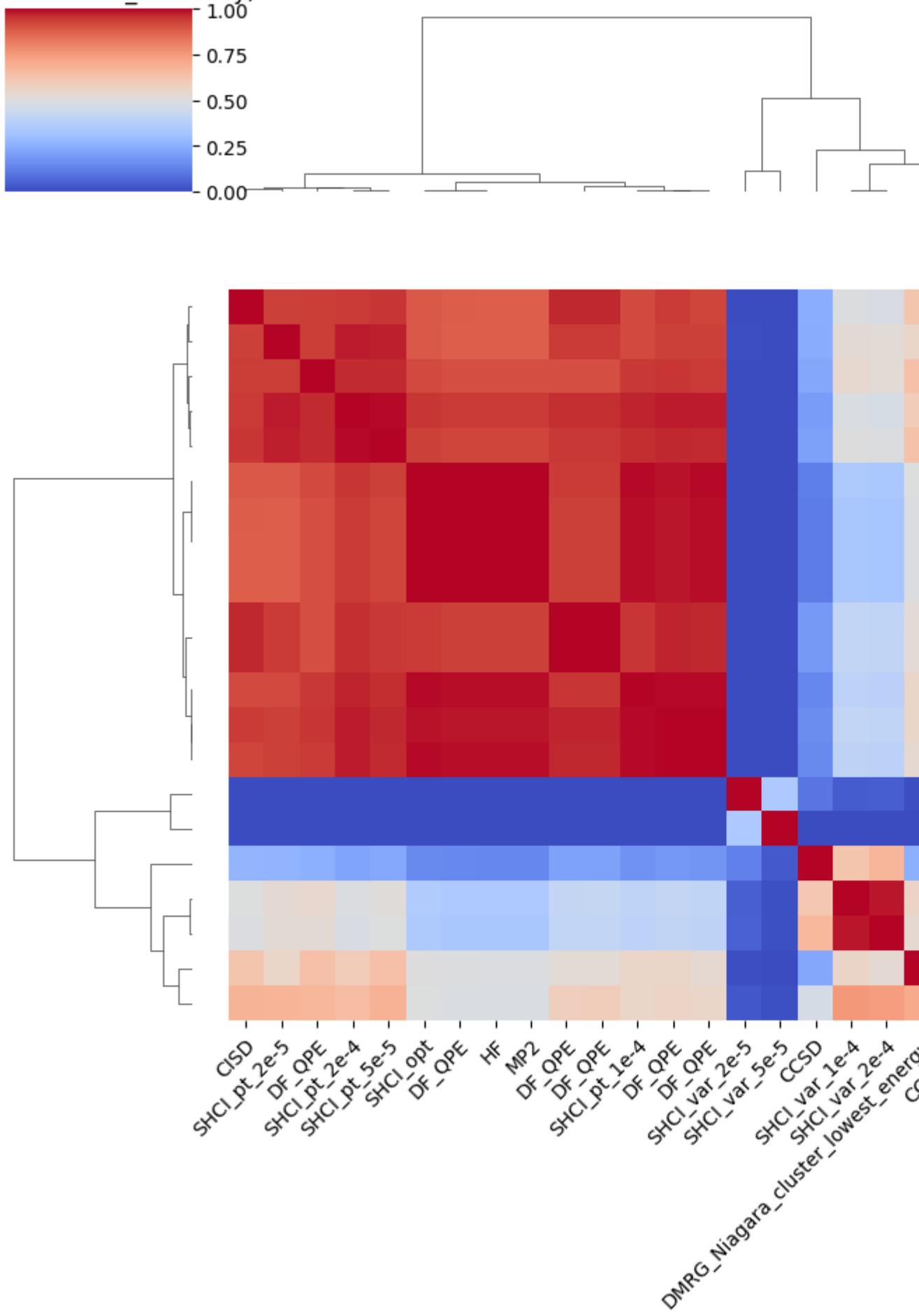
Solver points in PCA space
(PCA space of SHAP_summary)

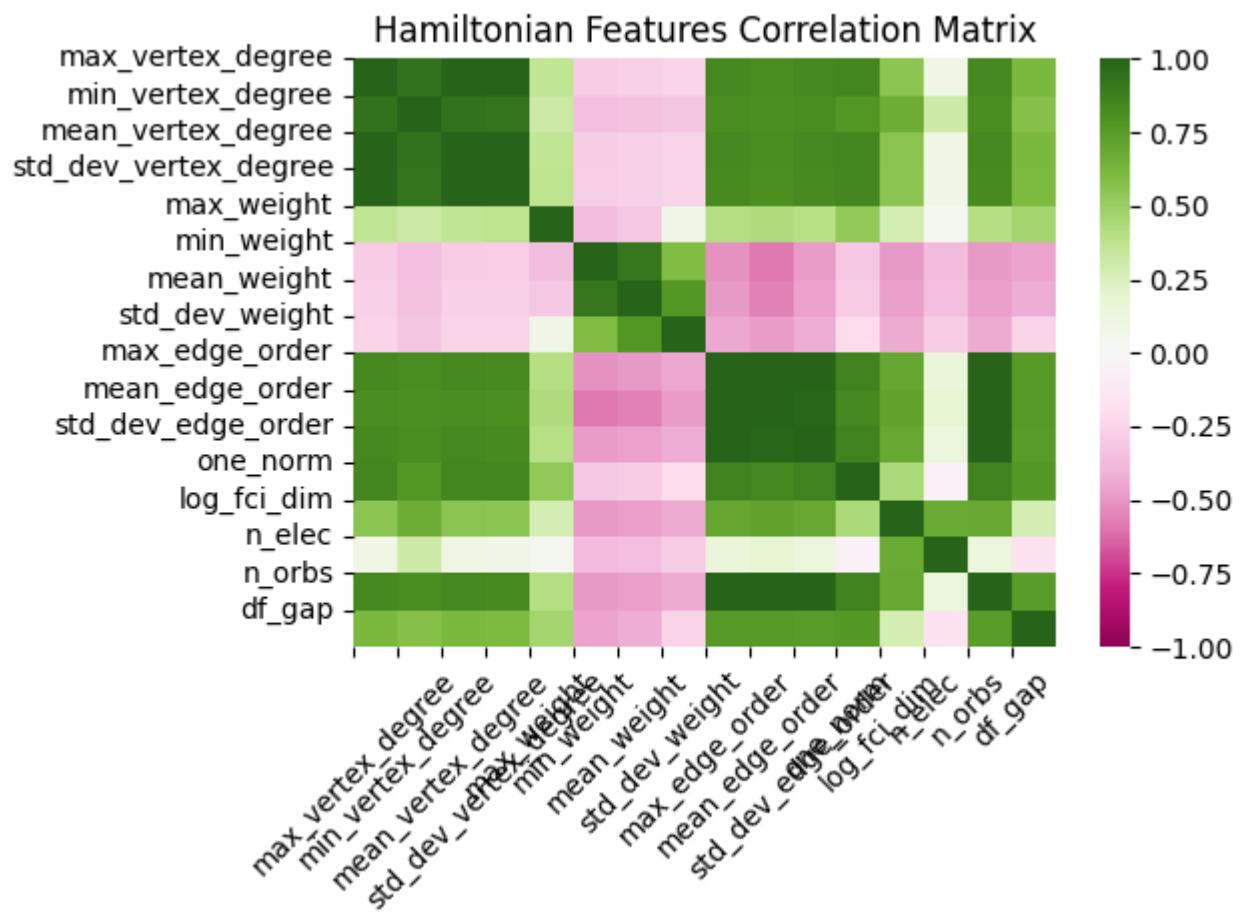


Solver similarity matrix
(based on Area_Summary)

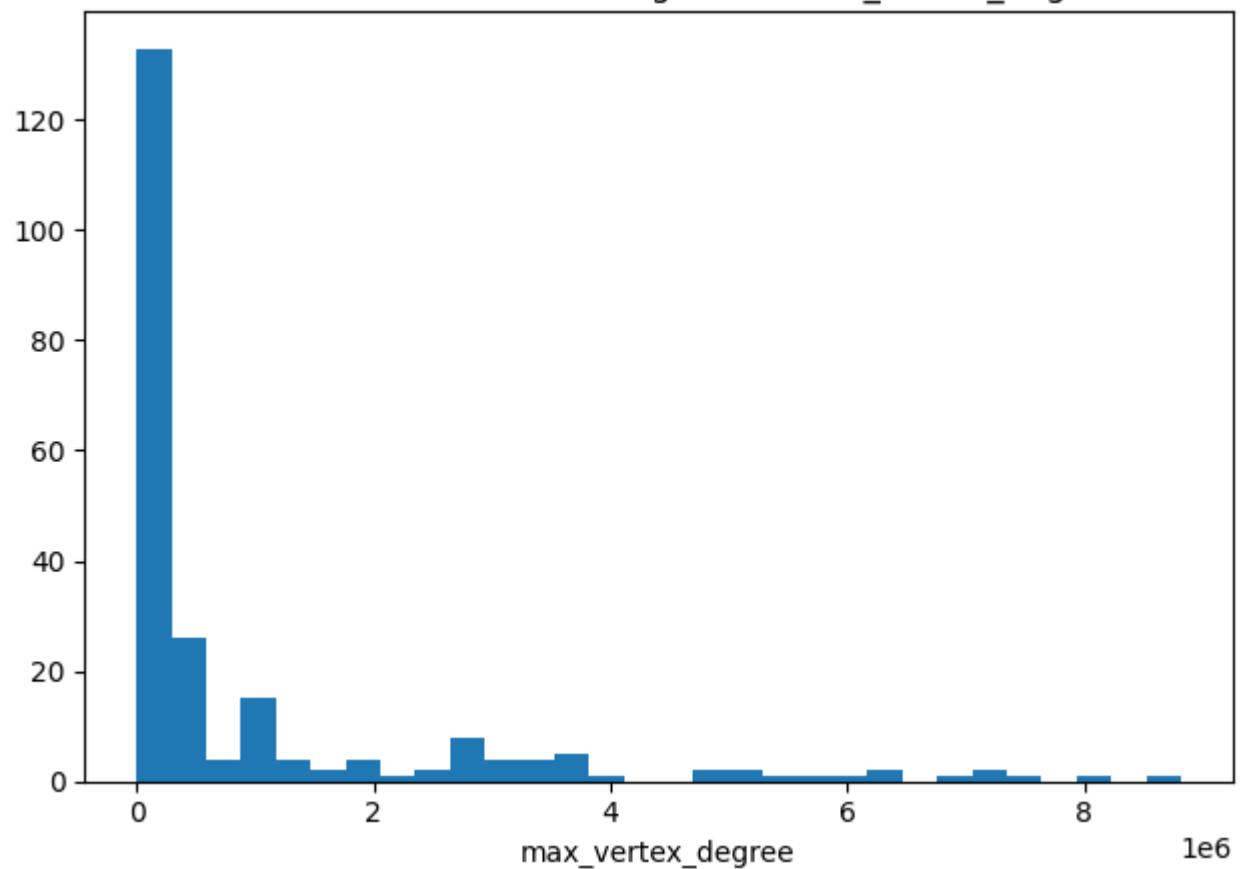


Solver similarity matrix
(based on SHAP_summary)

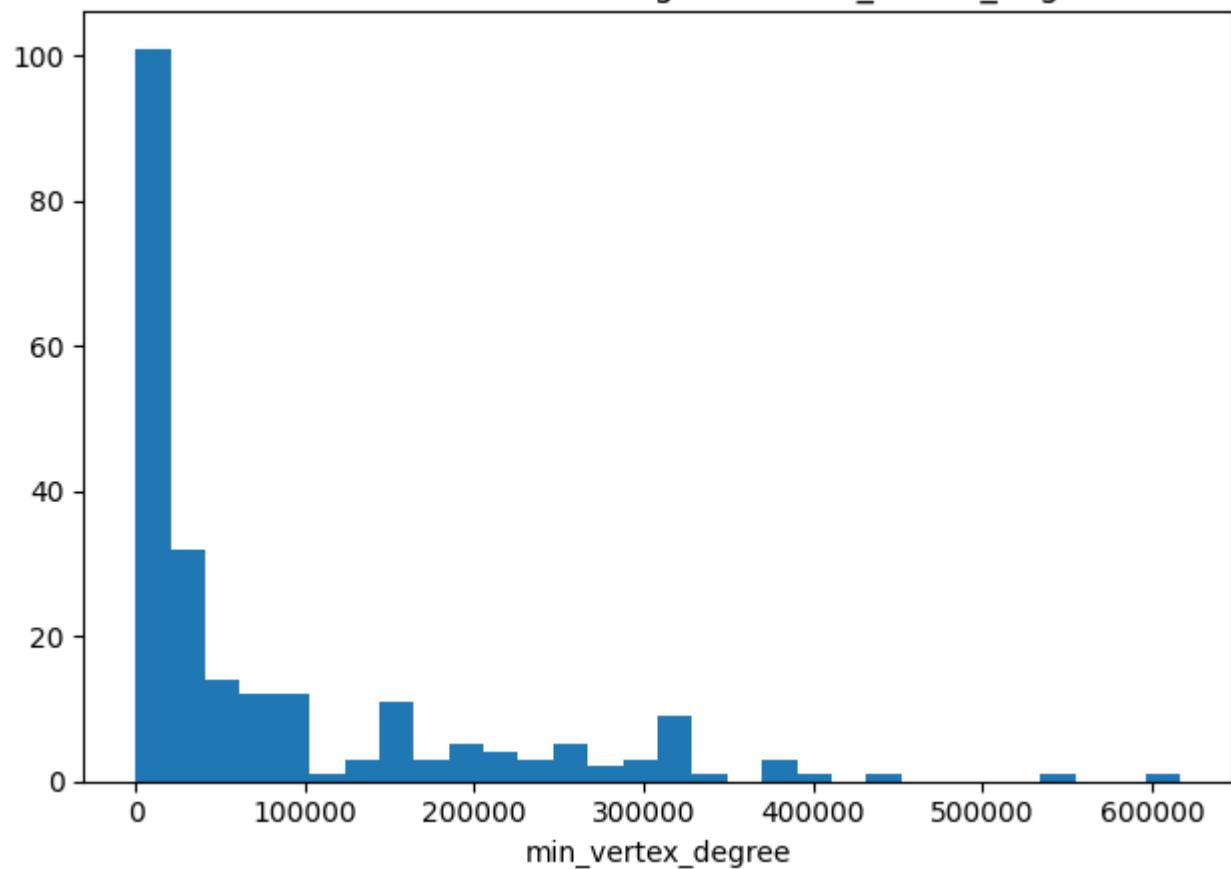




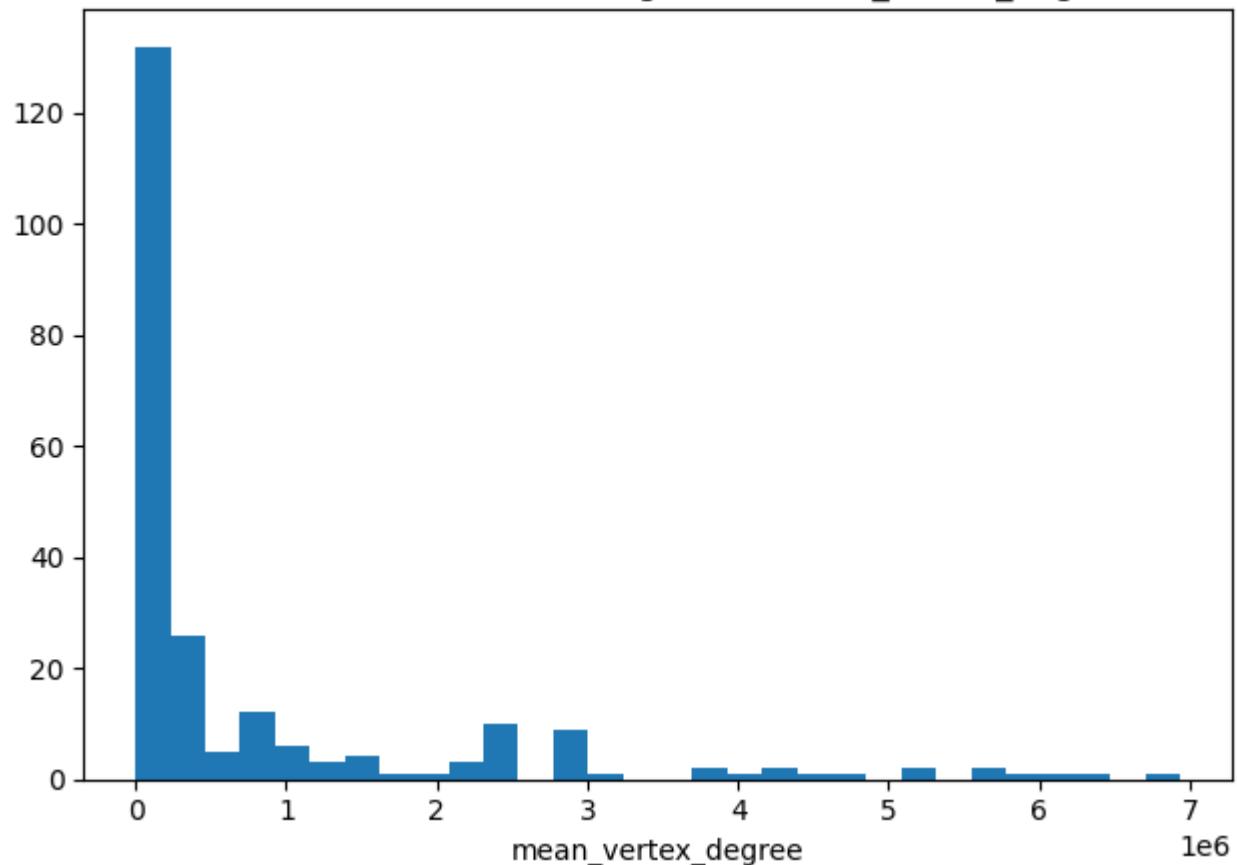
Hamiltonian features: histogram of max_vertex_degree



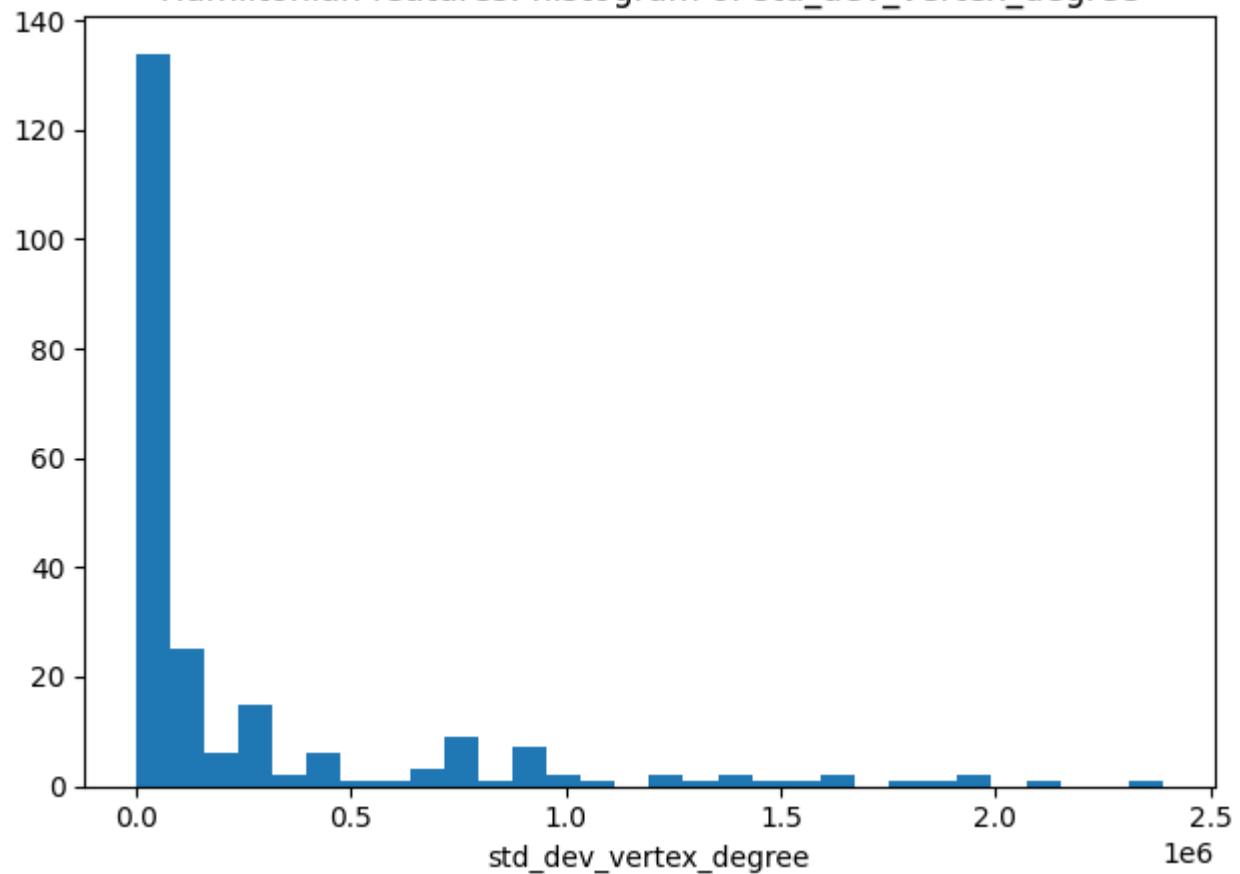
Hamiltonian features: histogram of min_vertex_degree



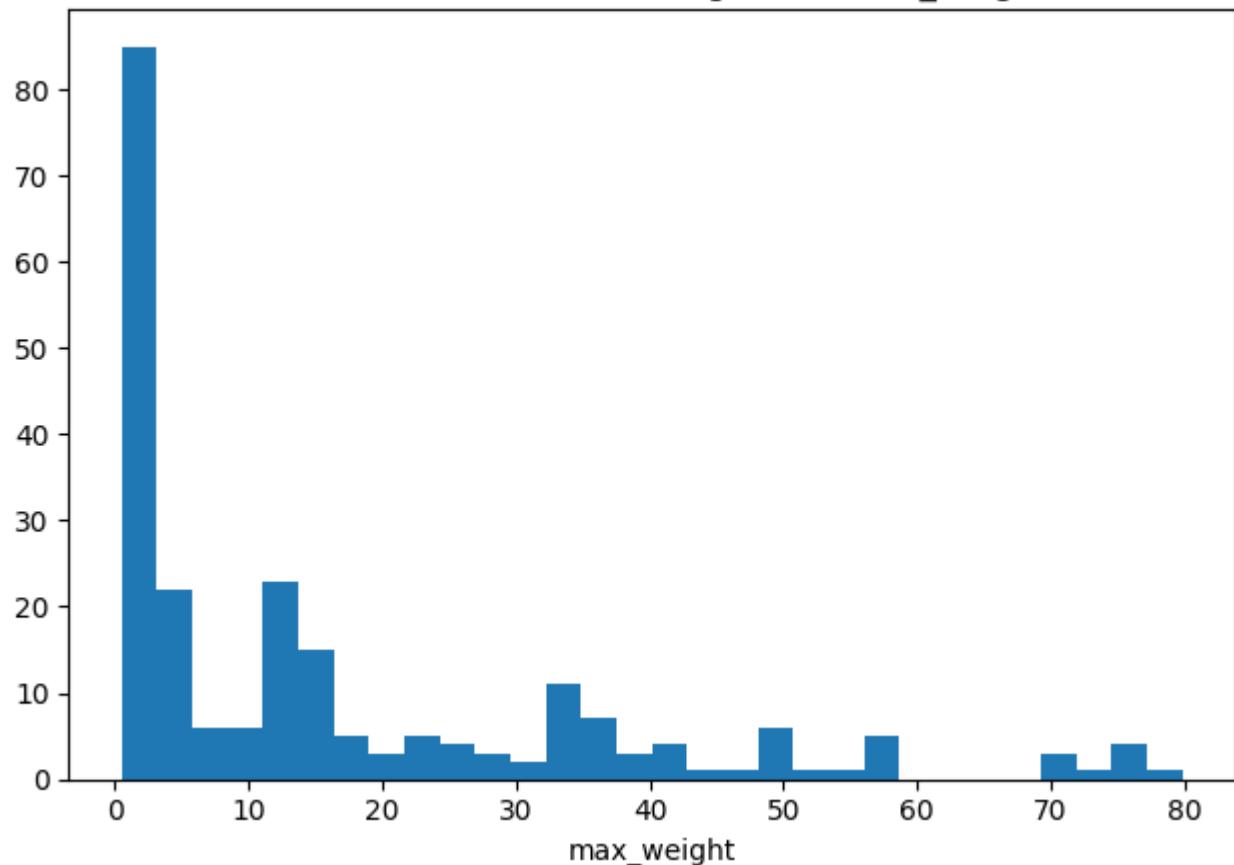
Hamiltonian features: histogram of mean_vertex_degree



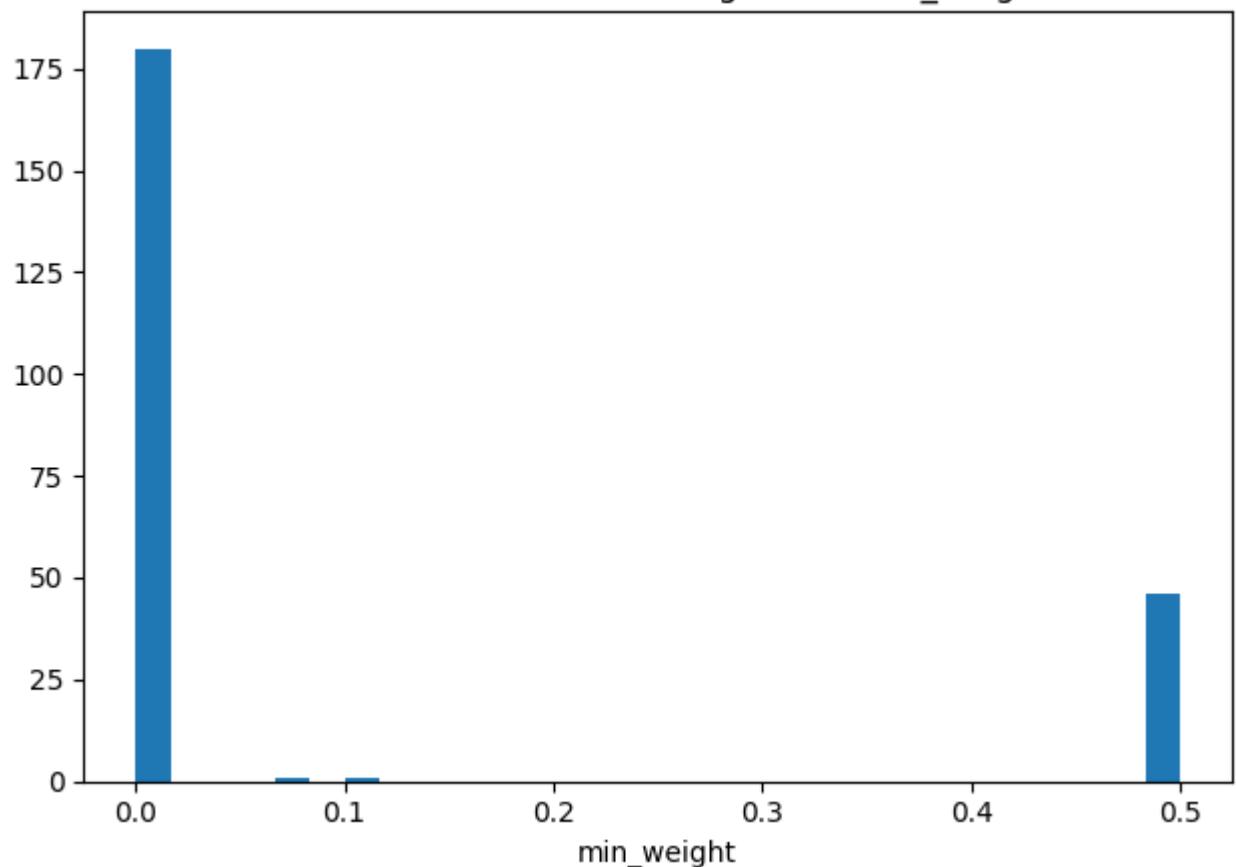
Hamiltonian features: histogram of std_dev_vertex_degree



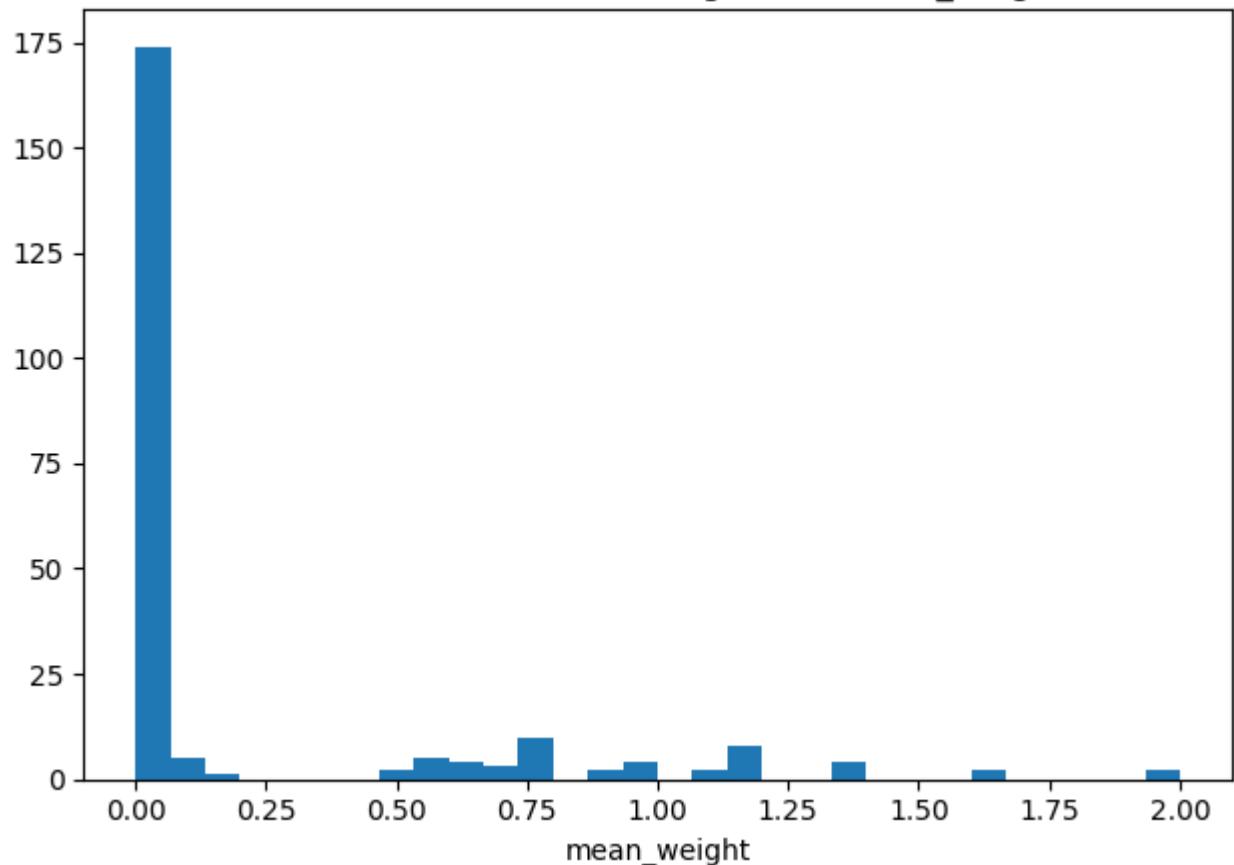
Hamiltonian features: histogram of max_weight



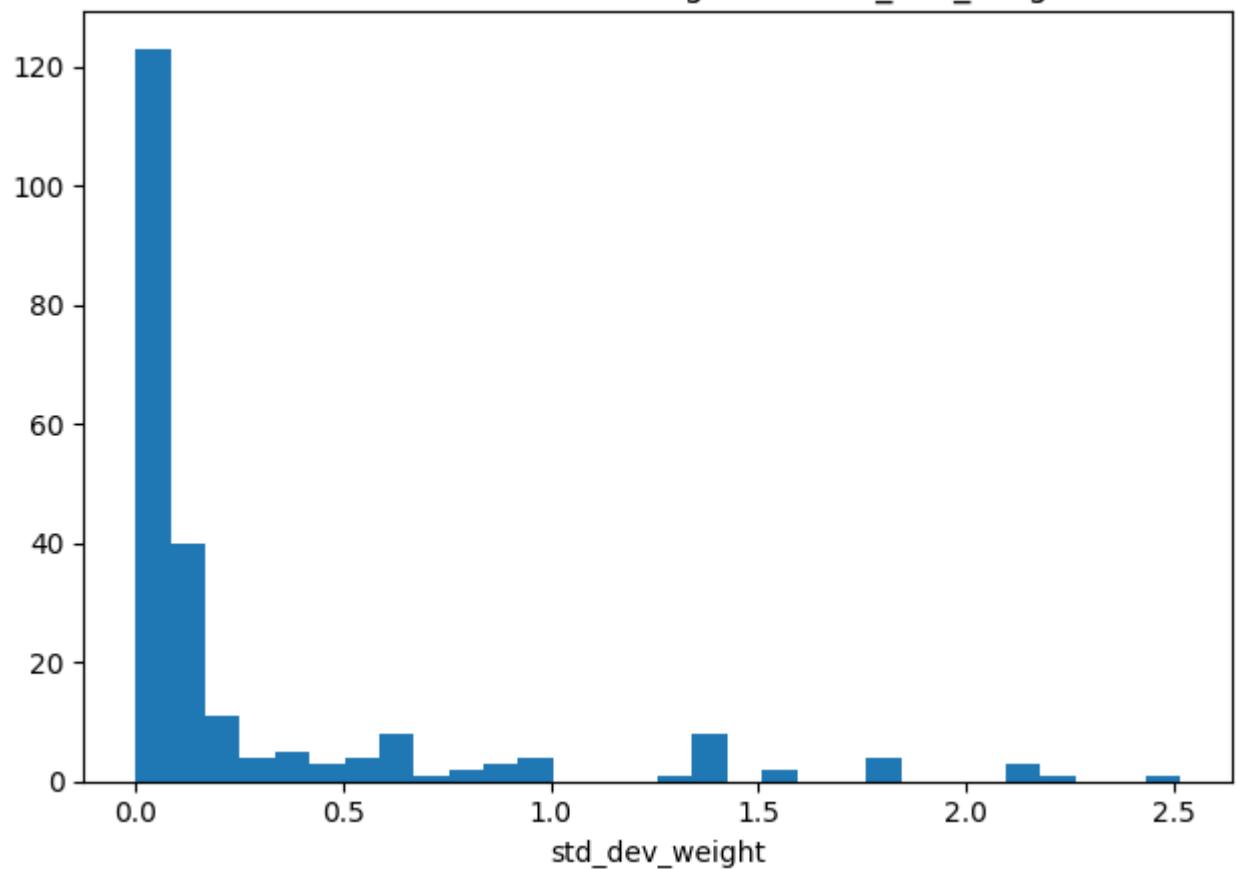
Hamiltonian features: histogram of min_weight



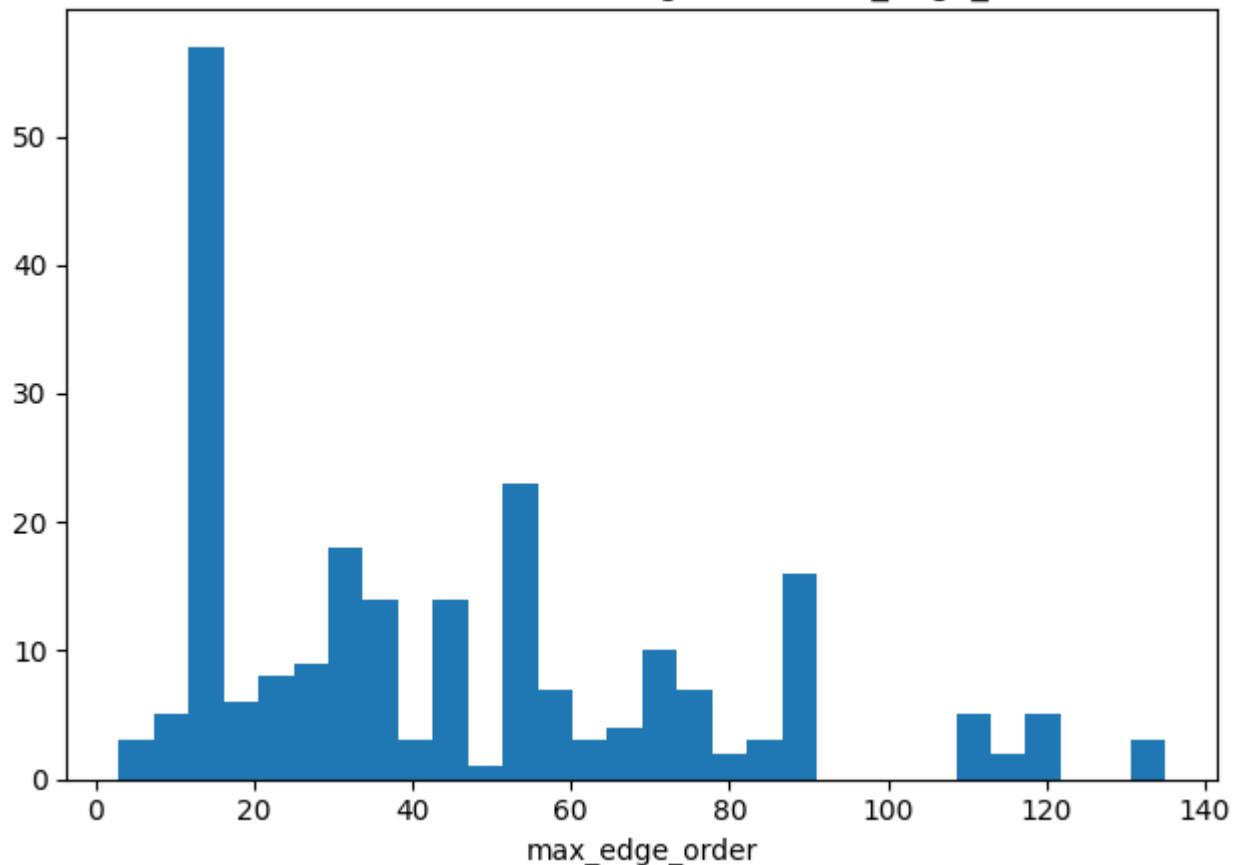
Hamiltonian features: histogram of mean_weight



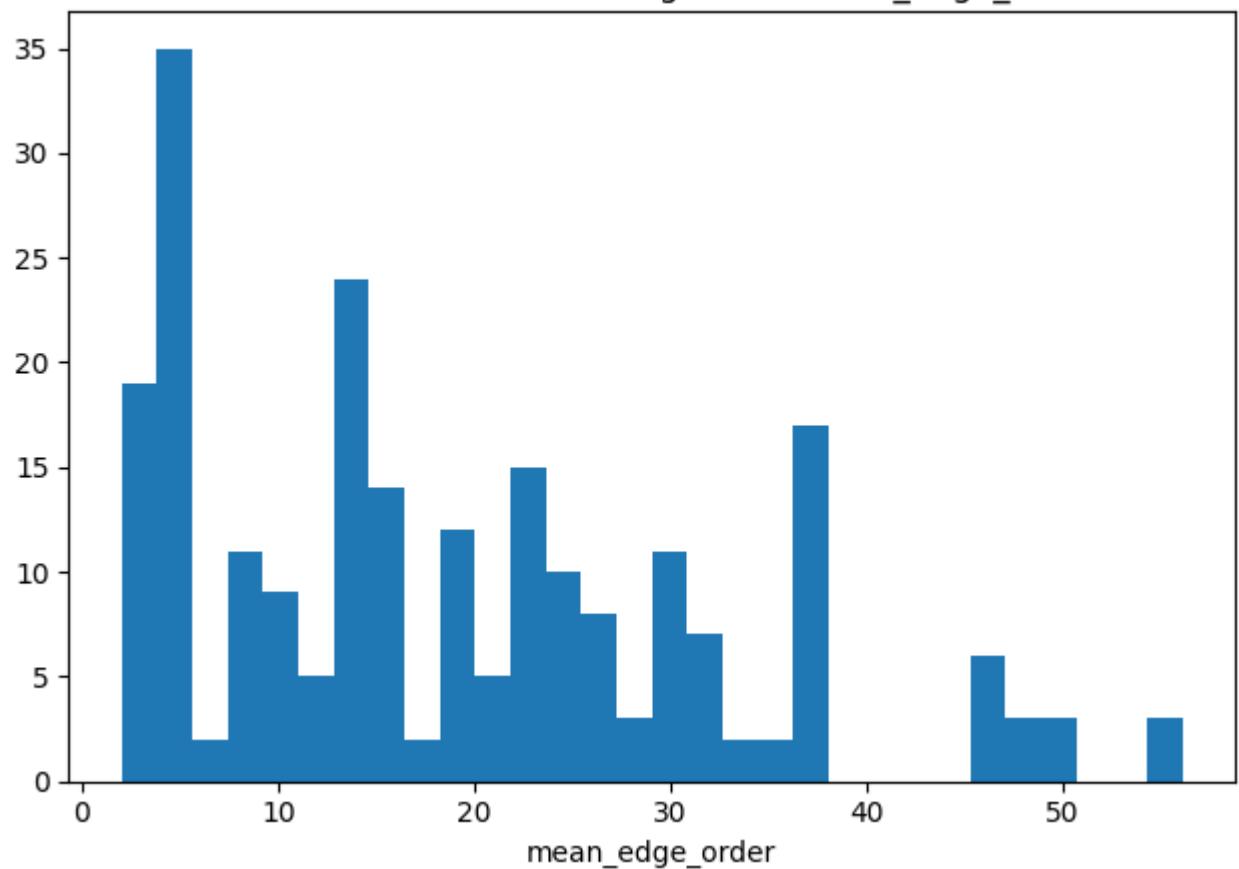
Hamiltonian features: histogram of std_dev_weight



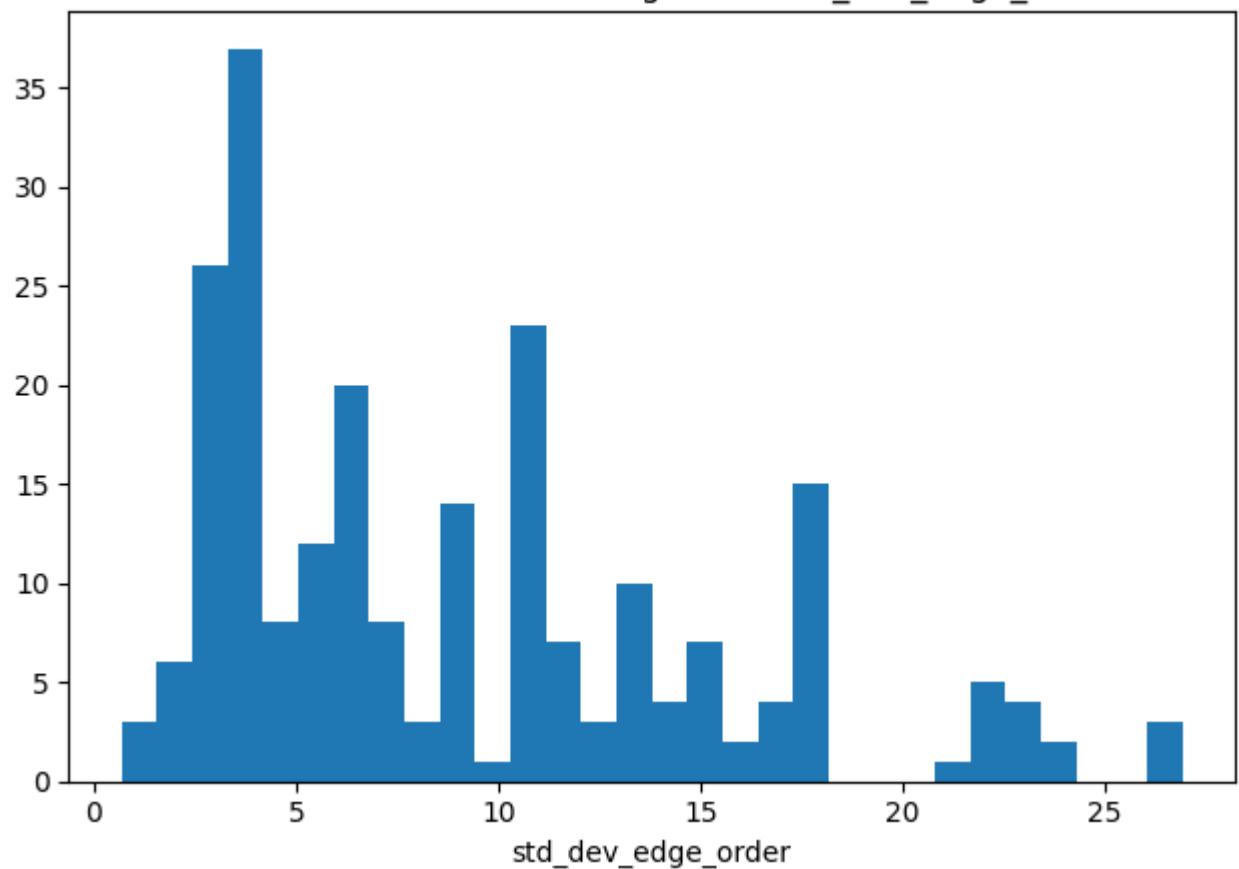
Hamiltonian features: histogram of max_edge_order



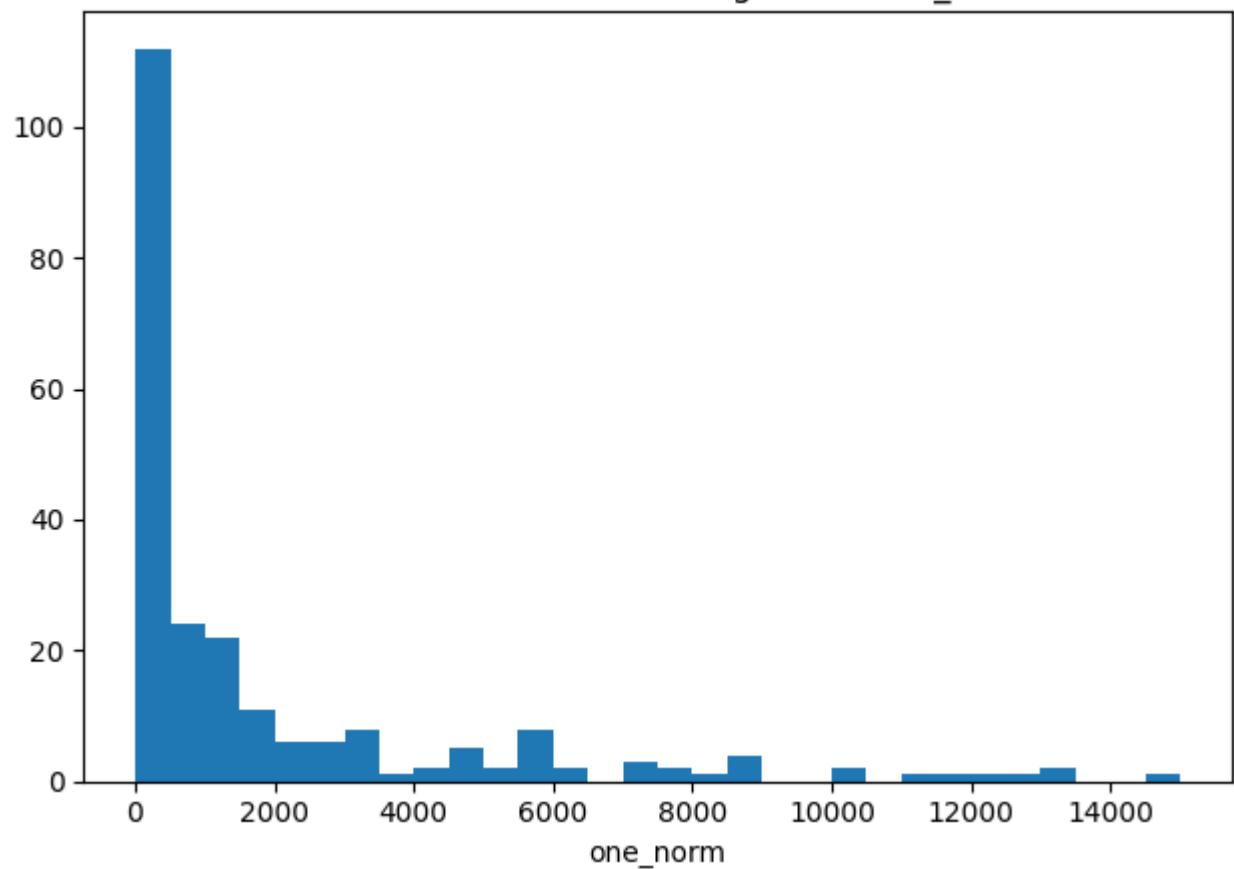
Hamiltonian features: histogram of mean_edge_order



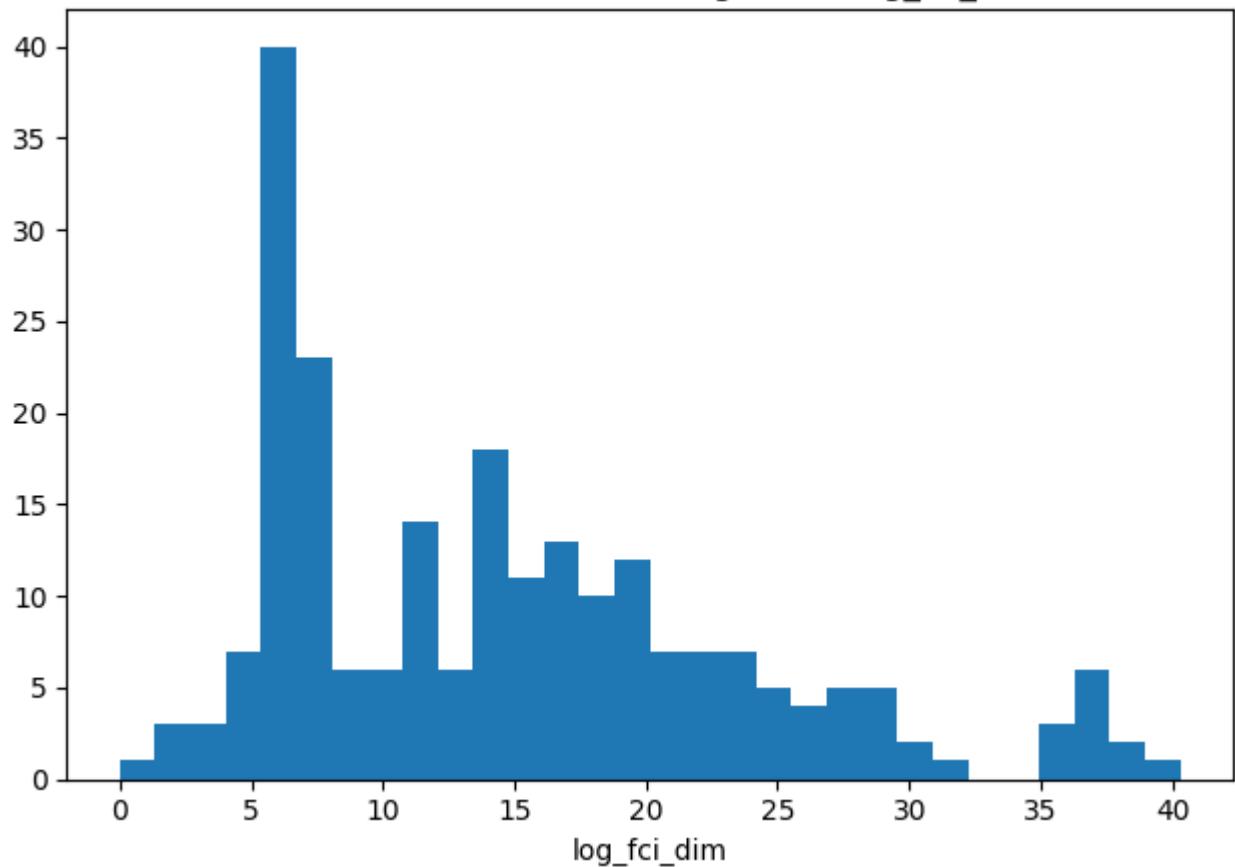
Hamiltonian features: histogram of std_dev_edge_order



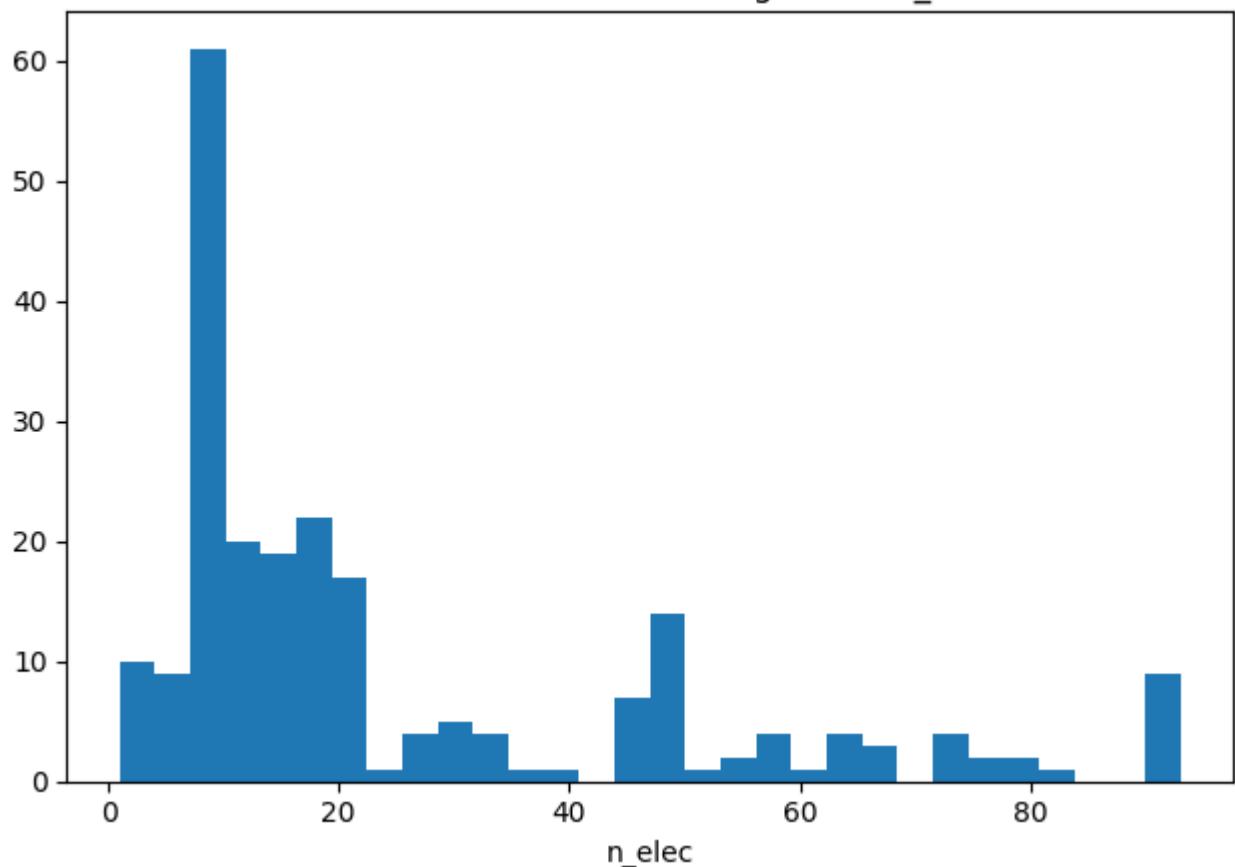
Hamiltonian features: histogram of one_norm



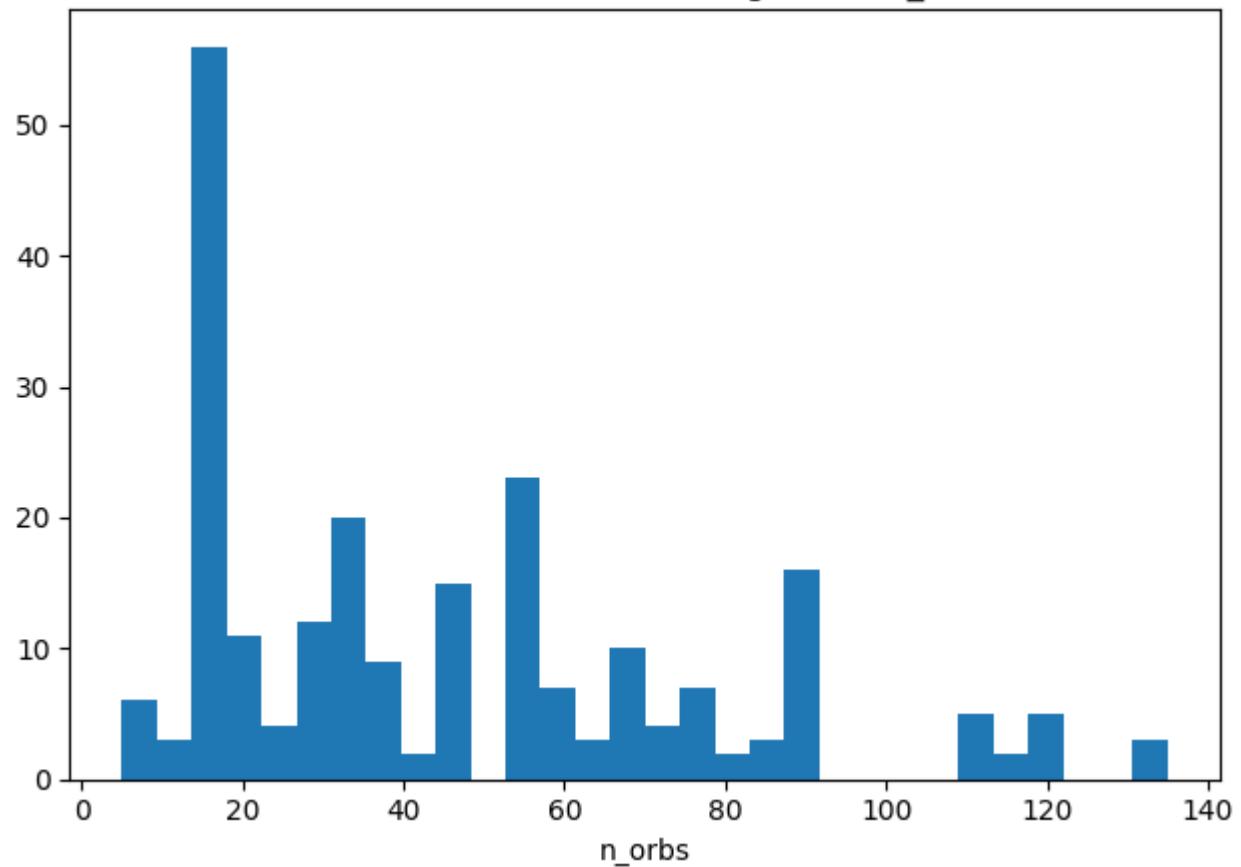
Hamiltonian features: histogram of log_fci_dim



Hamiltonian features: histogram of n_elec



Hamiltonian features: histogram of n_orbs



Hamiltonian features: histogram of df_gap

