

GSEE Benchmark Standard Report

Report based on data from 2025-02-19T18:26:13.854054+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Wed Feb 19 07:47:55 2025

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

Latest creation time for a `problem_instance.json` file: Wed Feb 19 12:32:46 2025

Latest creation time for a `solution.json` file: Tue Feb 18 15:25:53 2025

Problem Instance Summary Statistics

number of `problem_instances`: 88.

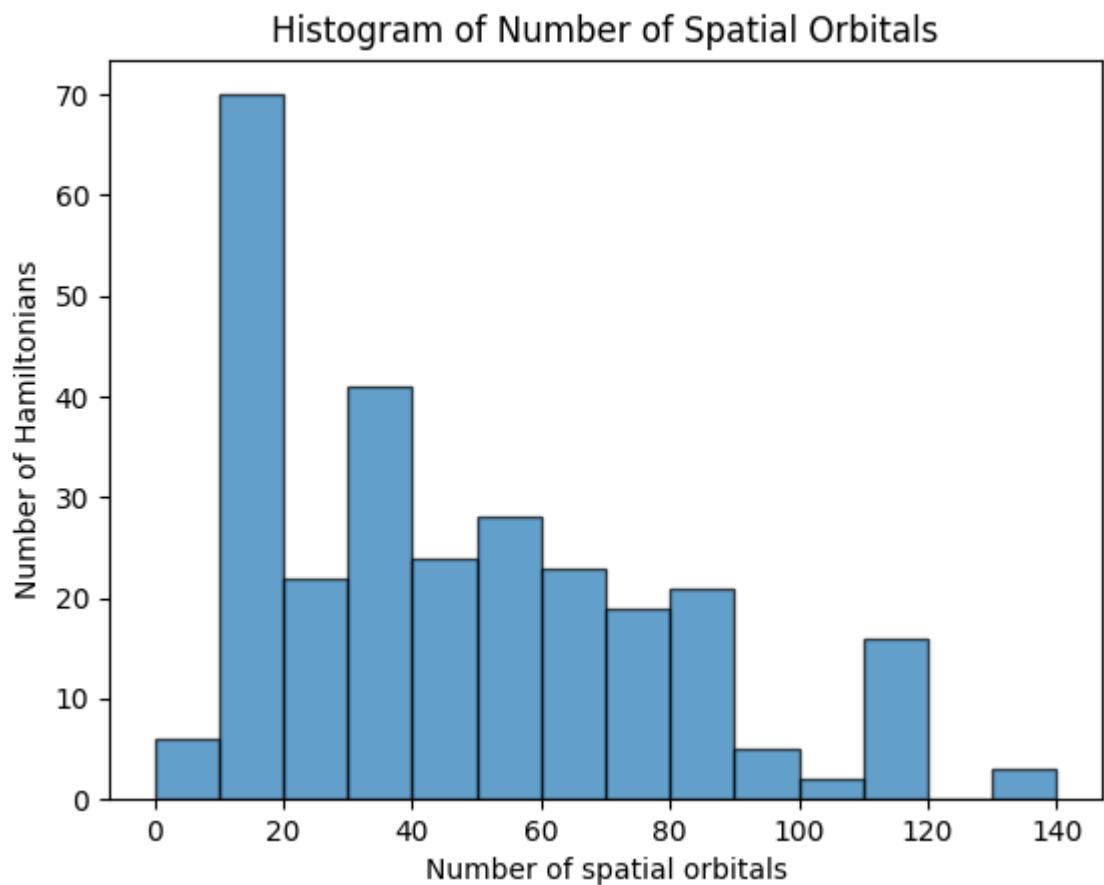
`problem_instance.json` with the most tasks: 30 (`hubbard_square/614c4444-a31a-4348-b24d-01040208651c`)

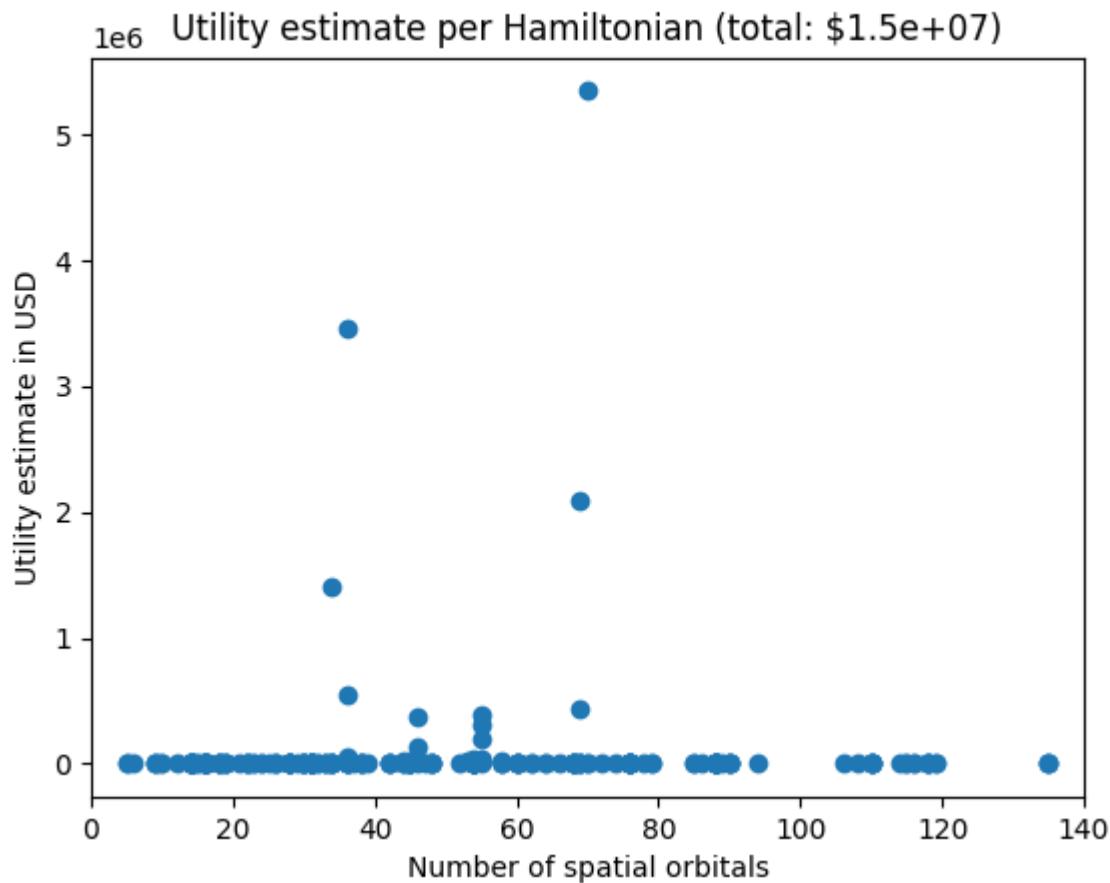
number of Hamiltonians (i.e., tasks) we have features calculated for: 280

minimum number of orbitals: 5

median number of orbitals: 42.0

maximum number of orbitals: 135





Solver Summary Statistics

number of unique participating solvers: 21

Solver: DF_QPE/2610d8de-bd3a-469e-9a80-473e8988755f, Model could not be calculated.

Solver: SHCI_opt/2dde727e-a881-44fa-aabf-bba6248e4baf, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.69230769 0.97315436]

Solver: DF_QPE/4b07b89f-c66f-4e72-8c24-df3e4222cb41, Model could not be calculated.

Solver: SHCI_pt_1e-4/4ed500f1-0650-41e3-af00-e4d0359394b4, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.66666667 0.96219931]

Solver: SHCI_var_1e-4/7e730dfb-57ee-480b-a8a1-4b73f5f07c54, ML Solvability Ratio: {'PCA': 0.3758, 'NNMF': 0.0115}, F1 Score: [0.95588235 0.96808511]

Solver: SHCI_pt_2e-4/ad964781-302e-4728-a26d-39918e0a6cdb, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.72413793 0.93984962]

Solver: SHCI_pt_2e-5/c71b90bd-3250-4c0c-b4e7-fc9878f141f6, ML
Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.3 0.95394737]

Solver: SHCI_pt_5e-5/d626506c-7aae-4ad6-802a-b29af5f2bb93, ML
Solvability Ratio: {'PCA': 0.991, 'NNMF': 0.6864}, F1 Score: [0.7
0.95774648]

Solver: SHCI_var_2e-4/0db183e3-a86d-491b-9125-599556e37c7a, ML
Solvability Ratio: {'PCA': 0.2602, 'NNMF': 0.452}, F1 Score: [0.96815287
0.97005988]

Solver: SHCI_var_2e-5/86bfe50c-9342-4d54-bb68-abc8abd95688, ML
Solvability Ratio: {'PCA': 0.5692, 'NNMF': 0.5177}, F1 Score: [0.83333333
0.96212121]

Solver: SHCI_var_5e-5/01949b95-c427-4693-9134-01f47f688c09, ML
Solvability Ratio: {'PCA': 0.5156, 'NNMF': 0.4165}, F1 Score: [0.80952381
0.93333333]

Solver: DF_QPE/5d768520-b3d0-4292-bbb4-9776fa128107, Model could not
be calculated.

Solver: DF_QPE/5dad4064-cd11-412f-85cb-d722afe3b3de, Model could not
be calculated.

Solver: CISD/418f060e-496b-4024-8d2d-9b1f8791e76d, ML Solvability
Ratio: {'PCA': 0.0498, 'NNMF': 0.012}, F1 Score: [0.97526502 0.82926829]

Solver: CCSD(T)/c09217e6-d0f7-4b0f-81c4-79210b7ac878, ML Solvability
Ratio: {'PCA': 0.2424, 'NNMF': 0.5231}, F1 Score: [0.92397661
0.91503268]

Solver: HF/5f5e617a-19c2-4d82-bebc-b2d6b3dcb012, ML Solvability Ratio:
'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98709677 0.71428571]

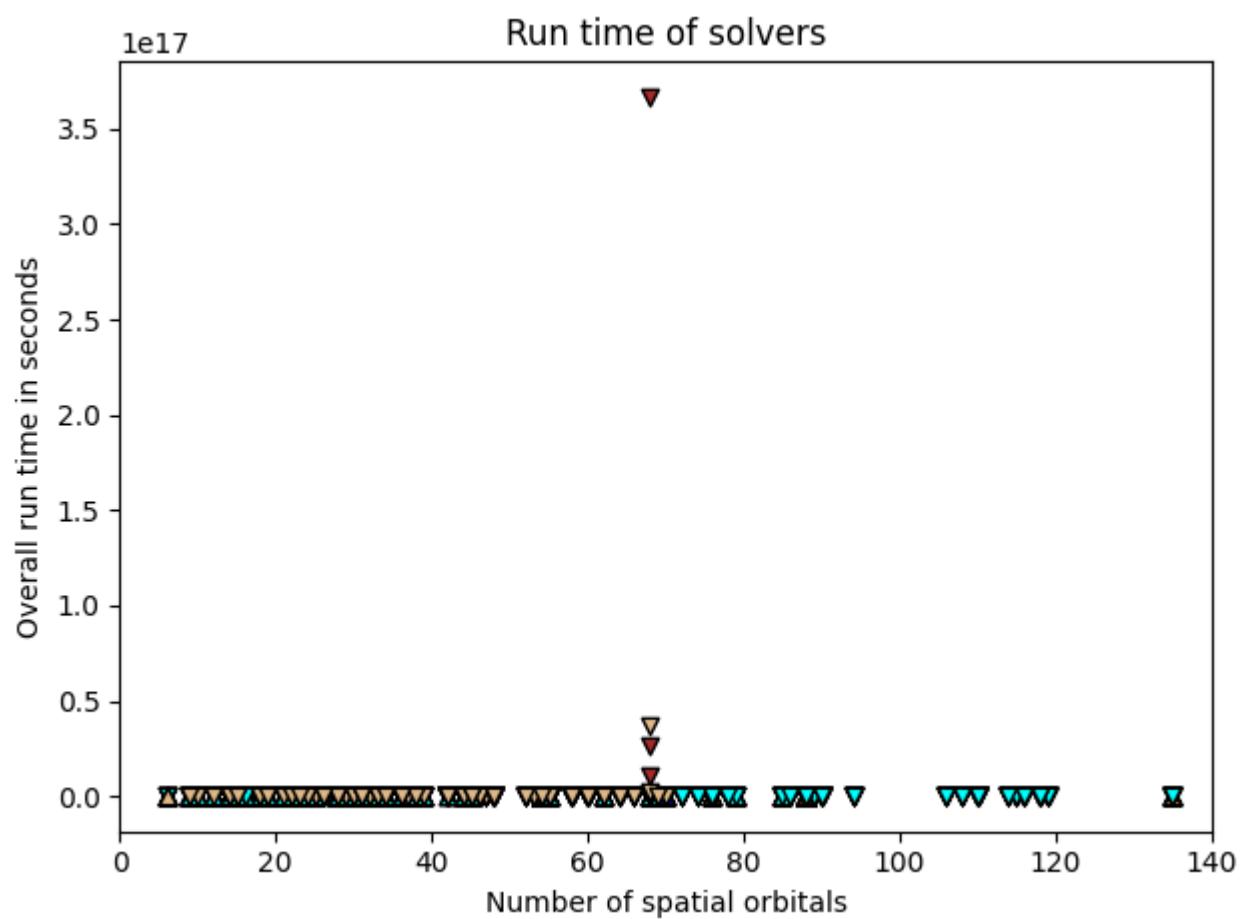
Solver: MP2/b420358b-5def-41e6-8c5d-b9d93b6aecd2, ML Solvability Ratio:
'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98709677 0.71428571]

Solver: CCSD/0a29e54f-bef9-4d19-bafa-d94b1c4b37aa, ML Solvability Ratio:
'PCA': 0.0, 'NNMF': 0.0164}, F1 Score: [0.98529412 0.92307692]

Solver: DMRG_Niagara_cluster_lowest_energy/16537433-9f4c-4eae-
a65d-787dc3b35b59, ML Solvability Ratio: {'PCA': 0.6263, 'NNMF':
0.4481}, F1 Score: [0.91836735 0.96460177]

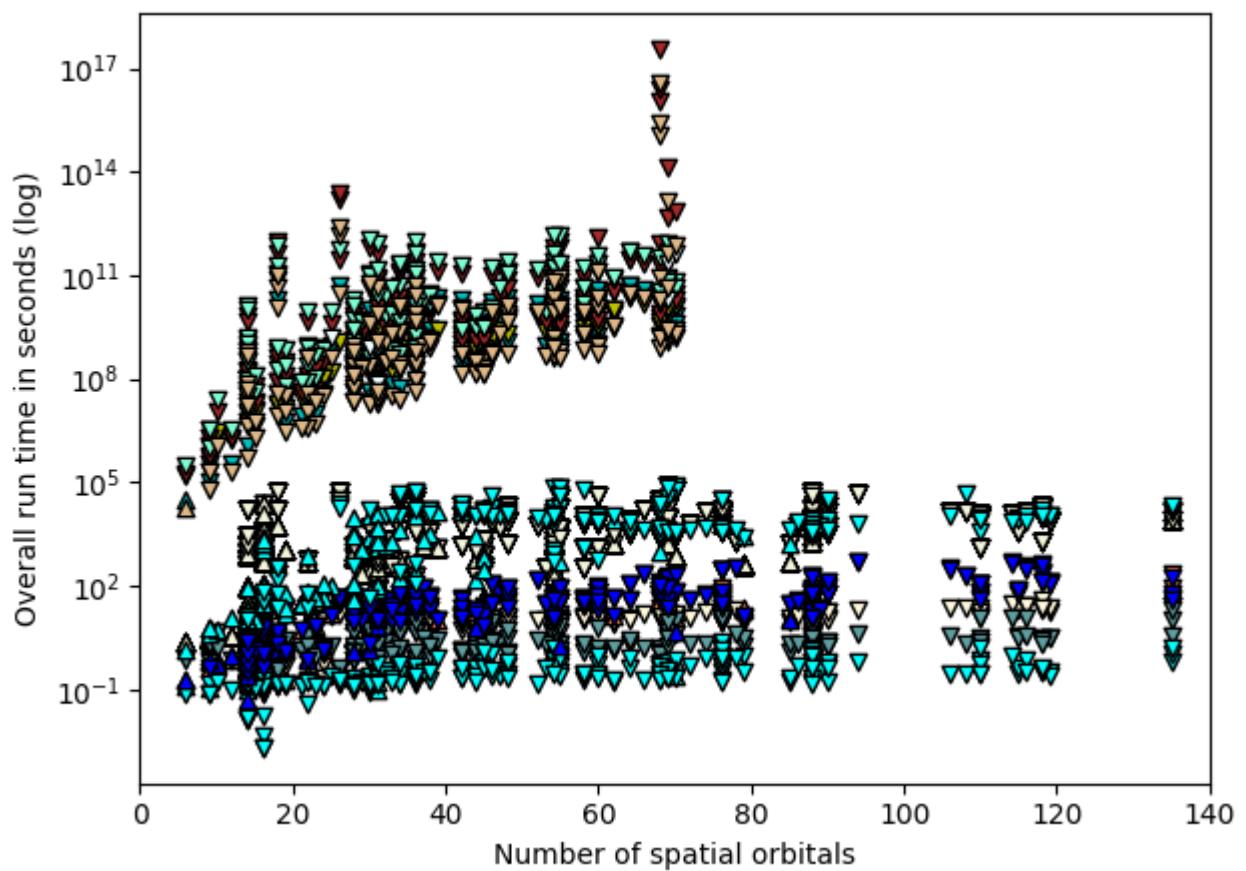
Solver: DF_QPE/6f385080-934b-4cbb-b813-39c2cb61349e, Model could not
be calculated.

Solver: DF_QPE/f6b36bde-be4a-4eee-975b-2c5f7e553f5f, Model could not be
calculated.



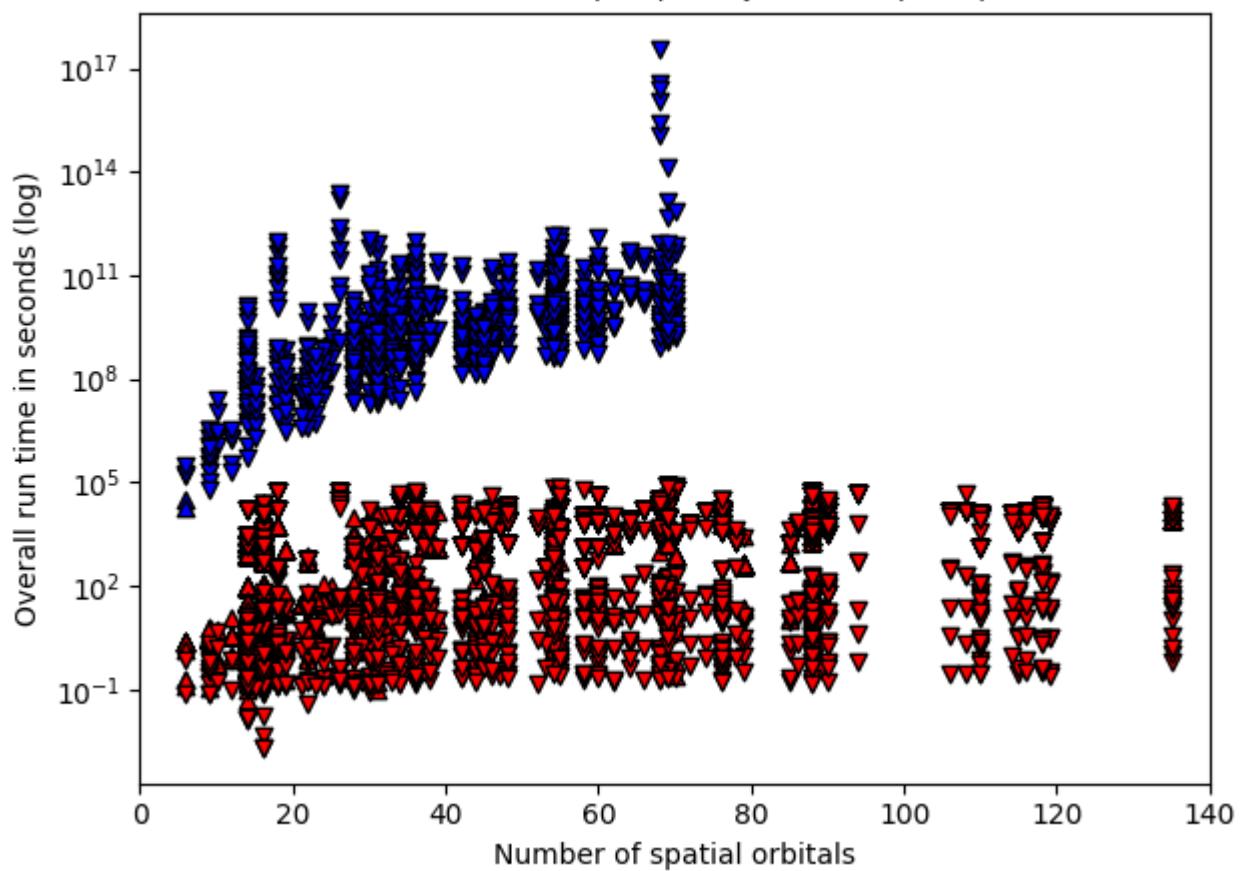
NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

Run time of solvers

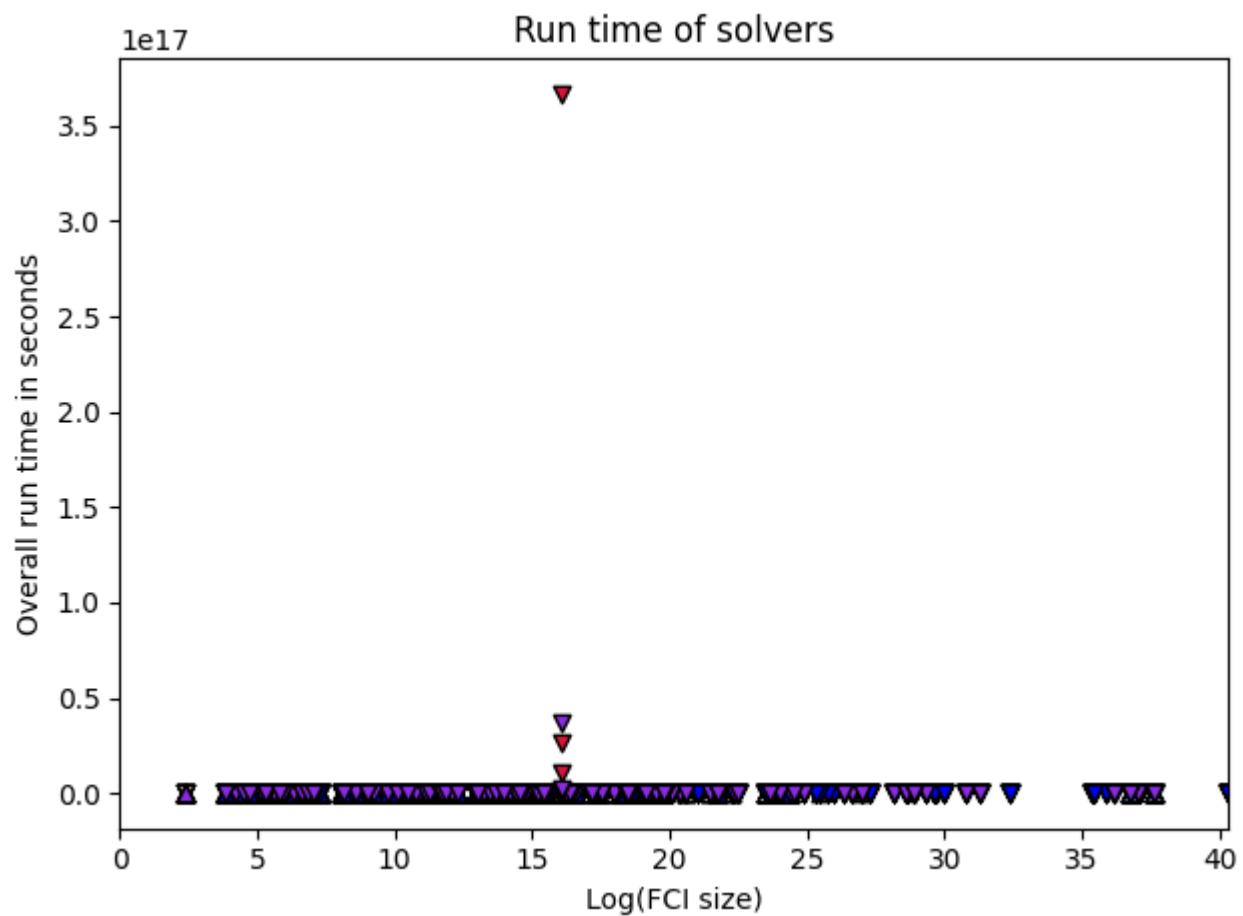


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

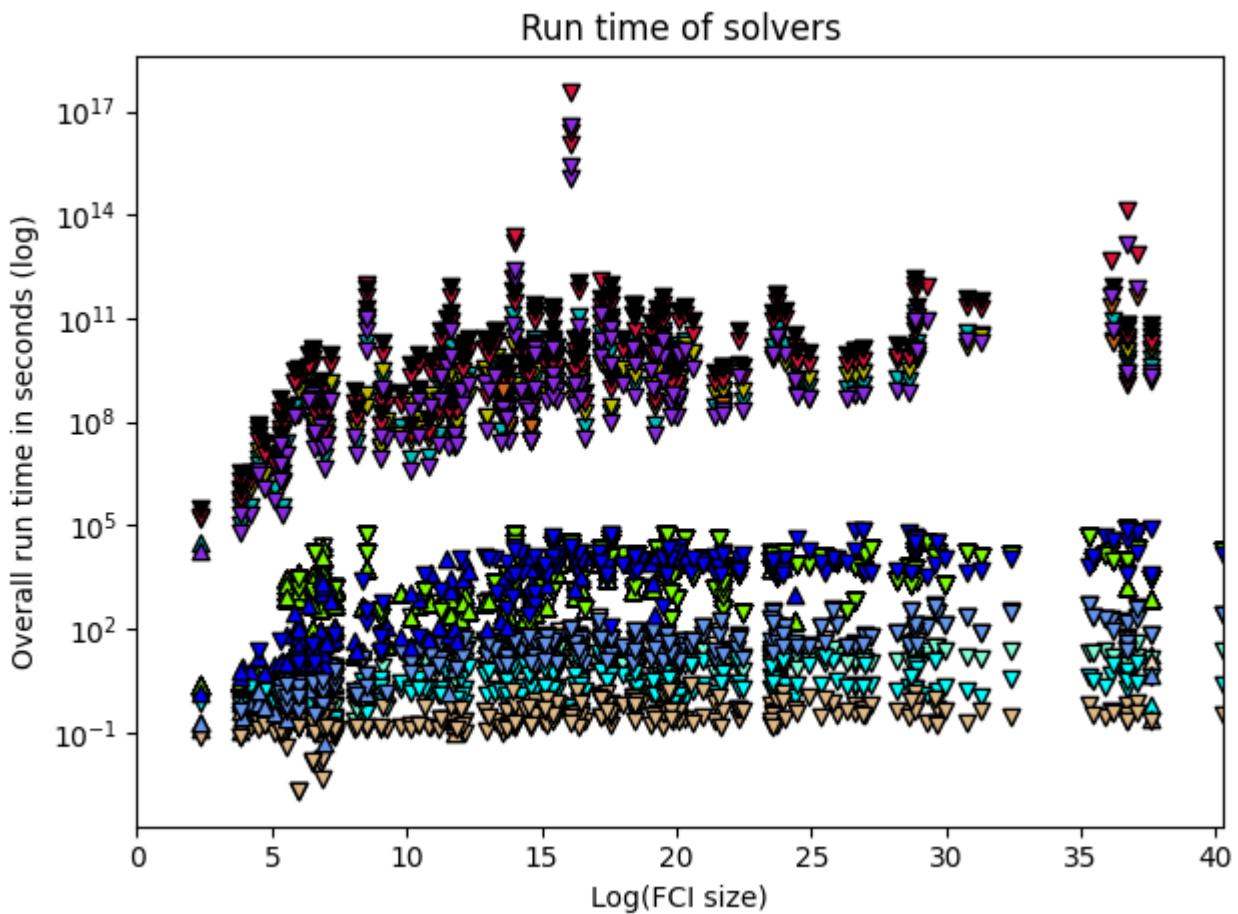
Run time of Classical (red) vs Quantum (blue) solvers



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



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.

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

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

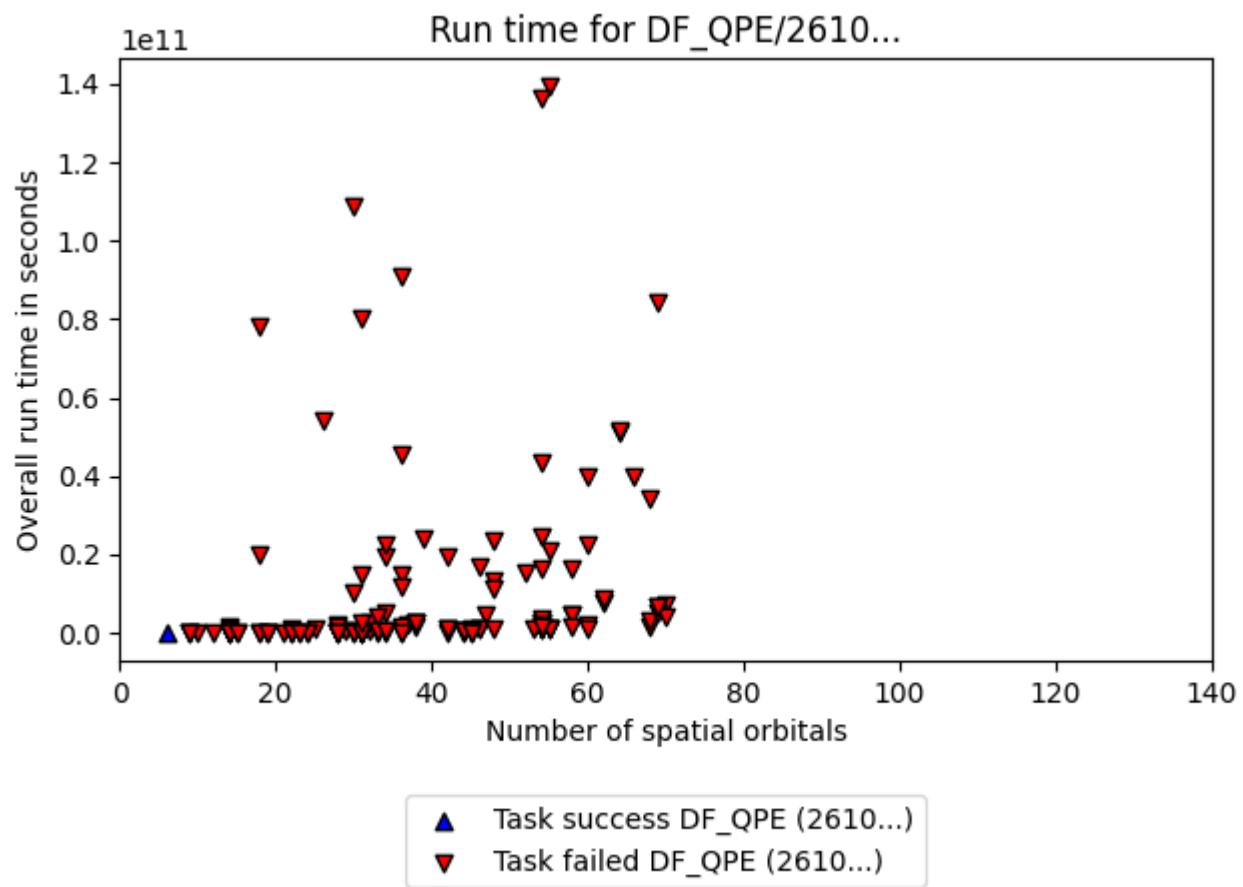
solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

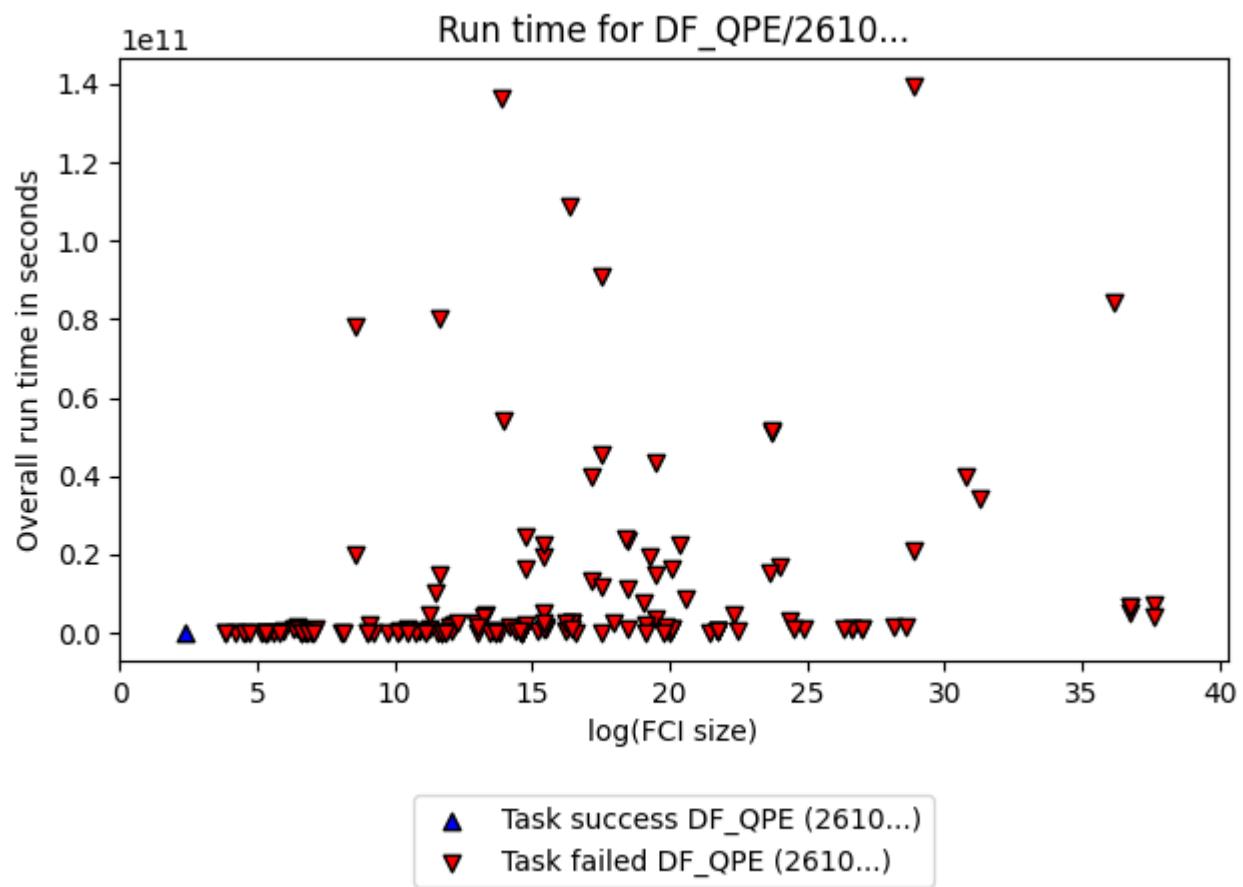
algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to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

software_details:[{'software_name': 'pyLIQTR', 'software_version': '1.3.4'}, {'software_name': 'qb-gsee-benchmark', 'software_version': '0.1.0a2.dev193+g879c00d'}, {'software_name': 'Python',

```
'software_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]',  
{'software_name': 'qualtran', 'software_version': '0.4.0'}]  
  
quantum_hardware_details: {'quantum_hardware_description': 'Ultra-  
optimistic hardware model based on the superconducting architecture  
described in https://arxiv.org/abs/2011.03494.',  
'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate':  
0.0001, 'cycle_time_microseconds': 0.1, 'parallelize_shots': False}}  
  
logical_resource_estimate_solution_uuid: 0be09ef6-6f34-4b70-  
a7e7-580d1c539c7c  
  
logical_resource_estimate_solver_uuid: f2d73e1f-3058-43c4-a634-  
b6c267c84ff1  
  
performance_metrics_uuid: 0a8978eb-4f5d-4980-a461-41c3658e0bf7  
  
creation_timestamp: 2025-02-19T18:26:13.854054+00:00  
  
number_of_problem_instances: 88  
  
number_of_problem_instances_attempted: 22  
  
number_of_problem_instances_solved: 0  
  
number_of_tasks: 280  
  
number_of_tasks_attempted: 154  
  
number_of_tasks_solved: 1  
  
number_of_tasks_solved_within_run_time_limit: 1  
  
number_of_tasks_solved_within_accuracy_threshold: 154  
  
max_run_time_of_attempted_tasks: 139406856747.7868  
  
sum_of_run_time_of_attempted_tasks: 1565254226637.0498  
  
solvability_ratio: None  
  
f1_score: None  
  
ml_metrics_calculator_version: 1  
  
comment: All labels were either all True or all False and we cannot create  
an ML model with only one class.
```



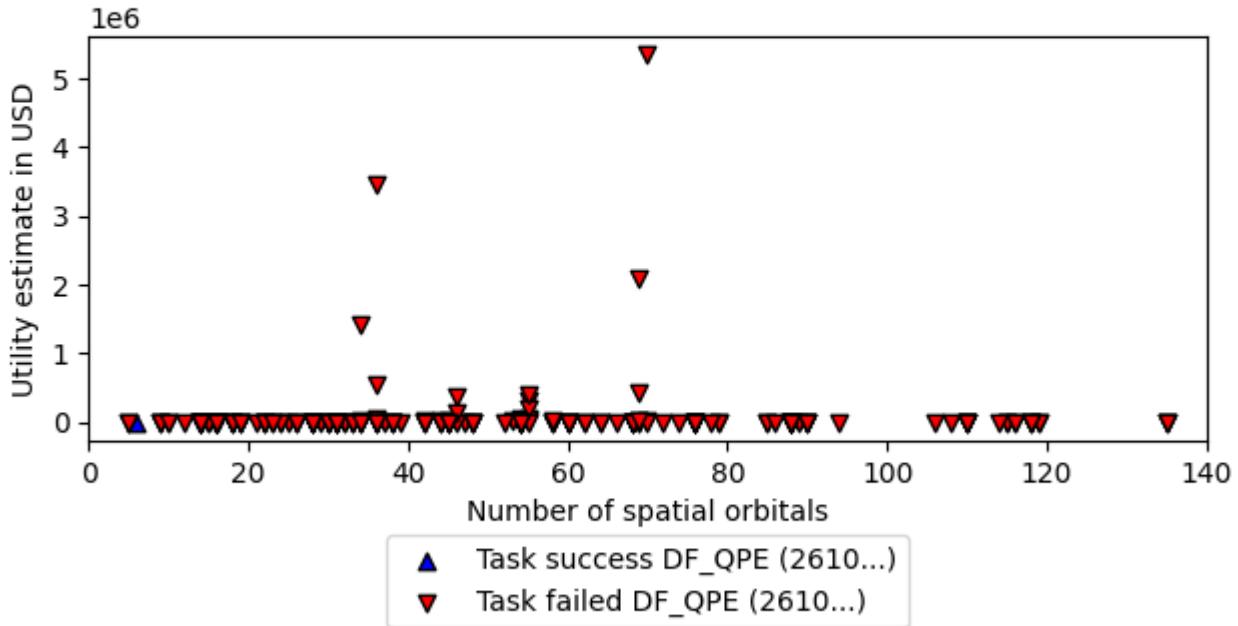
Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/2610...

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



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

solver uuid:2dde727e-a881-44fa-aabf-bba6248e4baf

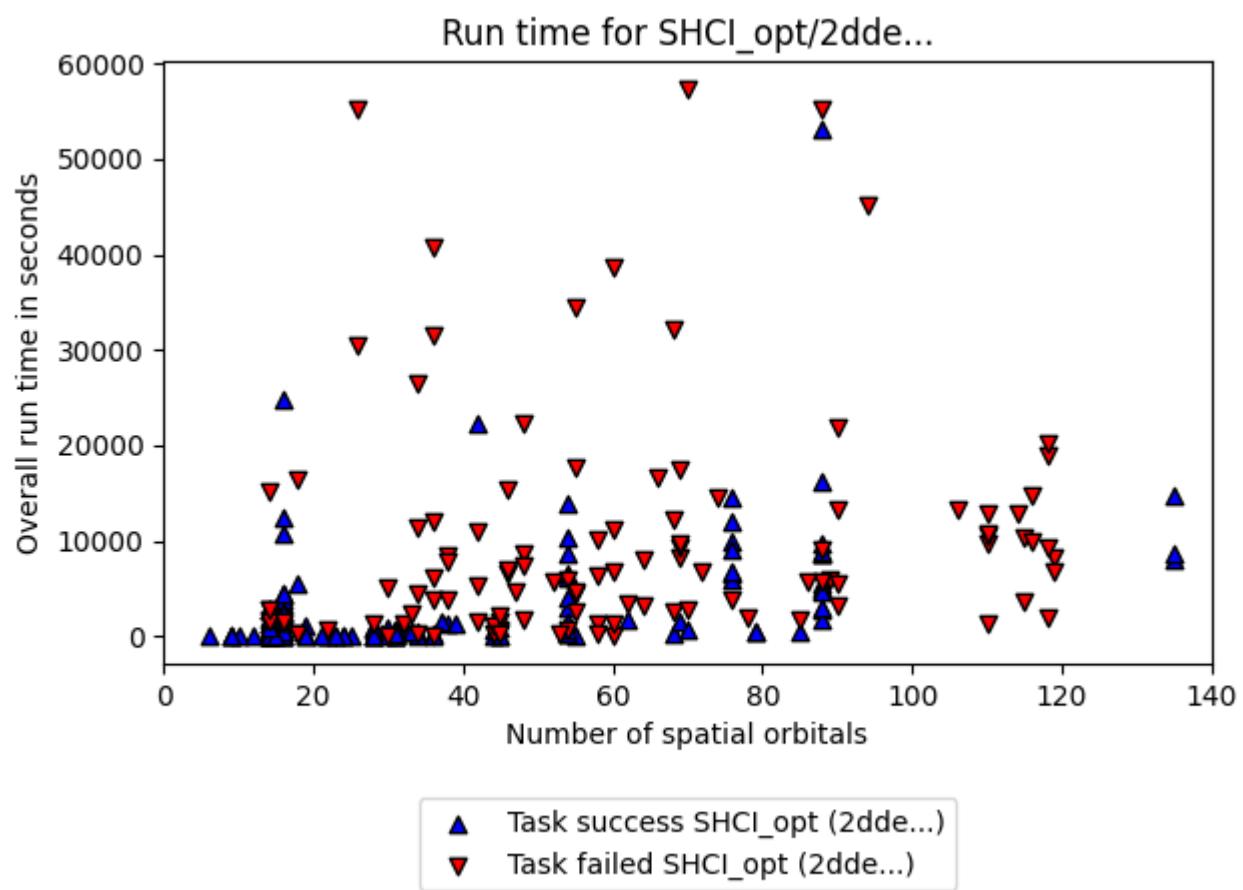
solver short name:SHCI opt

compute hardware type:classical computer

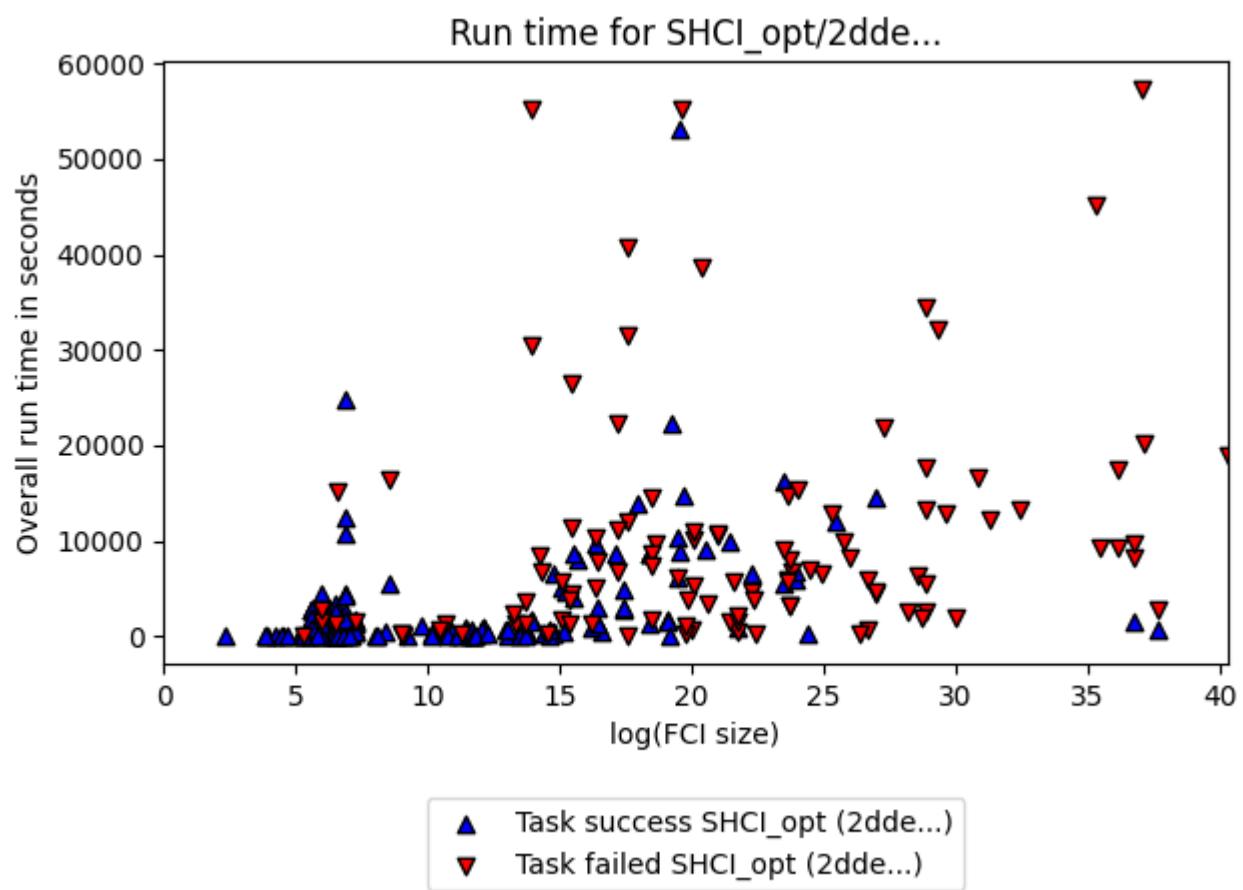
```
classical_hardware_details: {'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
```

algorithm details:SHCI with optimized orbitals followed by SHCI+PT

software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: c2d64bfd-66fc-43e0-a278-d4c0ed5be58a
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 80
number_of_problem_instances_solved: 33
number_of_tasks: 280
number_of_tasks_attempted: 265
number_of_tasks_solved: 153
number_of_tasks_solved_within_run_time_limit: 265
number_of_tasks_solved_within_accuracy_threshold: 153
max_run_time_of_attempted_tasks: 57334.2
sum_of_run_time_of_attempted_tasks: 1553340.6179999998
solvability_ratio: 1.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.6923076923076923, 0.9731543624161074]
ml_metrics_calculator_version: 1



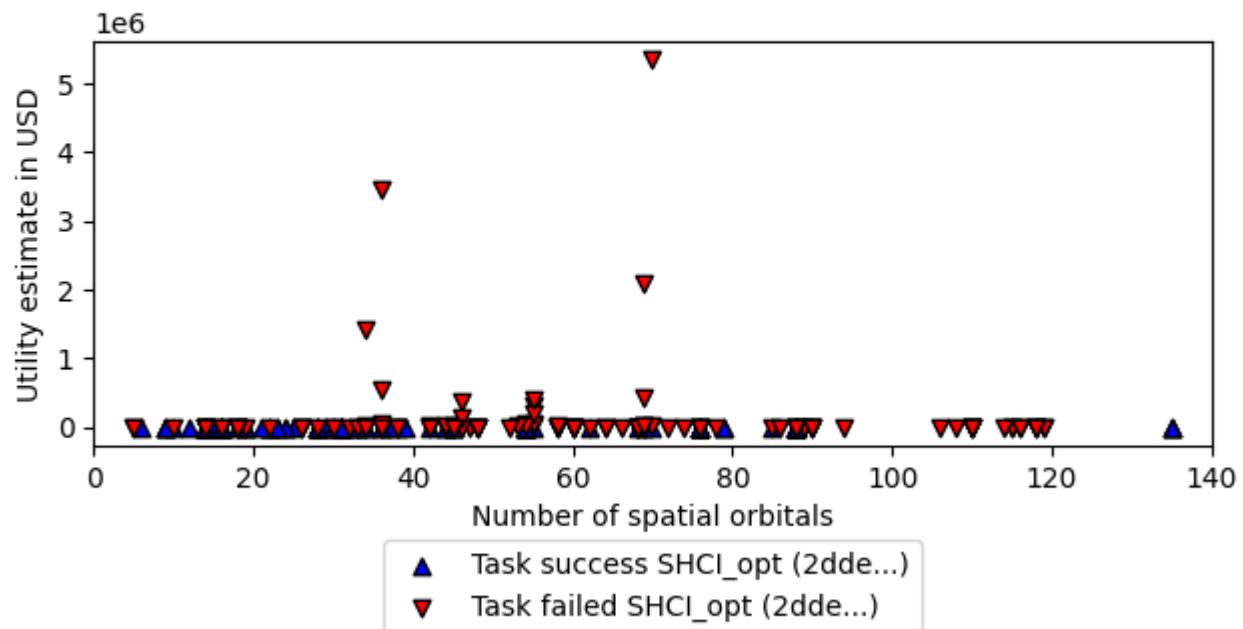
Note: plot only contains attempted tasks.



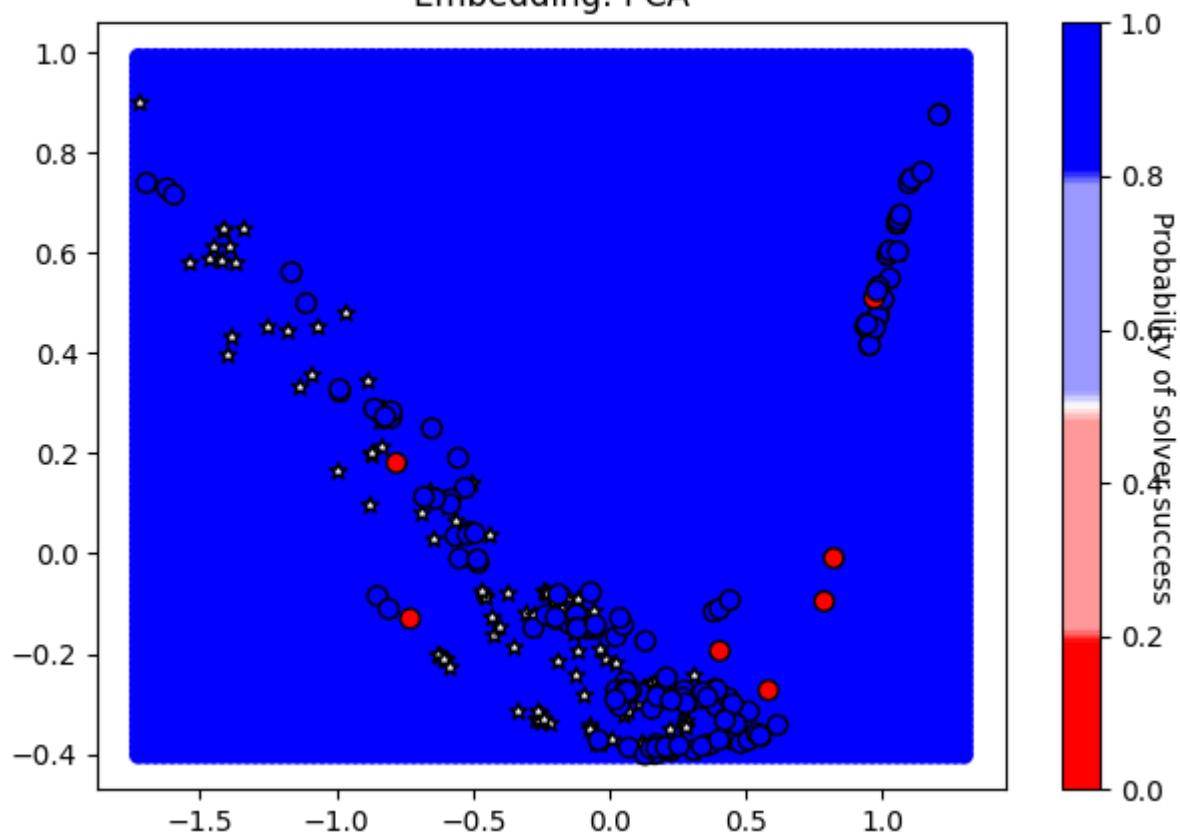
Note: plot only contains attempted tasks.

Utility capture from SHCI_opt/2dde...

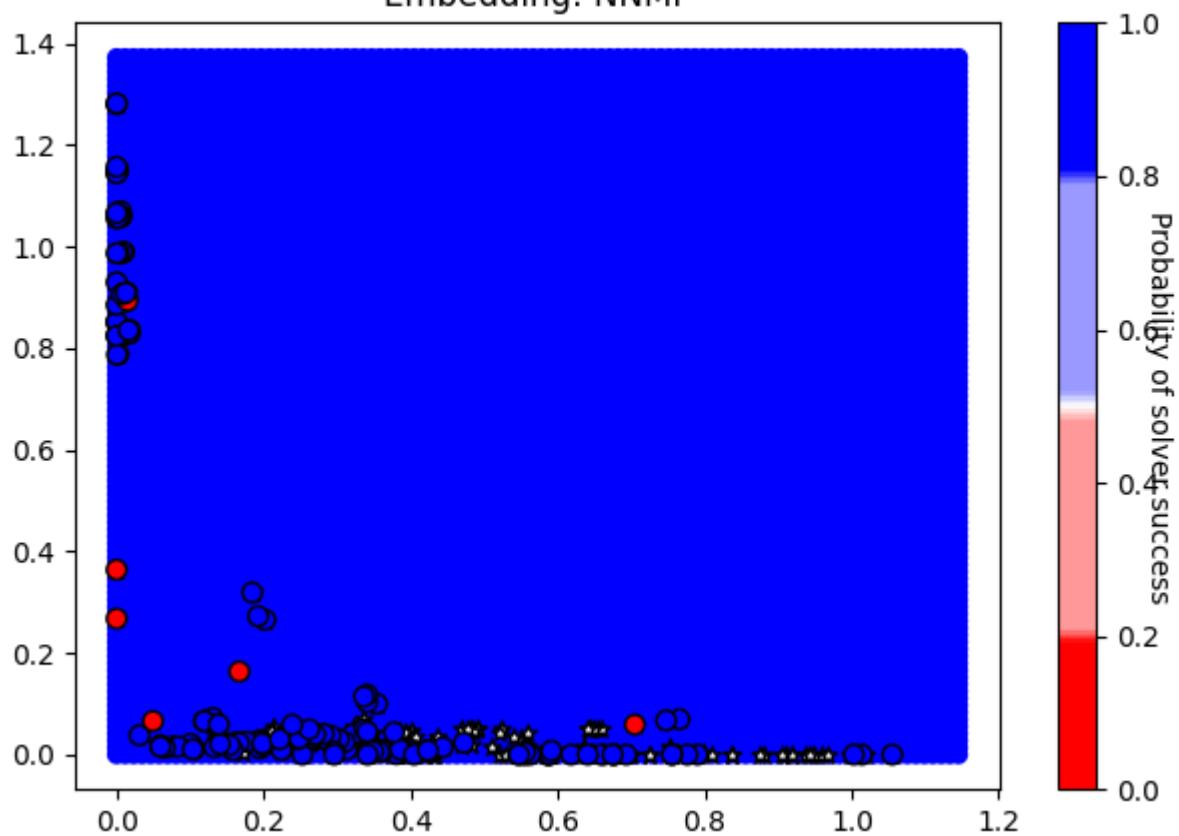
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



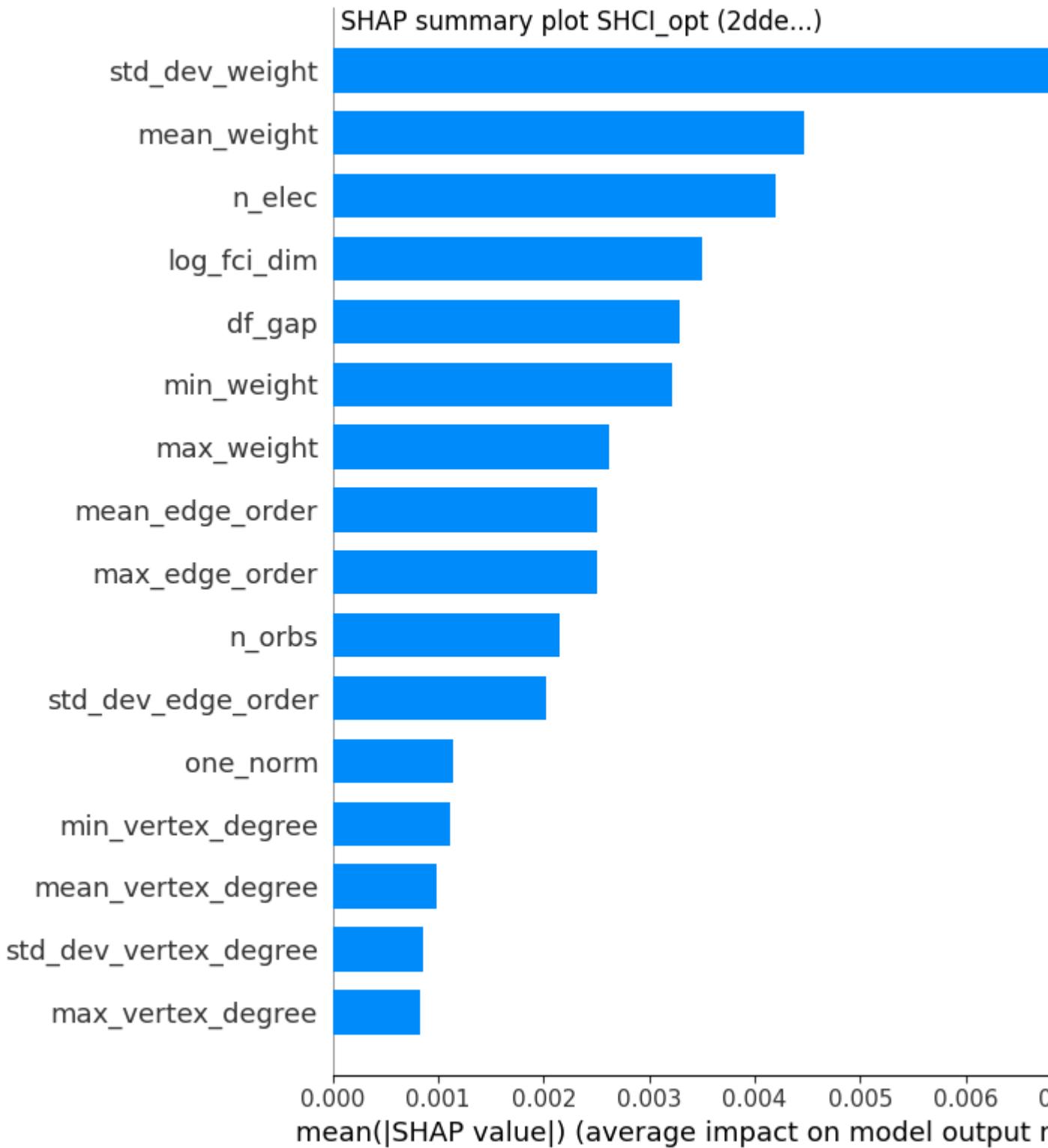
Solver SHCI_opt (2dde...)
Embedding: PCA



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



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



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

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

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

software_details:[{'software_name': 'pyLIQTR', 'software_version': '1.3.4'}, {'software_name': 'qb-gsee-benchmark', 'software_version': '0.1.0a2.dev193+g879c00d'}, {'software_name': 'Python', 'software_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]'}, {'software_name': 'qualtran', 'software_version': '0.4.0'}]

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

logical_resource_estimate_solution_uuid:
56513b7a-4644-4a2c-9467-46a2ba6ec2a8

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

performance_metrics_uuid: 72a0df89-1863-4a95-87d8-e5ac46e4fb6d

creation_timestamp: 2025-02-19T18:26:13.854054+00:00

number_of_problem_instances: 88

number_of_problem_instances_attempted: 22

number_of_problem_instances_solved: 0

number_of_tasks: 280

number_of_tasks_attempted: 154

number_of_tasks_solved: 0

number_of_tasks_solved_within_run_time_limit: 0

number_of_tasks_solved_within_accuracy_threshold: 154

max_run_time_of_attempted_tasks: 28597112908.874496

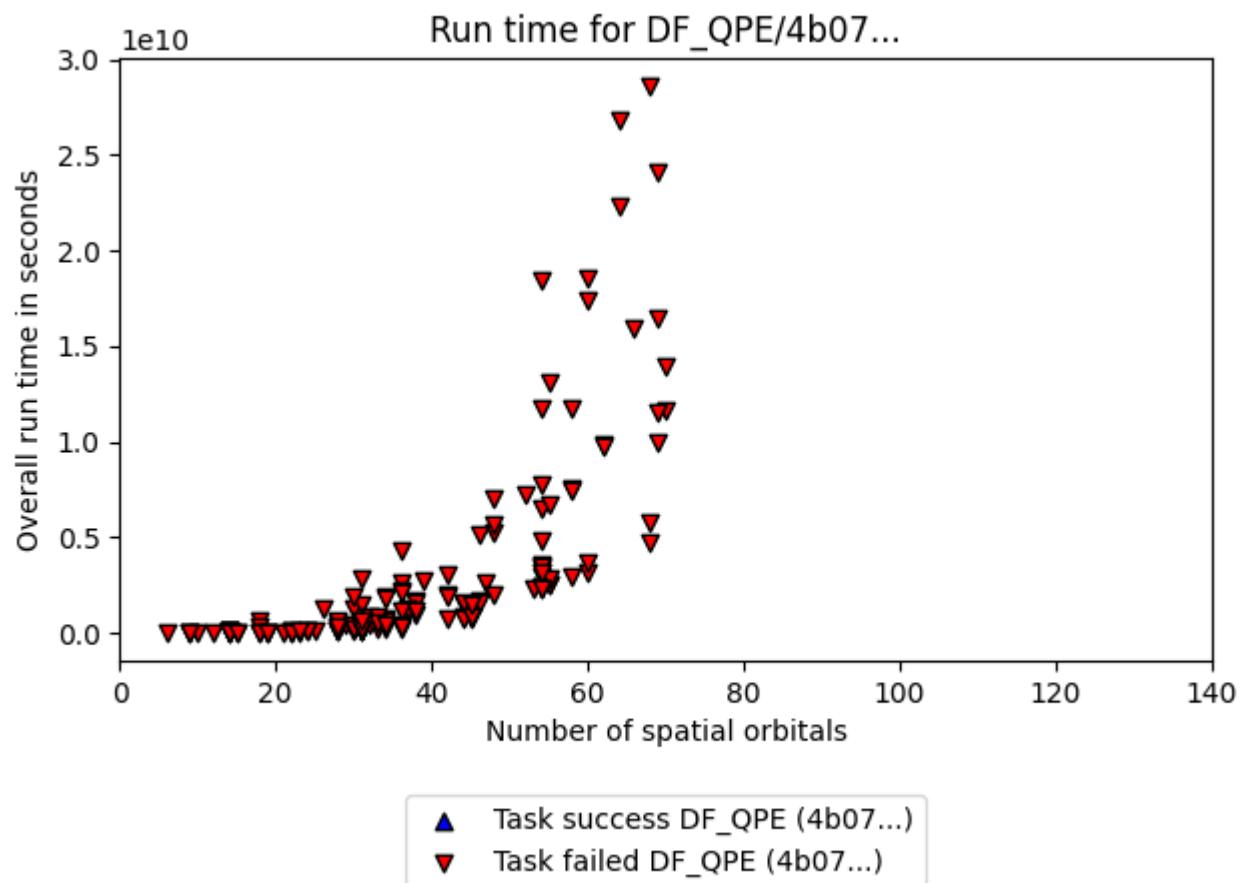
sum_of_run_time_of_attempted_tasks: 502121568076.6234

solvability_ratio: None

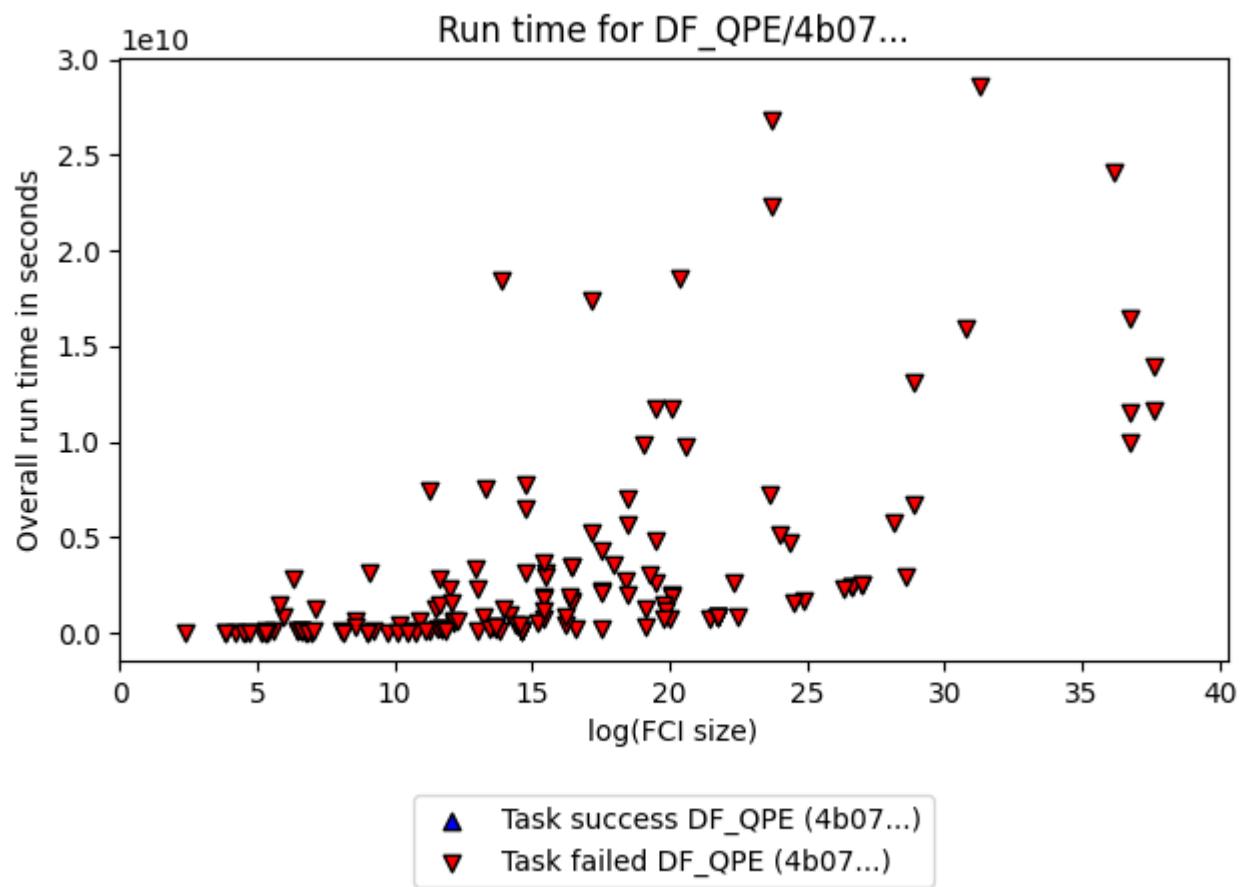
f1_score: None

ml_metrics_calculator_version: 1

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

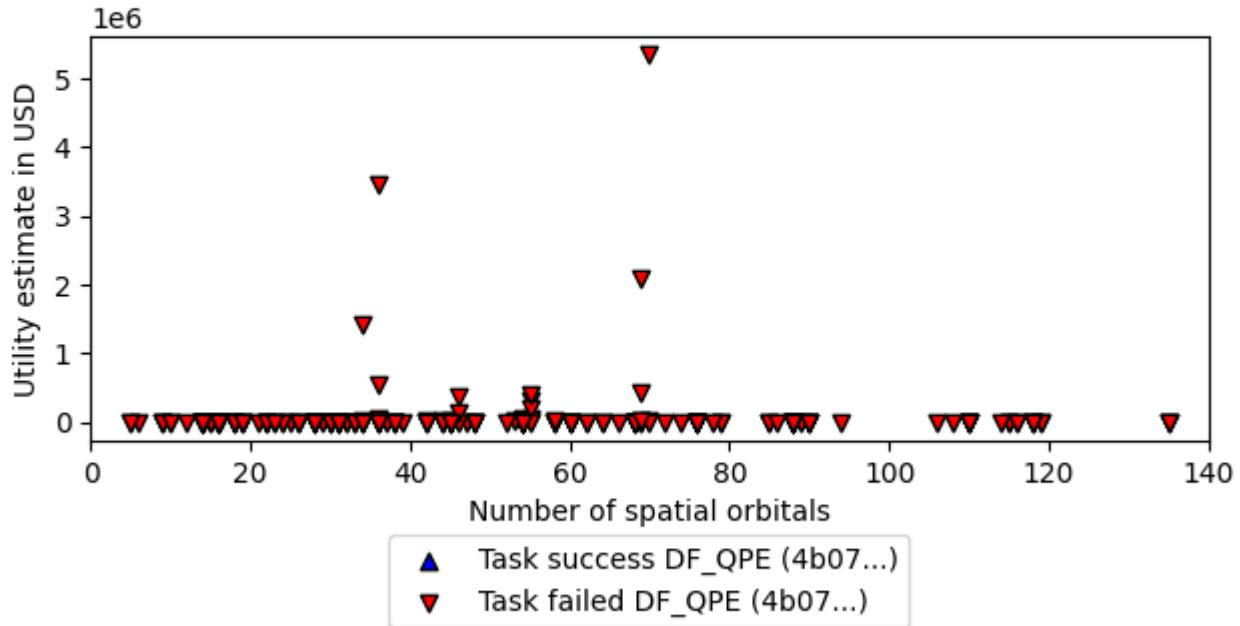


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/4b07...
 (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 SHCI_pt_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4

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

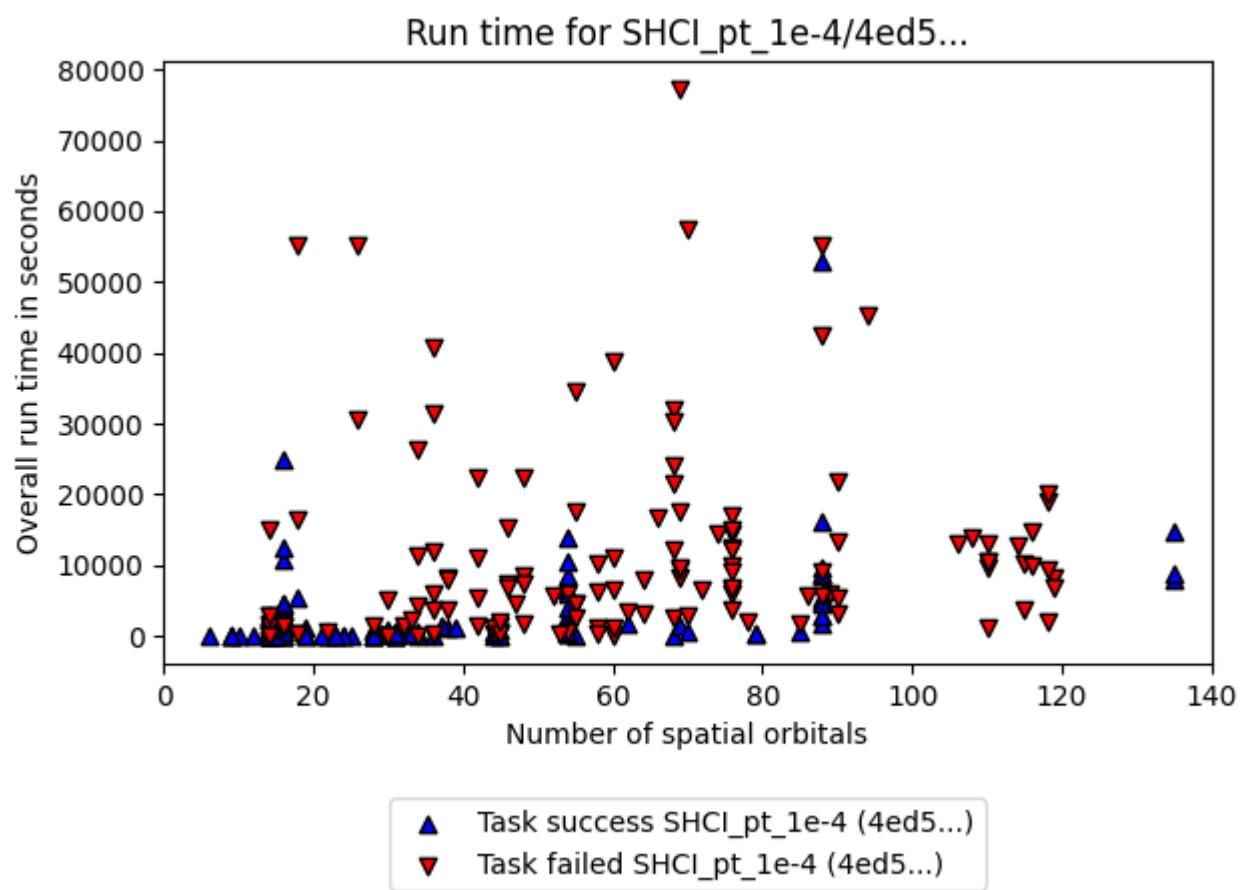
solver_short_name:SHCI_pt_1e-4

compute.hardware_type:classical_computer

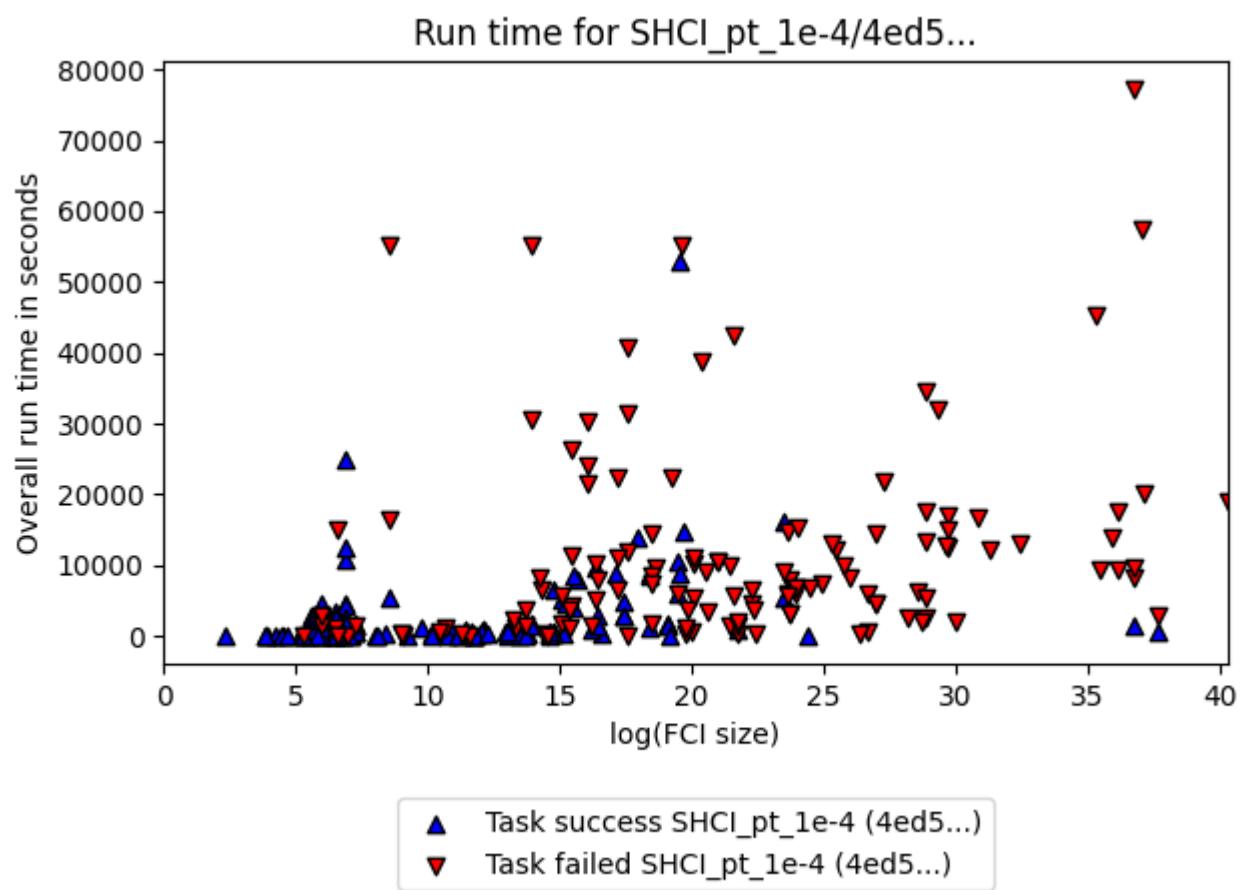
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}

algorithm_details:SHCI with eps_var 1e-4 + PT

software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: 940b2f10-5718-452b-8f0c-61d4b5faf1ea
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 22
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 140
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 140
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 1.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.6666666666666666, 0.9621993127147767]
ml_metrics_calculator_version: 1



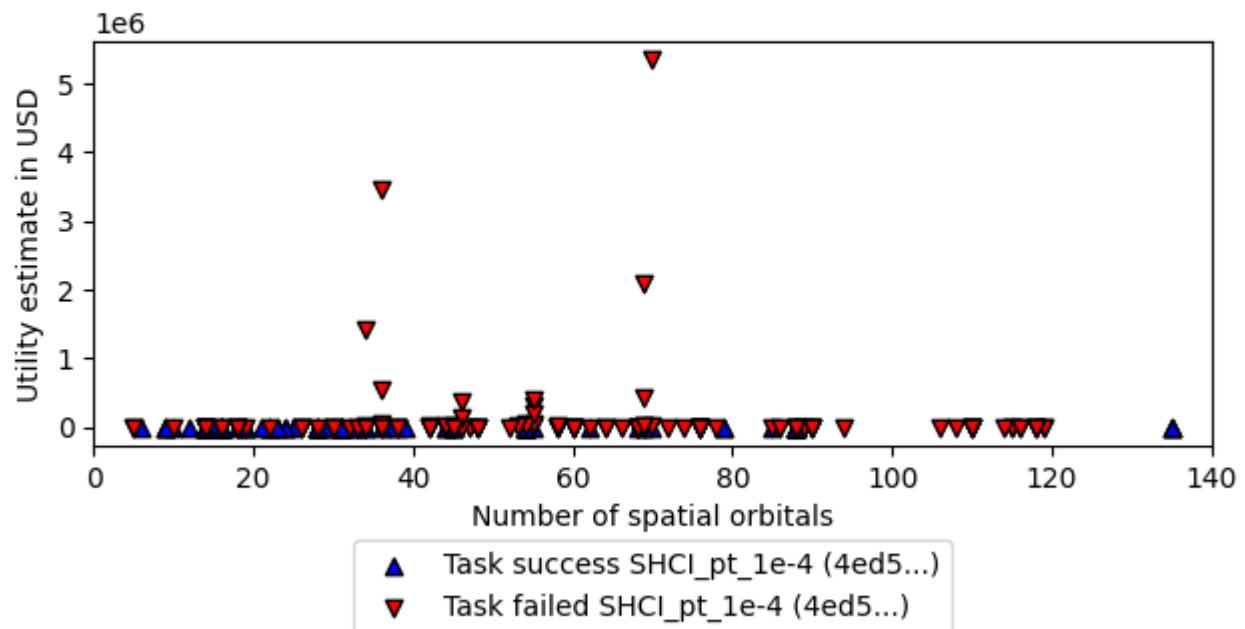
Note: plot only contains attempted tasks.



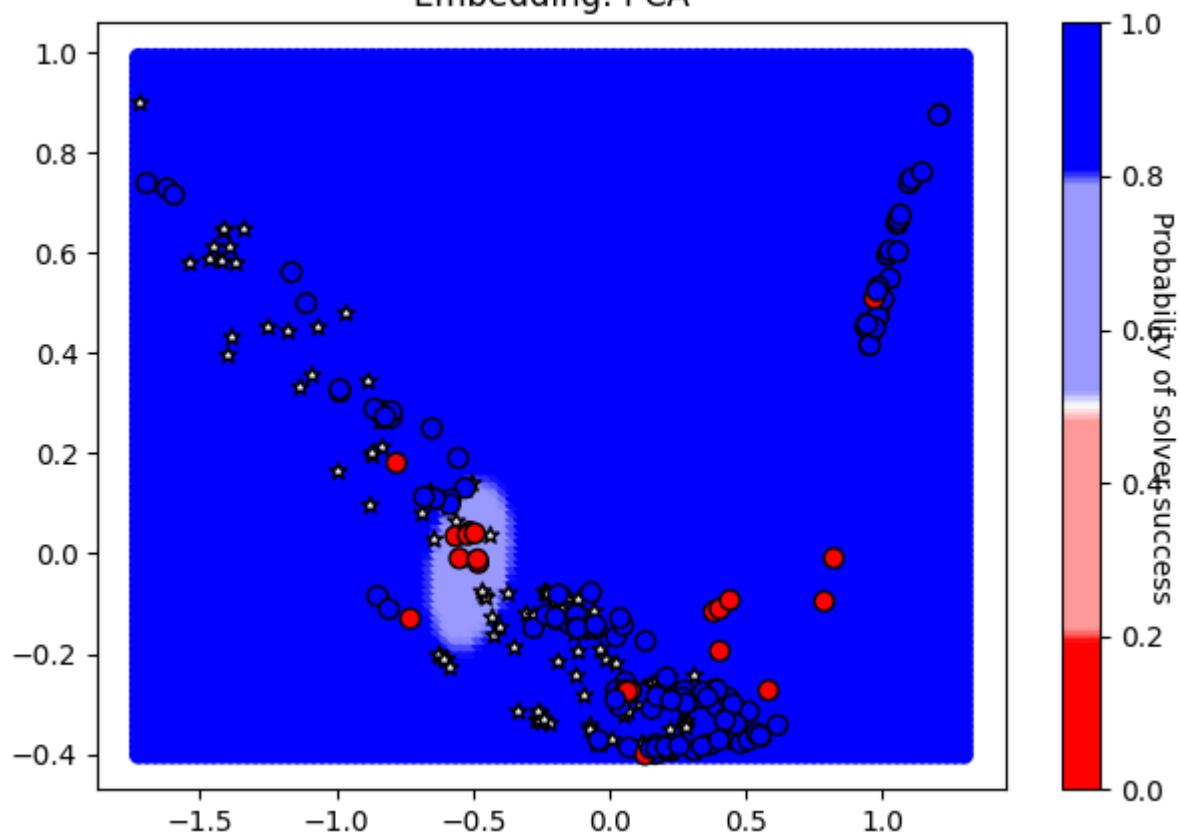
Note: plot only contains attempted tasks.

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

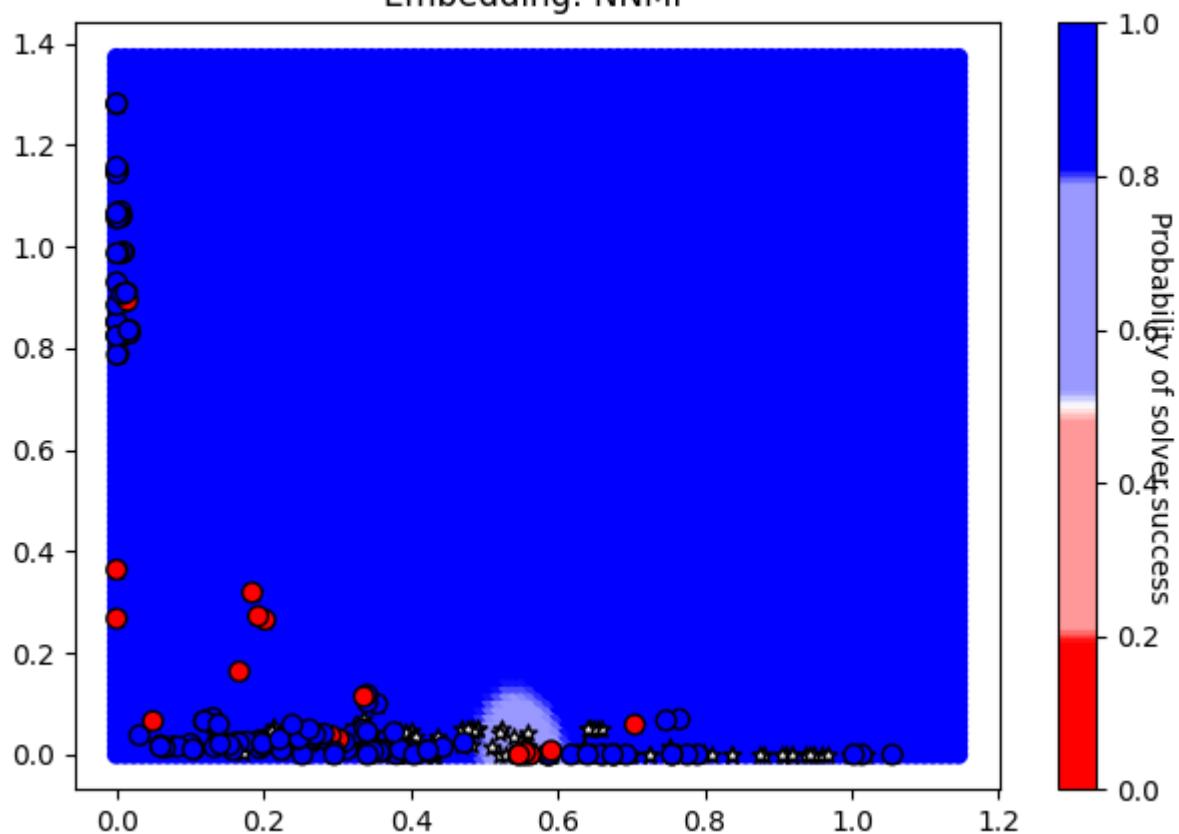
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



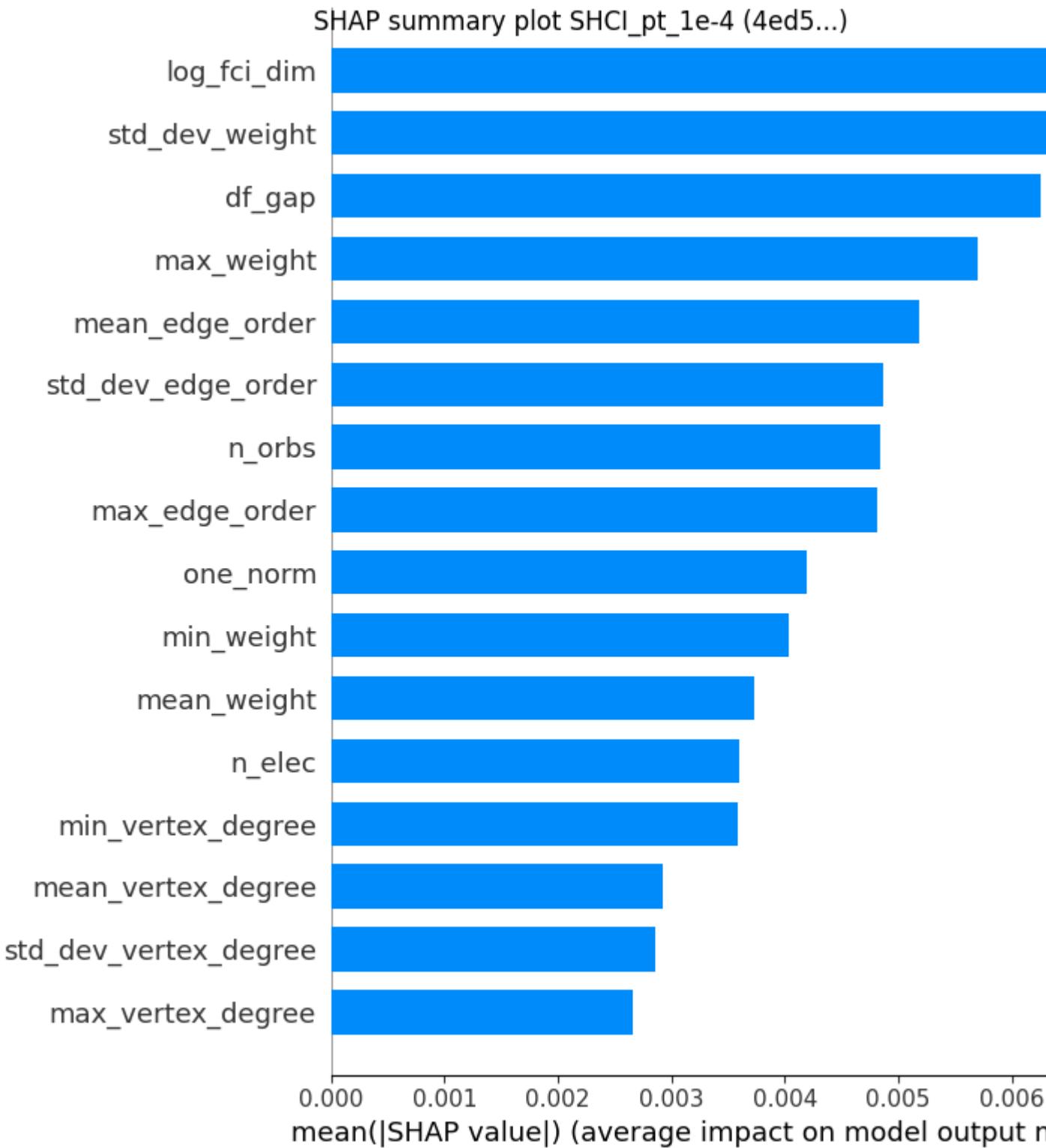
Solver SHCI_pt_1e-4 (4ed5...)
Embedding: PCA



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



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

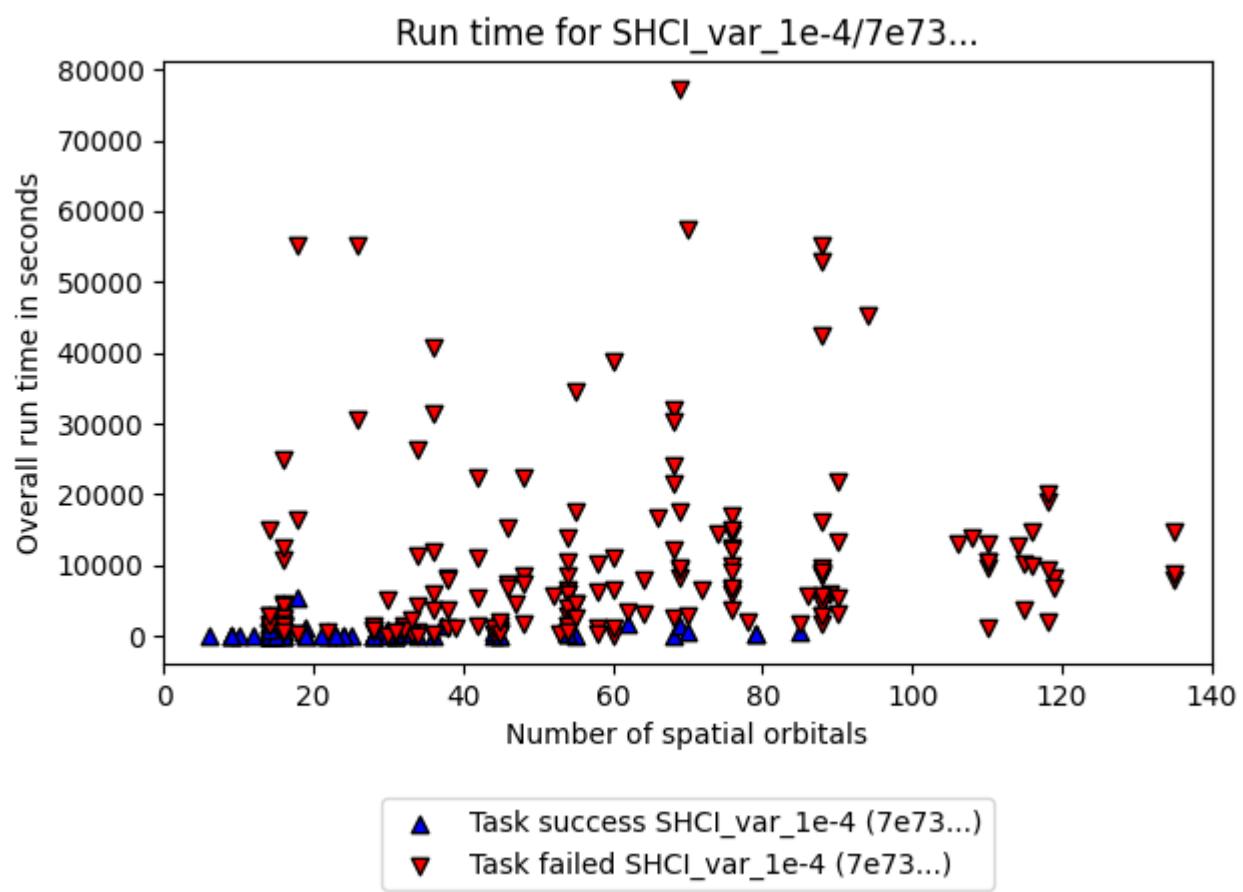


Solver SHCI_var_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54

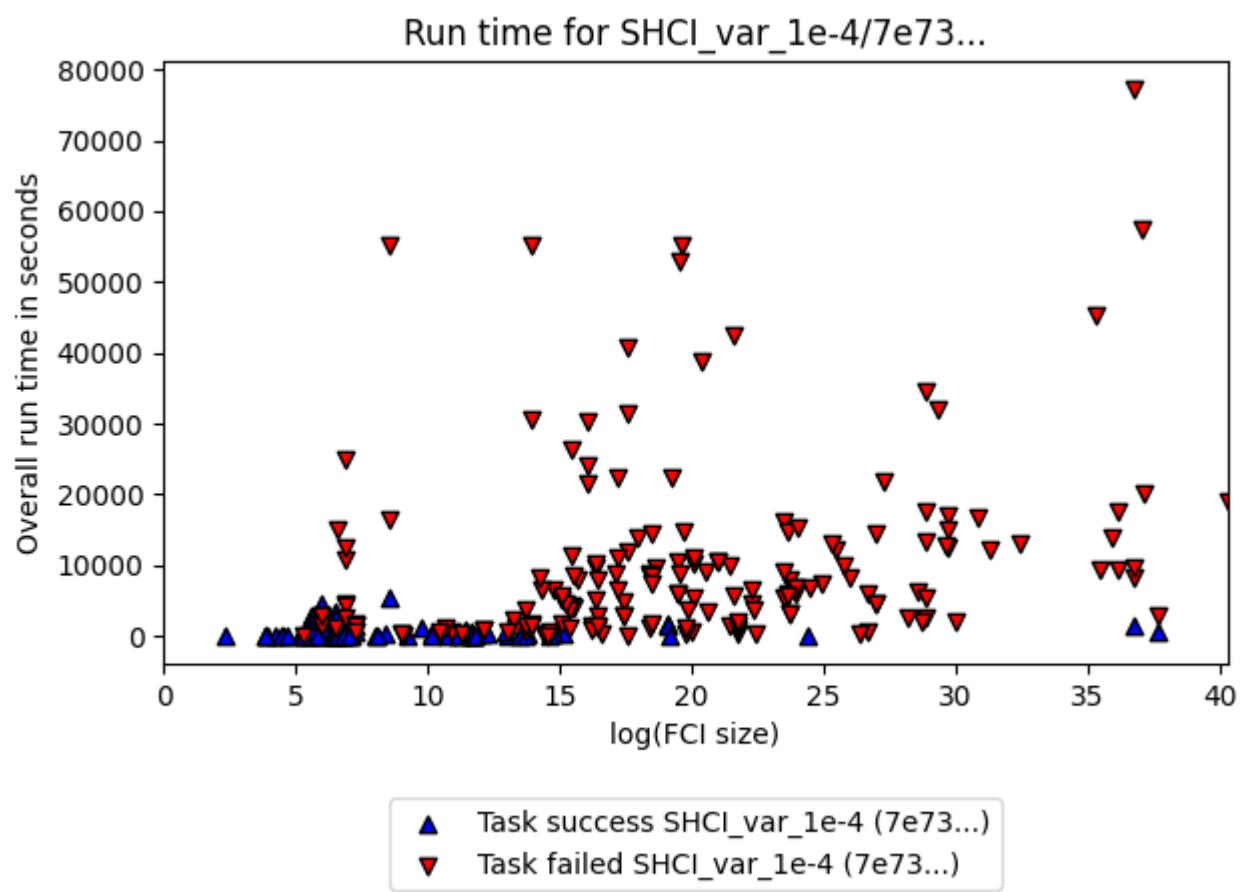
solver_uuid:7e730dfb-57ee-480b-a8a1-4b73f5f07c54

solver_short_name:SHCI_var_1e-4

compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 1e-4
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: 0de6d309-91f1-44e3-938c-0637a8e4247b
creation.timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 13
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 95
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 95
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 0.3758
comment: solvability ratio based on PCA embedding.
f1_score: [0.9558823529411765, 0.9680851063829787]
ml.metrics_calculator_version: 1



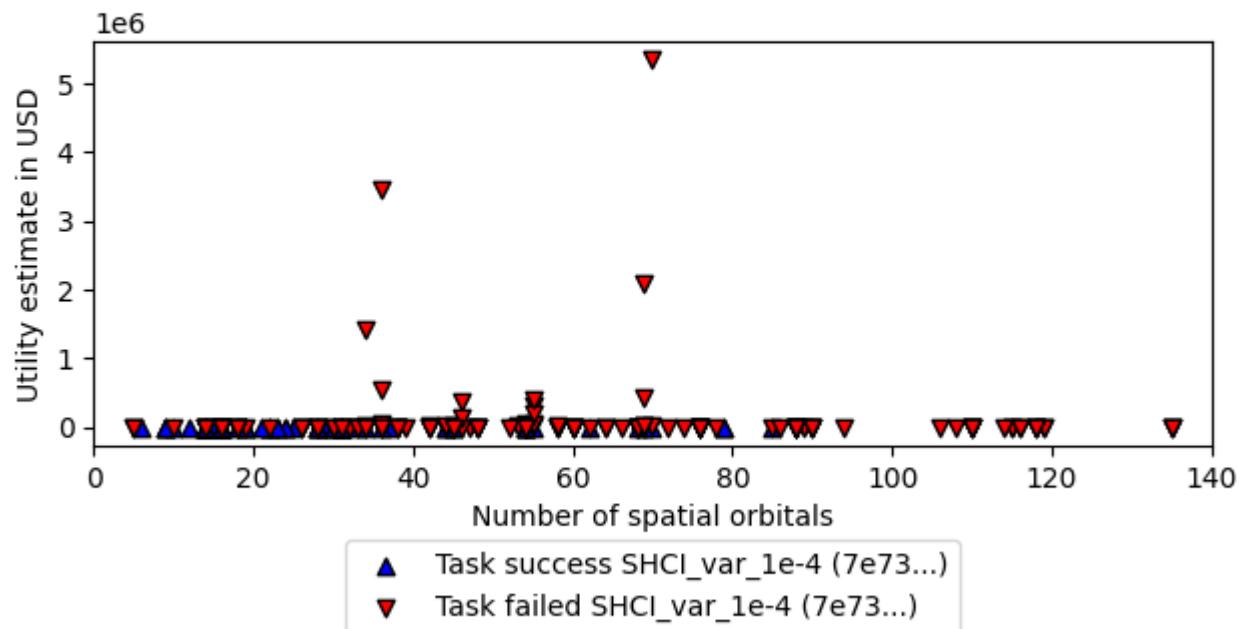
Note: plot only contains attempted tasks.



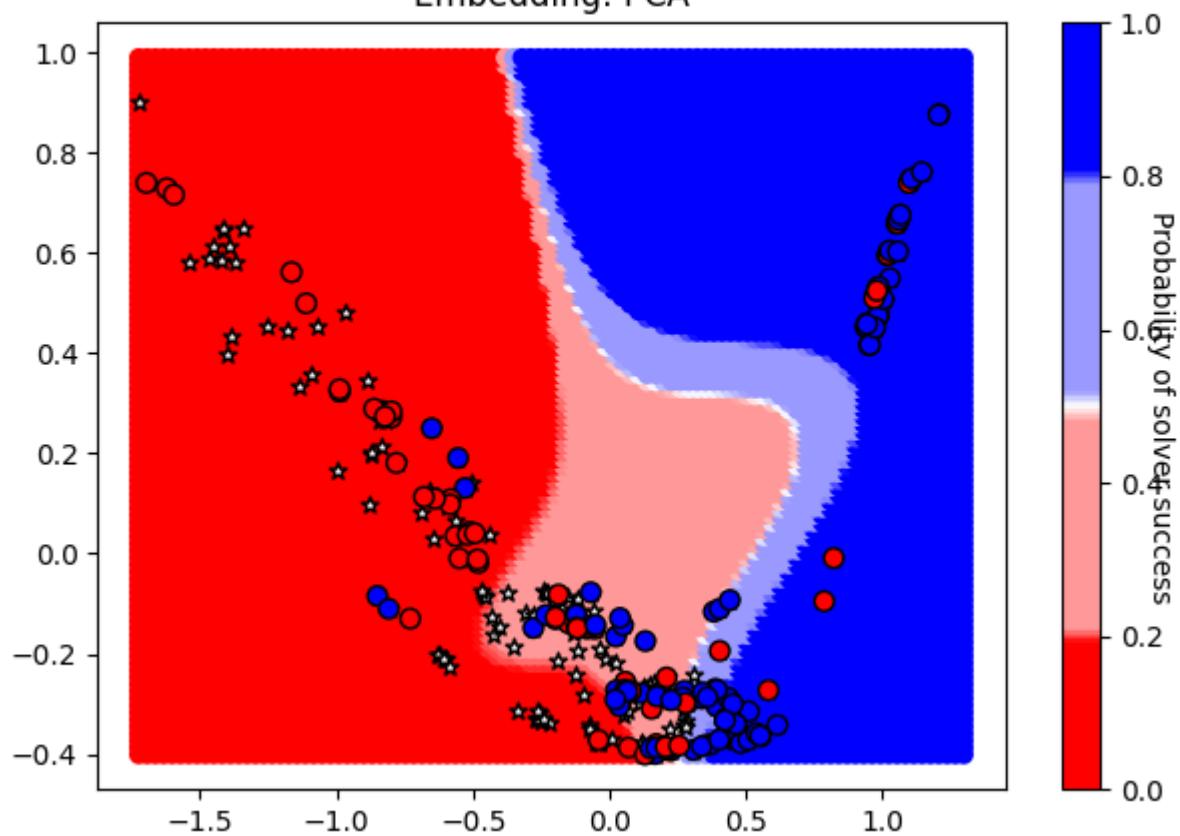
Note: plot only contains attempted tasks.

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

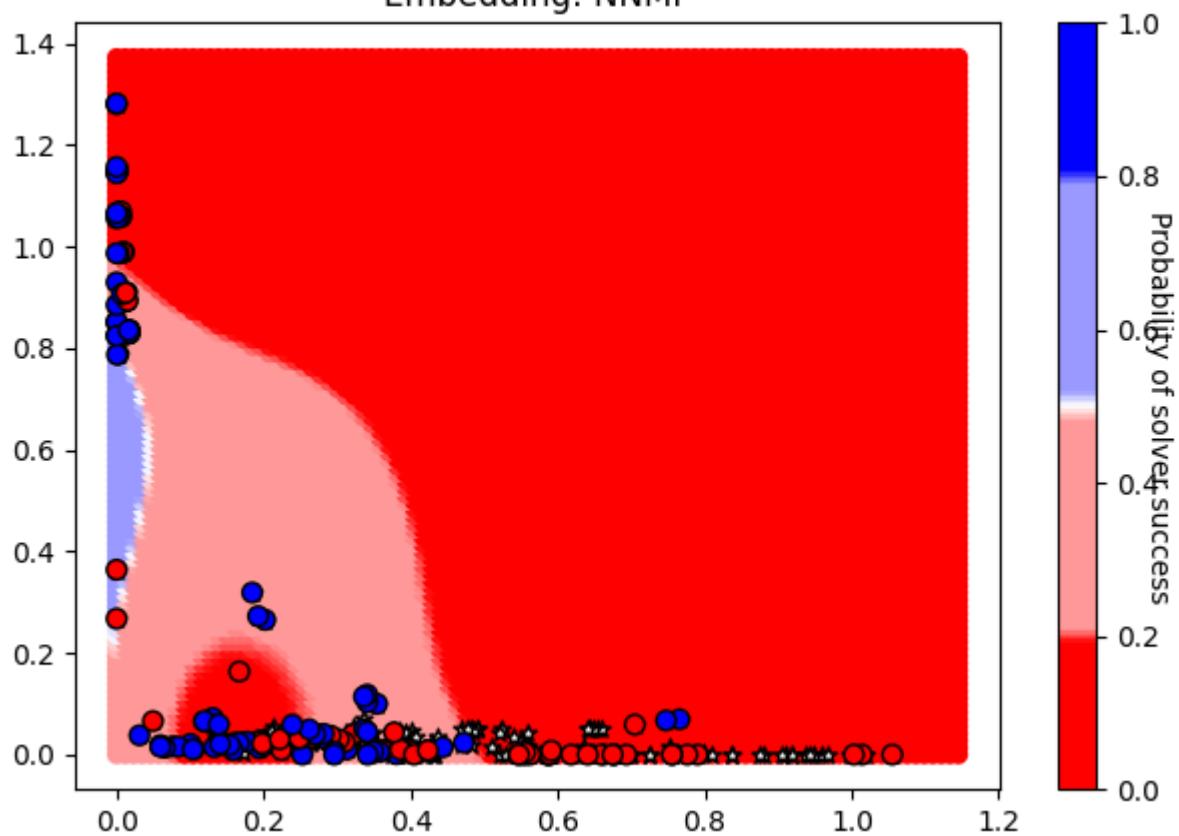
(captured: \$1.0e+02/1.5e+07, approximately 6.8e-04%)



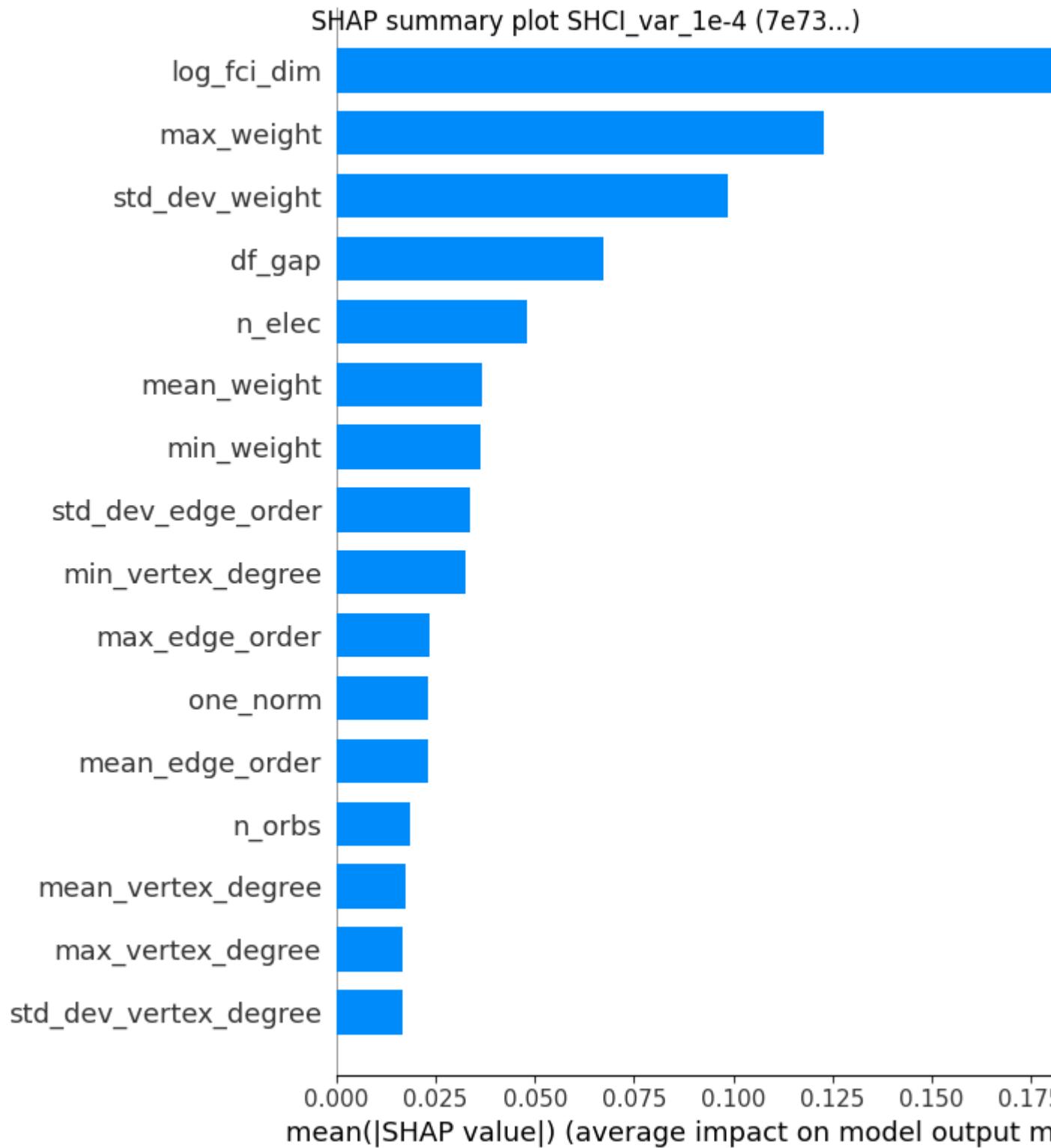
Solver SHCI_var_1e-4 (7e73...)
Embedding: PCA



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



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



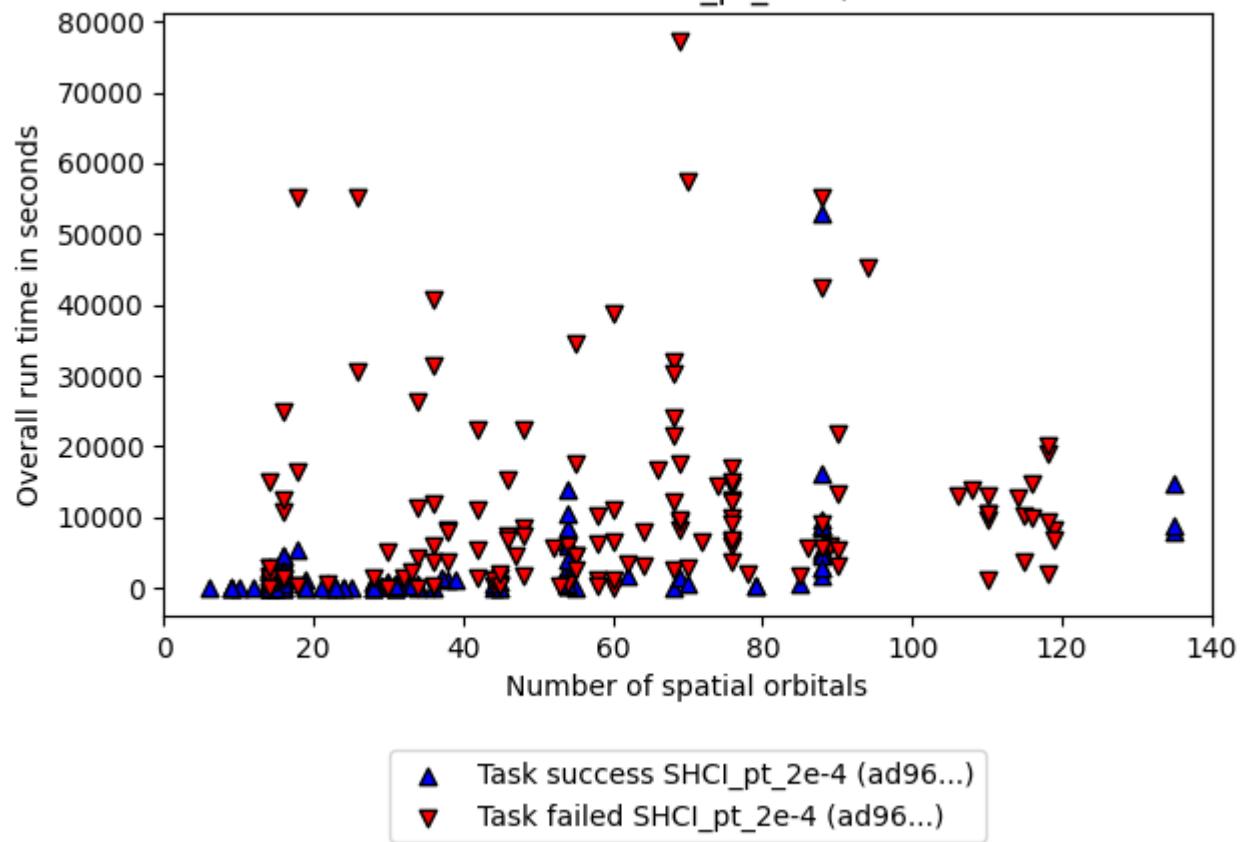
Solver SHCI_pt_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb

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

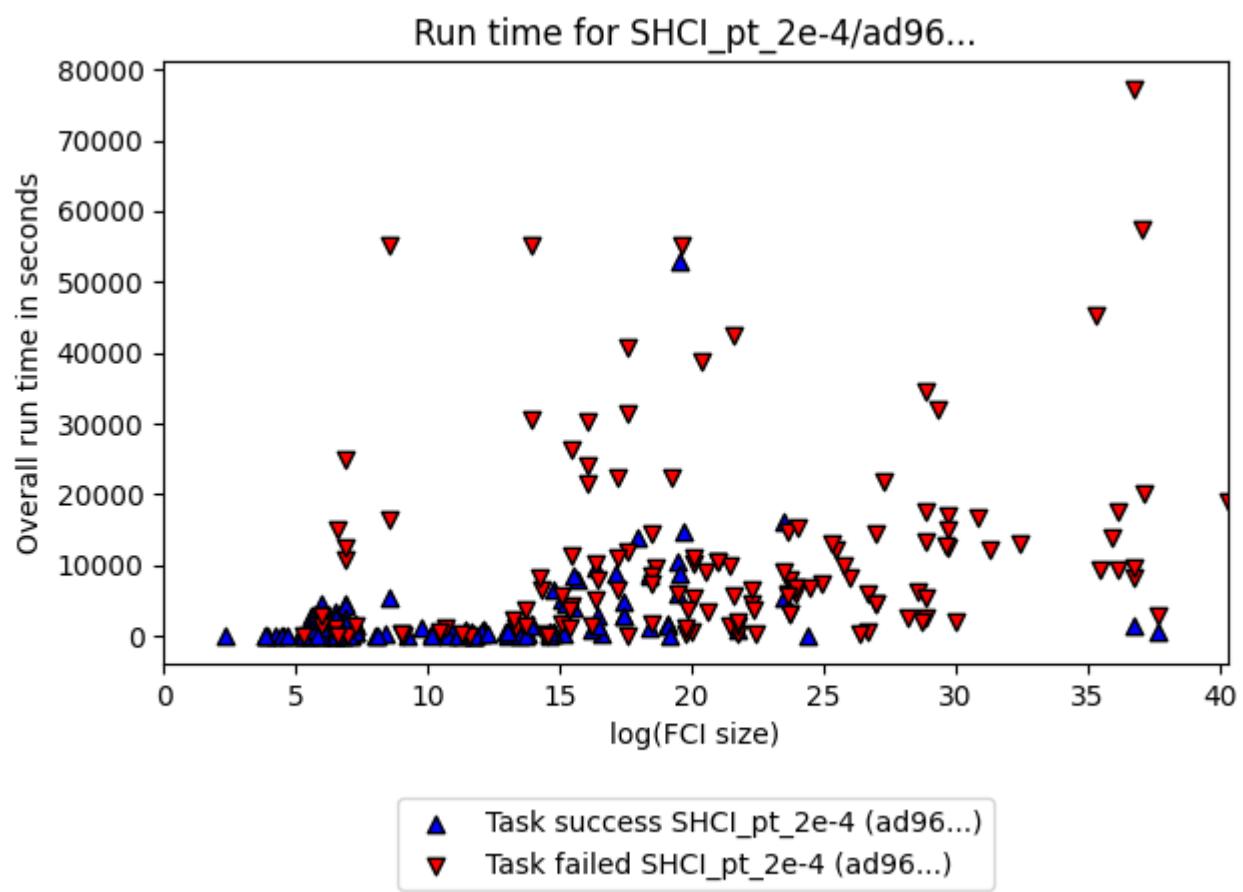
solver_short_name:SHCI_pt_2e-4

compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-4 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: f69a261a-fb4d-49bb-a2b6-9127710c71c4
creation.timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 22
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 137
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 137
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 1.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.7241379310344828, 0.9398496240601504]
ml.metrics_calculator_version: 1

Run time for SHCl_pt_2e-4/ad96...



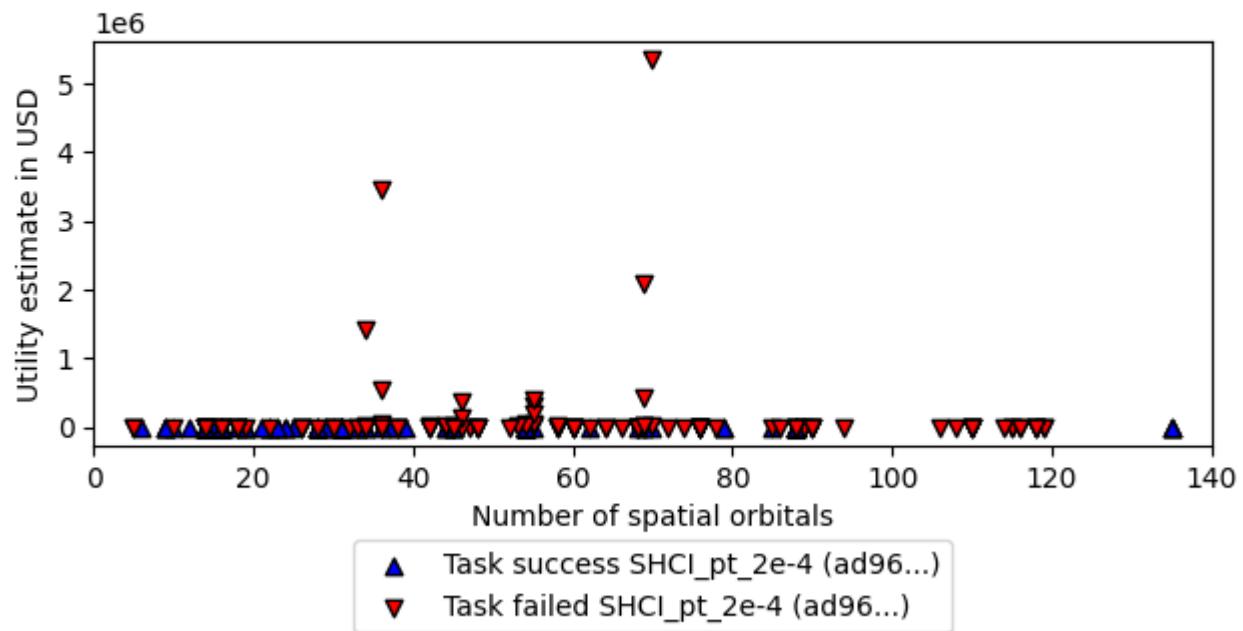
Note: plot only contains attempted tasks.



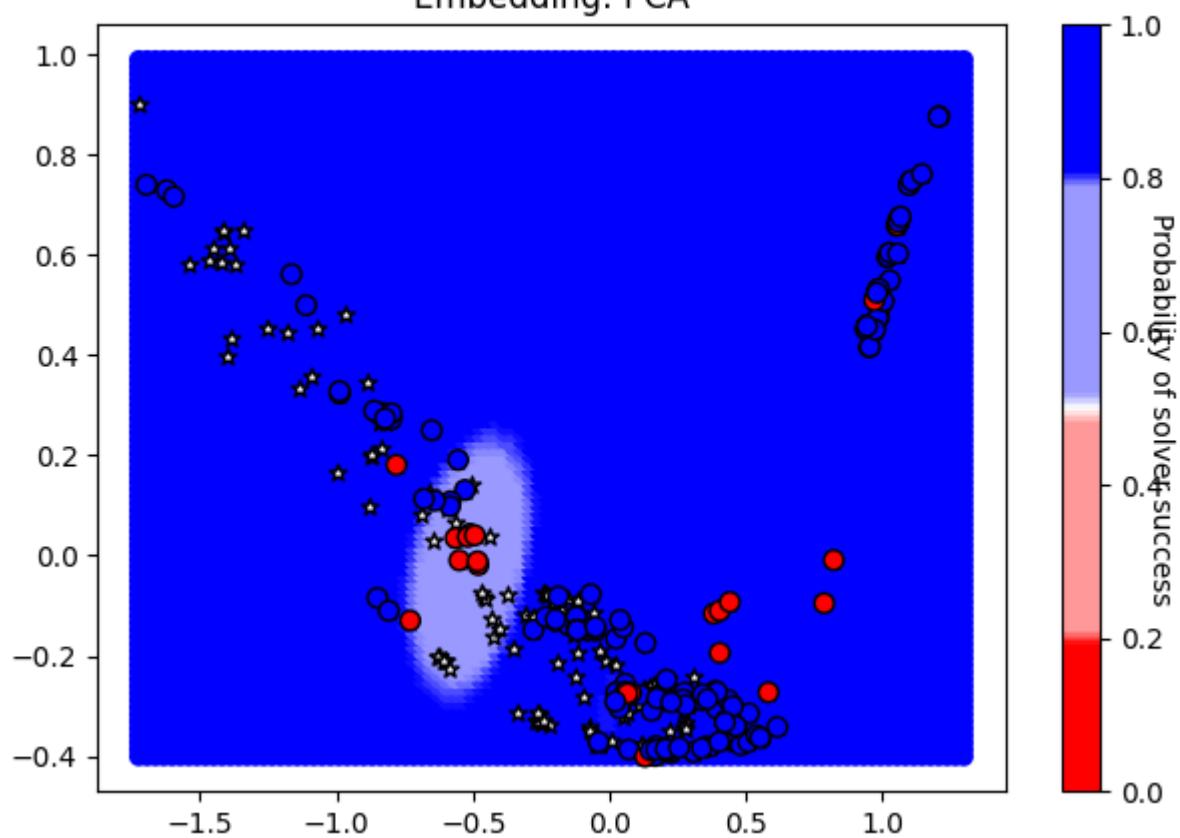
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-4/ad96...

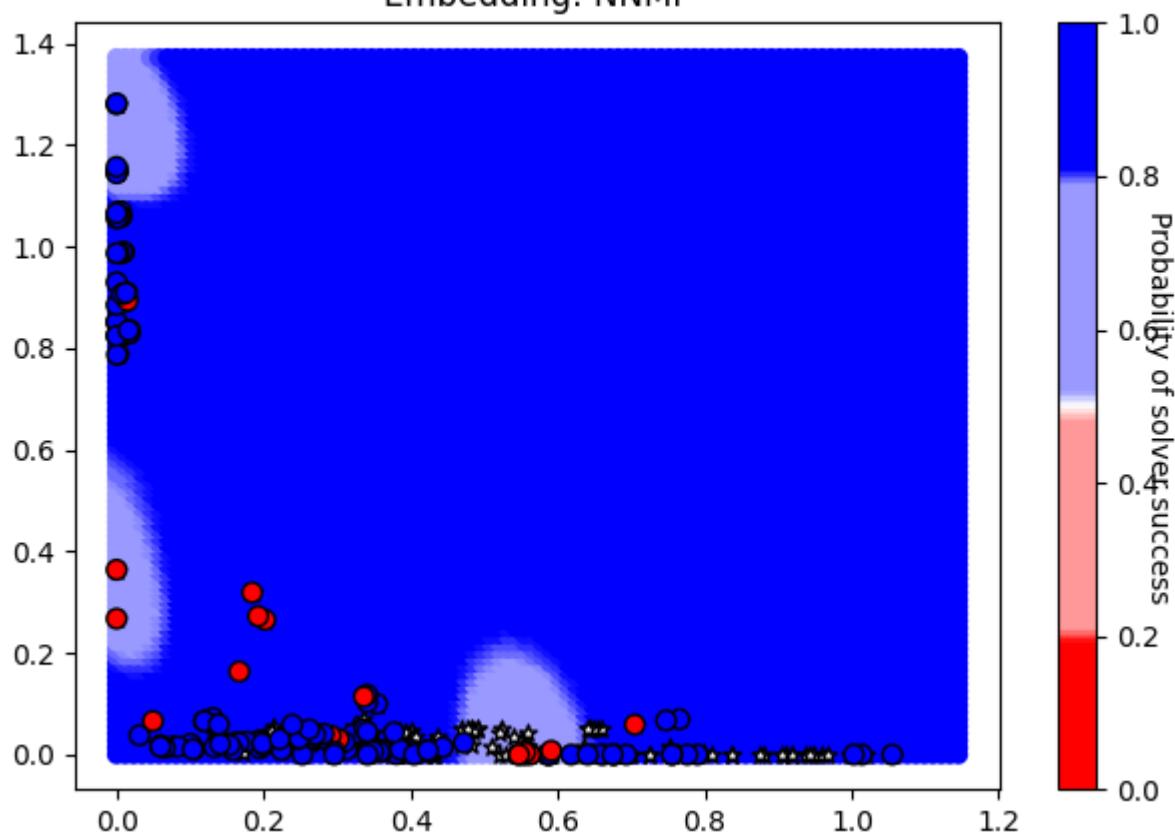
(captured: \$4.9e+02/1.5e+07, approximately 3.3e-03%)



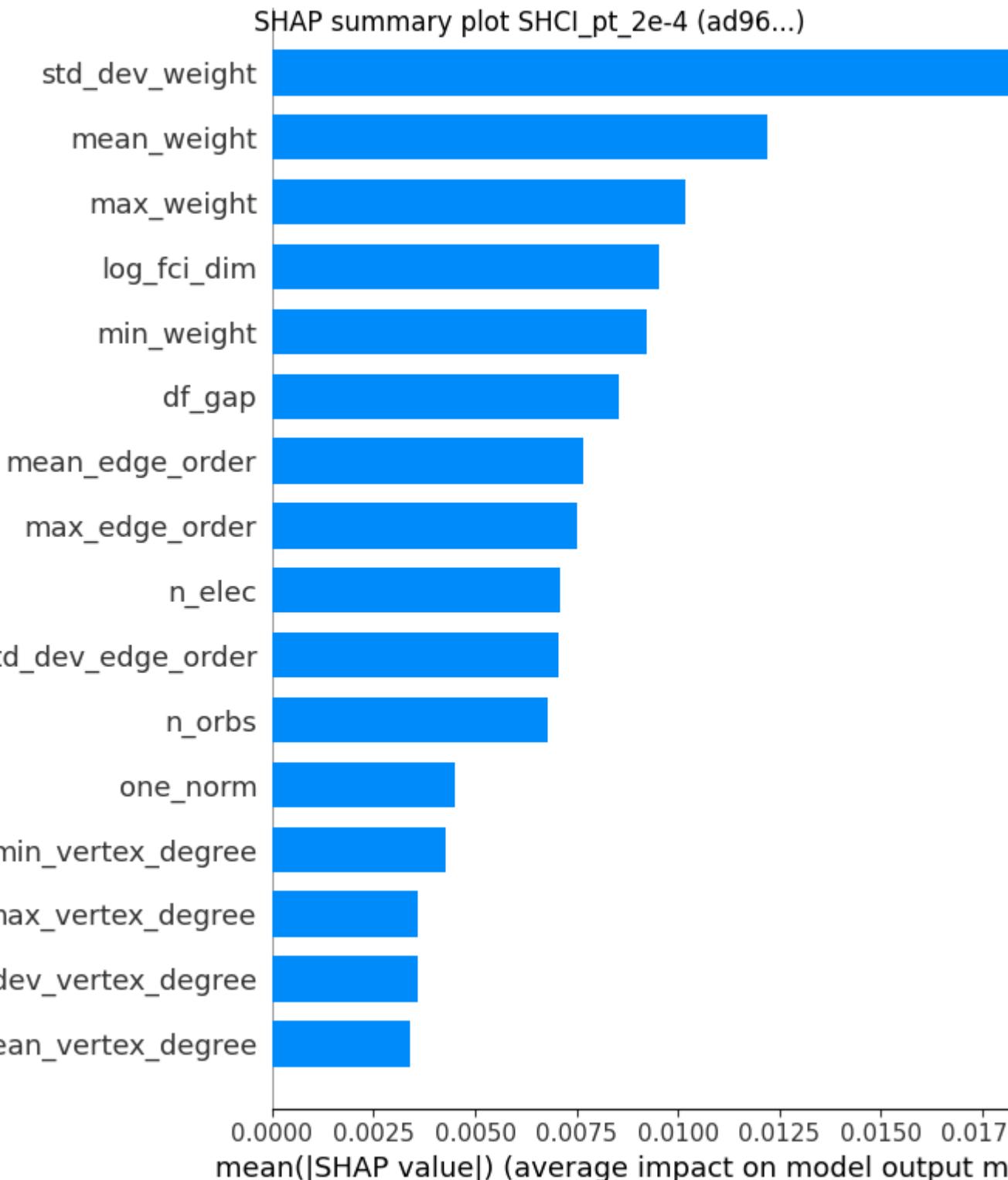
Solver SHCI_pt_2e-4 (ad96...)
Embedding: PCA



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



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



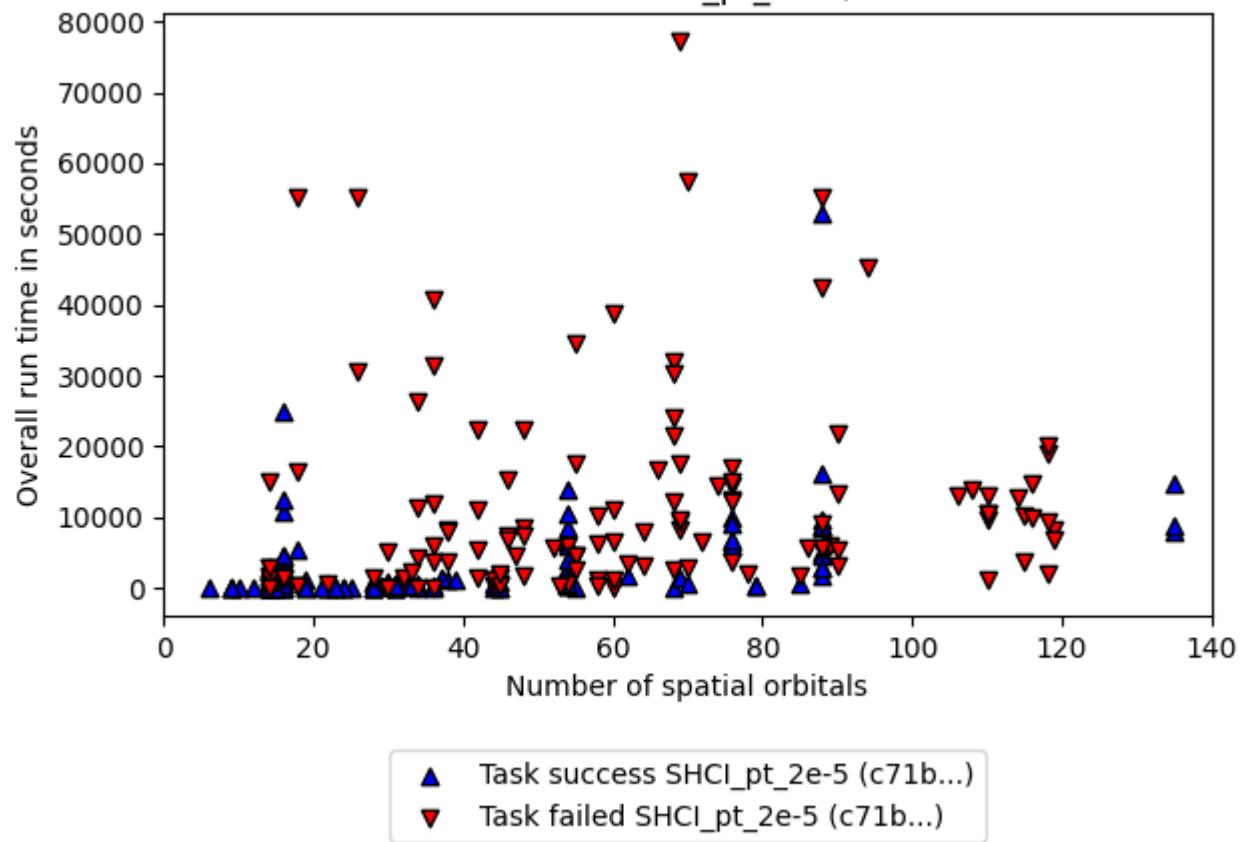
Solver SHCI_pt_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6

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

solver_short_name:SHCI_pt_2e-5

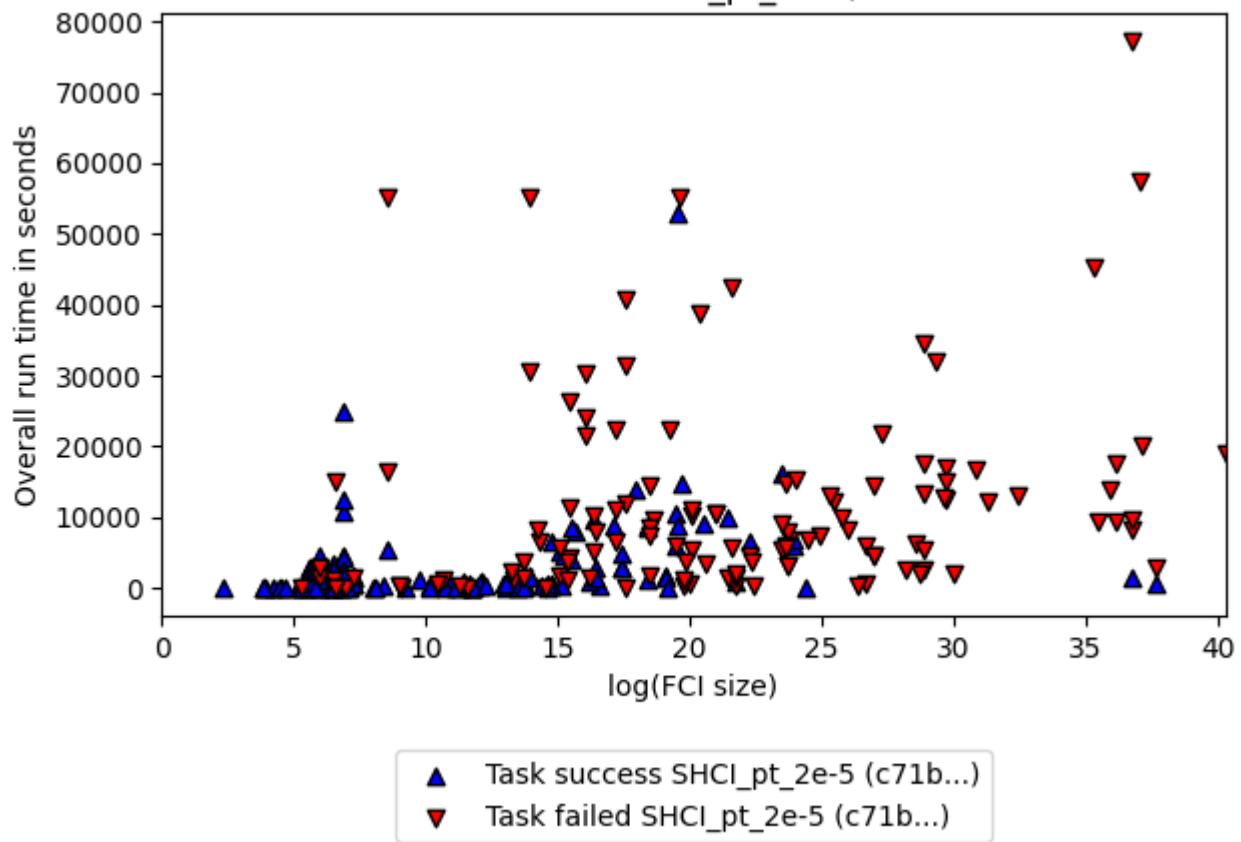
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-5 + PT
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: 654ee62d-1812-4a83-bc37-e1c420ac4b53
creation.timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 26
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 145
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 145
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 1.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.3, 0.9539473684210527]
ml.metrics_calculator_version: 1

Run time for SHCI_pt_2e-5/c71b...



Note: plot only contains attempted tasks.

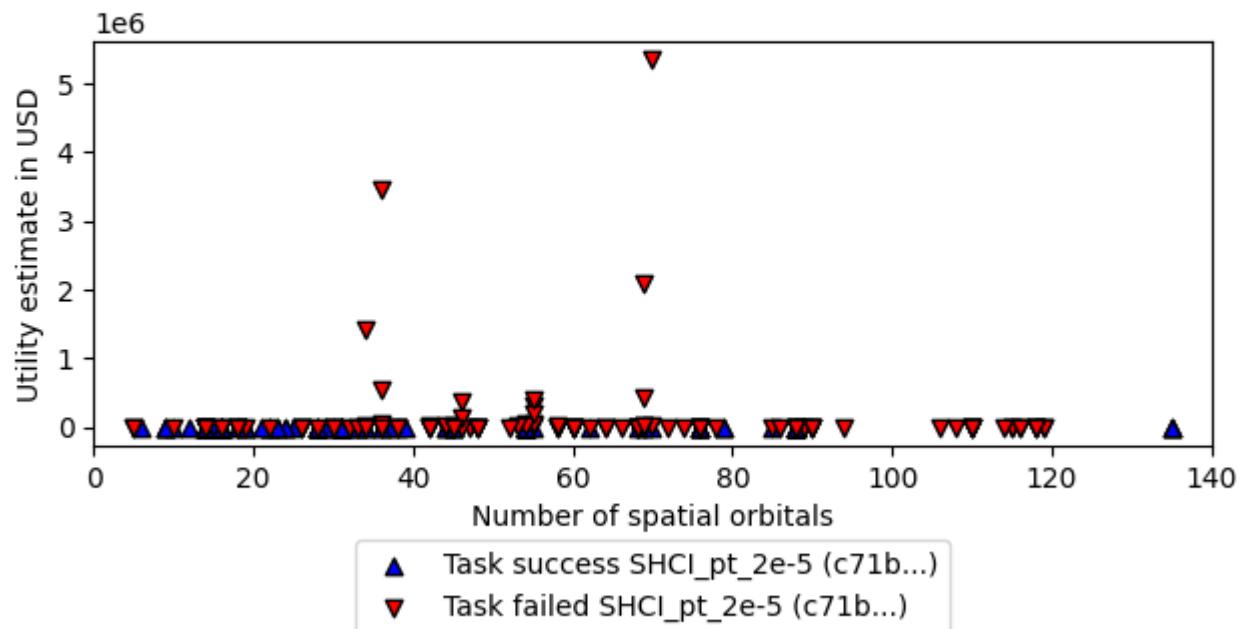
Run time for SHCI_pt_2e-5/c71b...



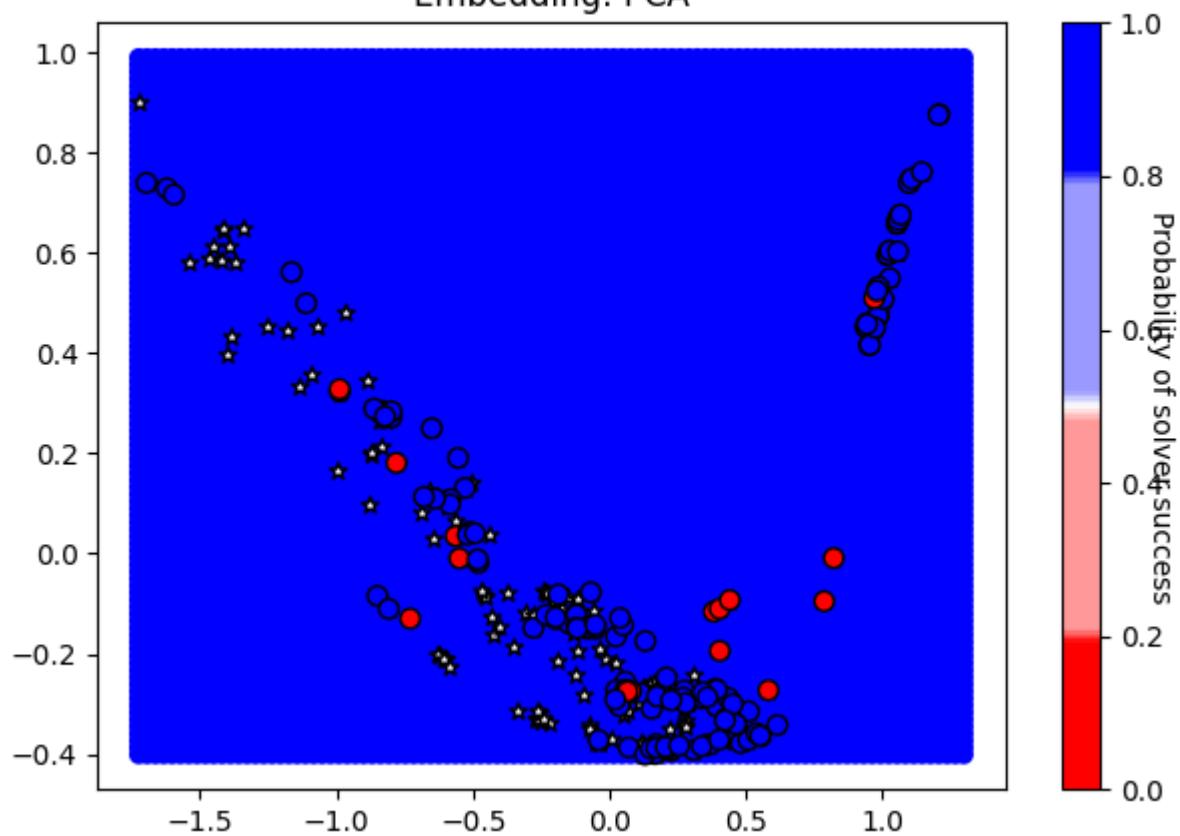
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_2e-5/c71b...

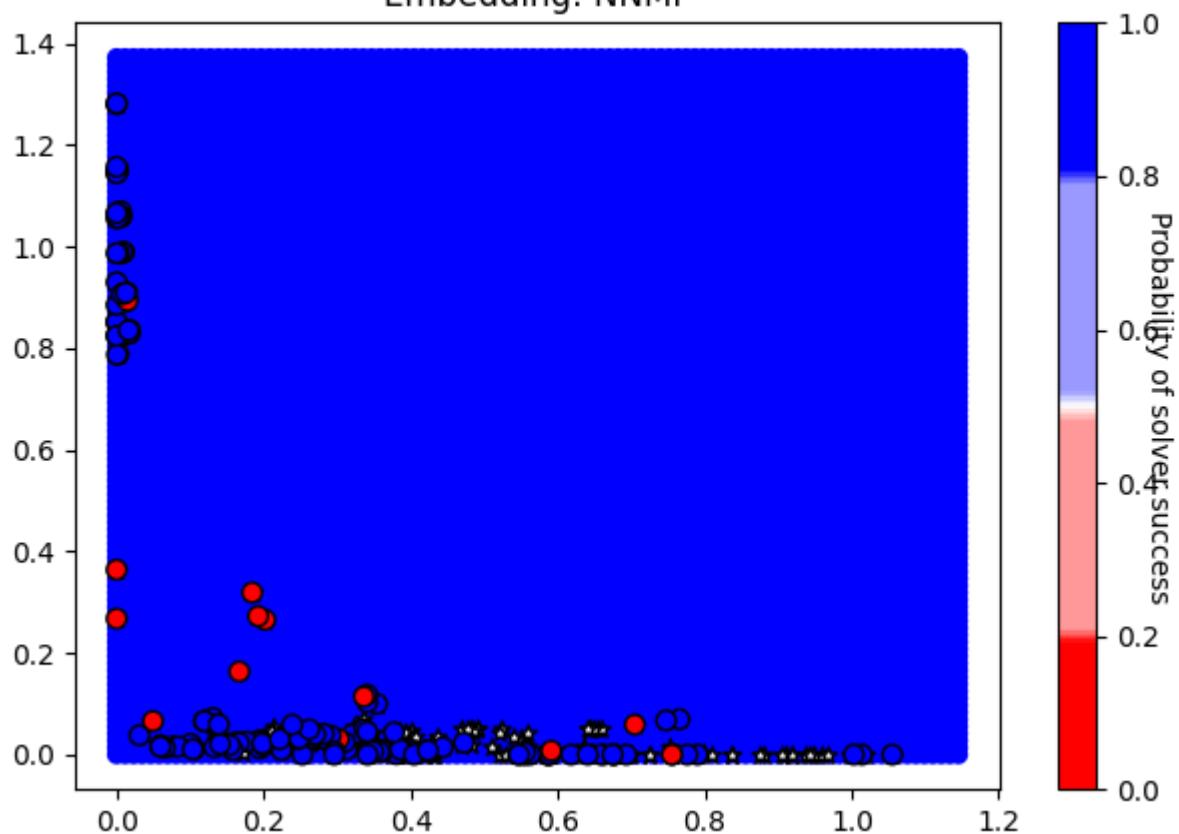
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



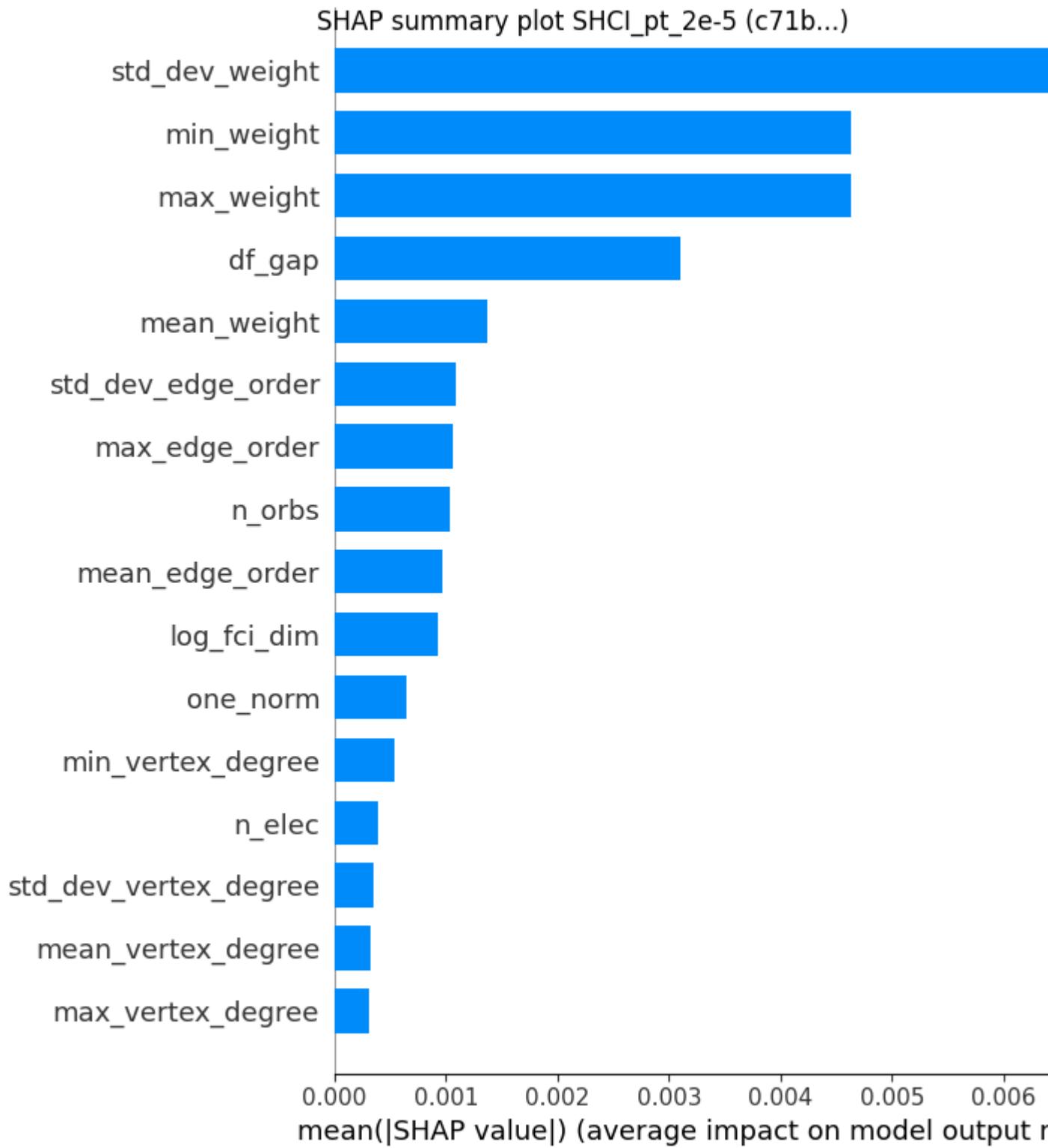
Solver SHCI_pt_2e-5 (c71b...)
Embedding: PCA



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



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

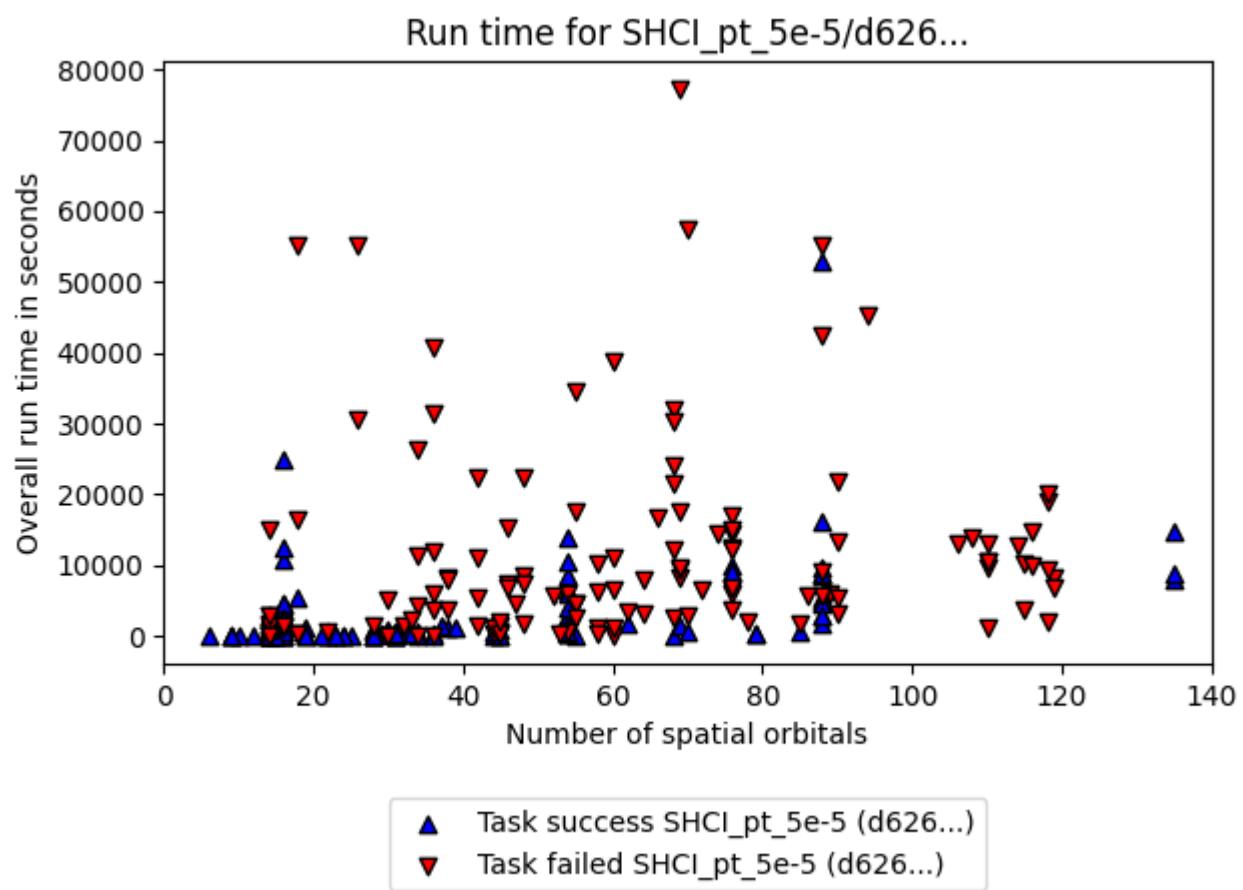


Solver SHCI_pt_5e-5, d626506c-7aae-4ad6-802a-b29af5f2bb93

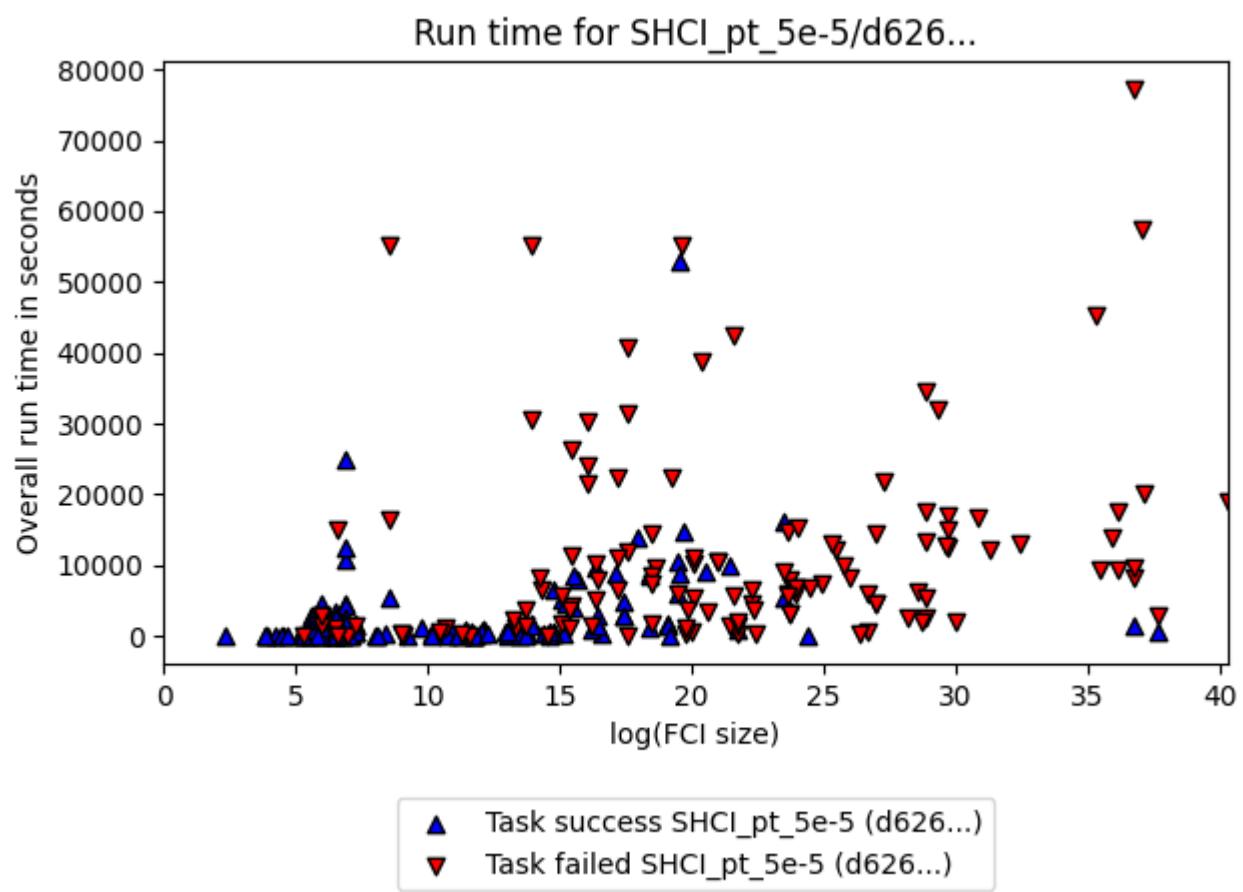
solver_uuid:d626506c-7aae-4ad6-802a-b29af5f2bb93

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: 1c93c3f6-3af1-448b-a64b-2e9b1c6f4306
creation.timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 24
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 143
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 143
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 0.991
comment: solvability ratio based on PCA embedding.
f1_score: [0.7, 0.9577464788732394]
ml.metrics_calculator_version: 1



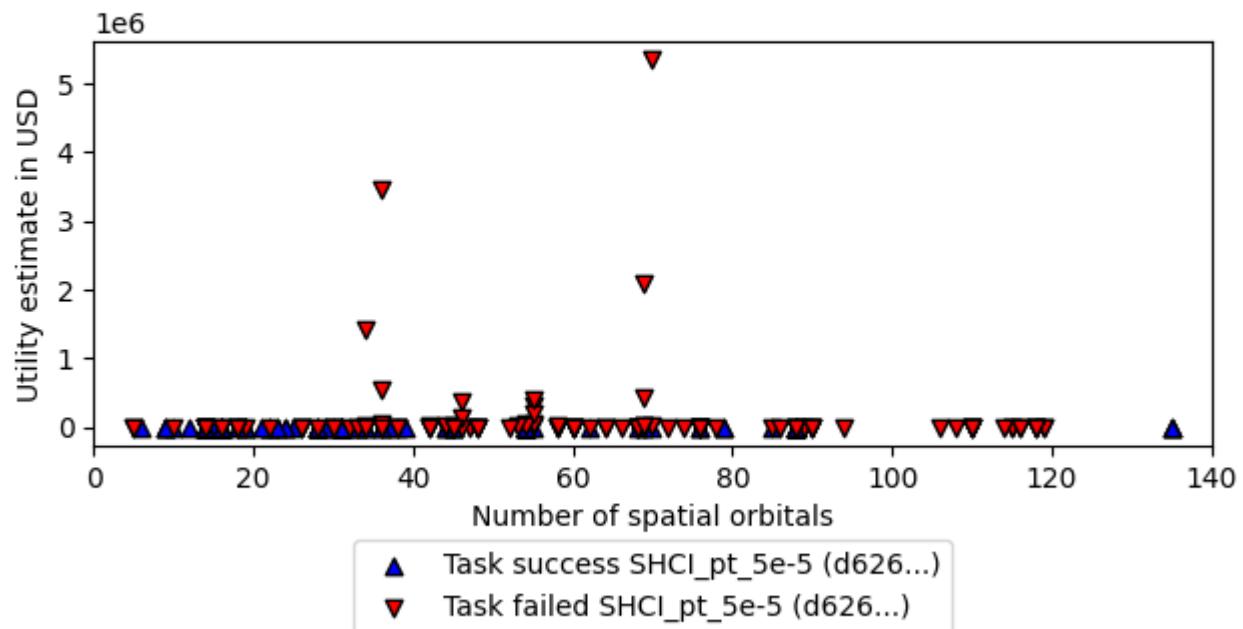
Note: plot only contains attempted tasks.



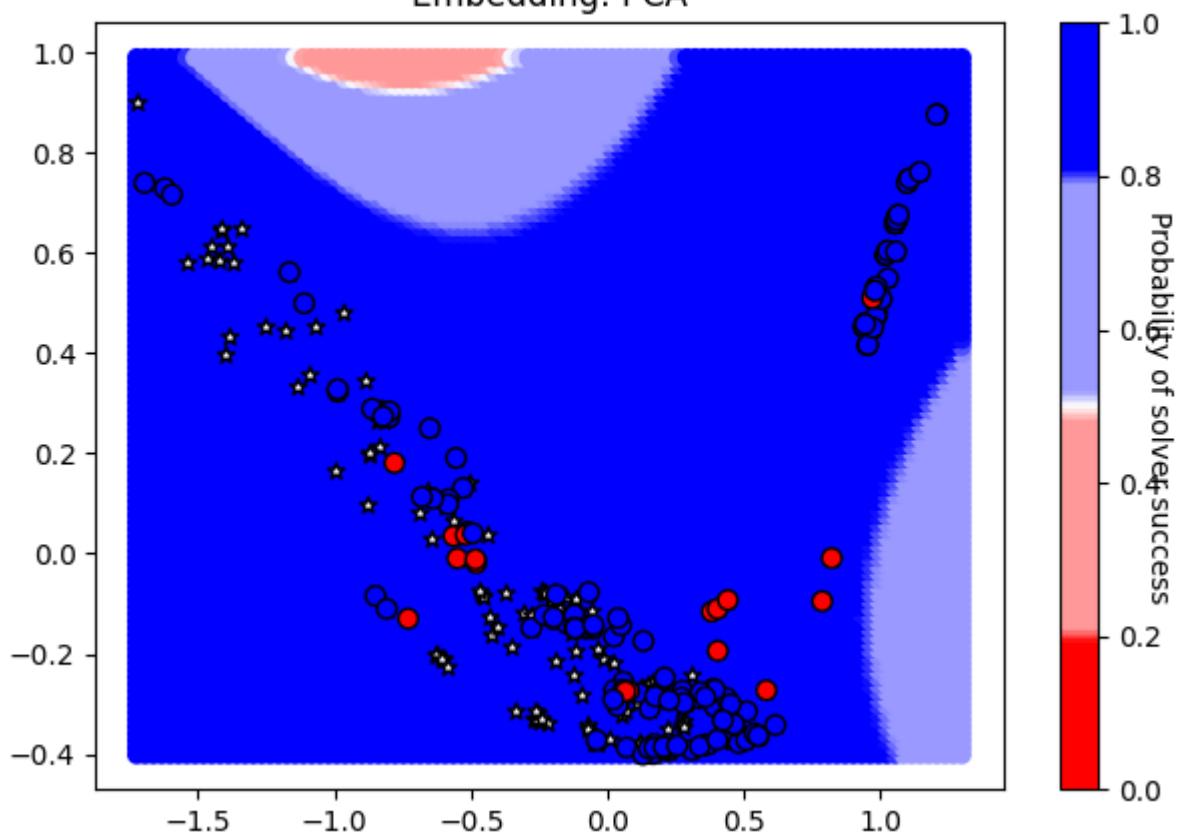
Note: plot only contains attempted tasks.

Utility capture from SHCI_pt_5e-5/d626...

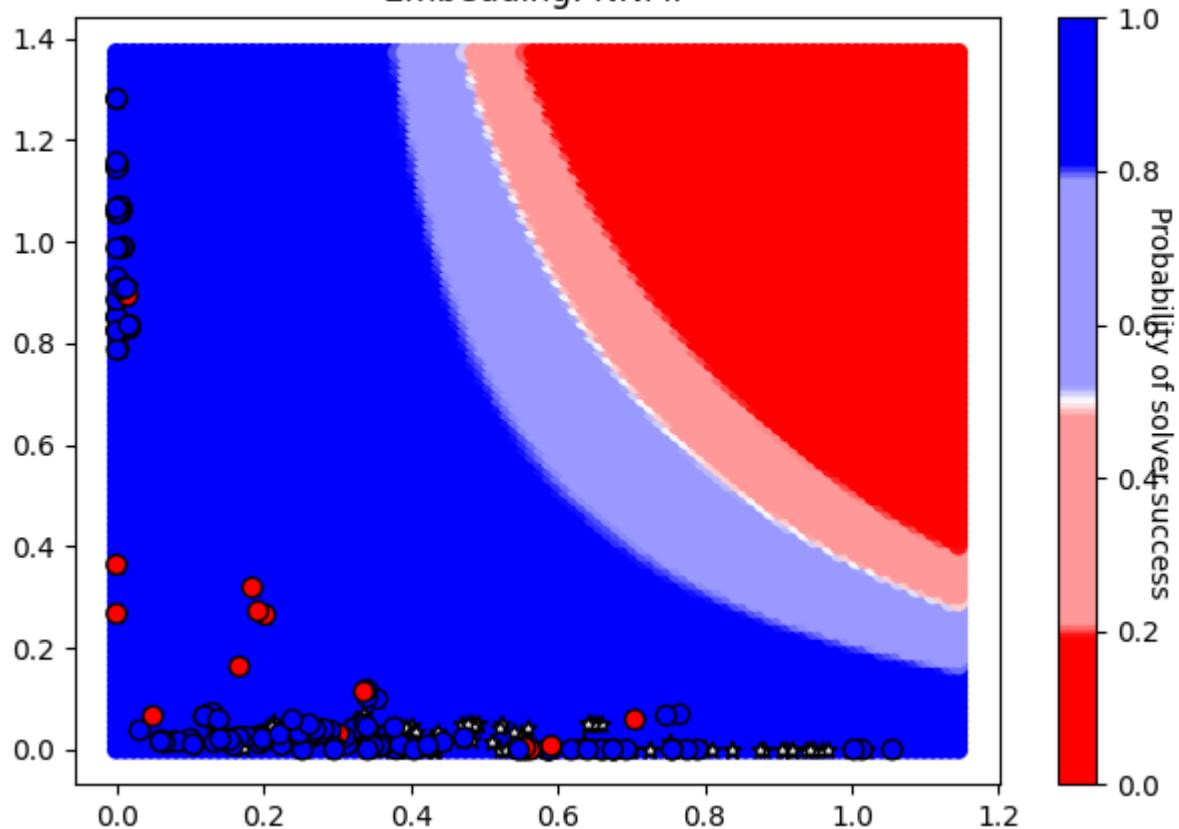
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



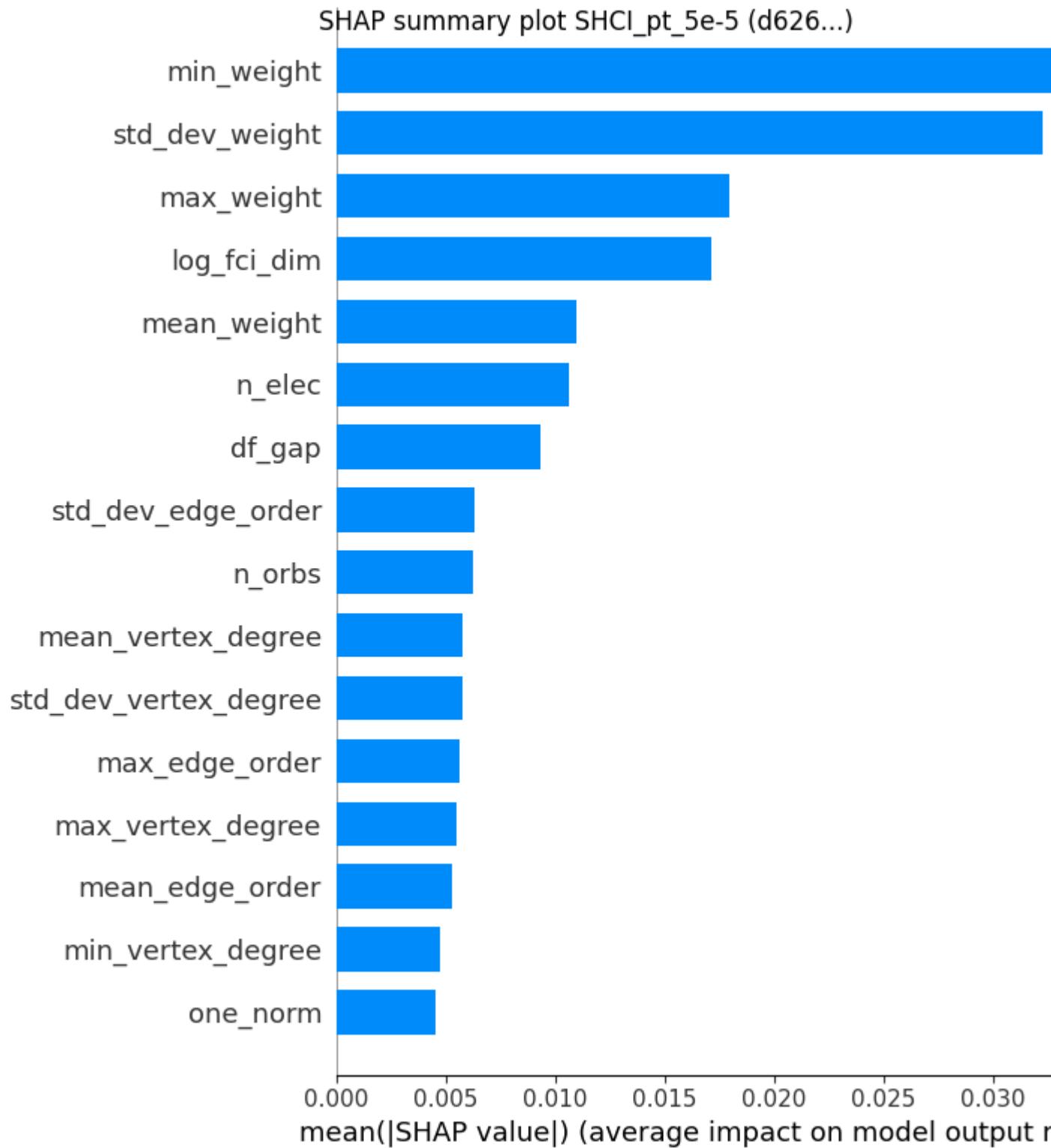
Solver SHCI_pt_5e-5 (d626...)
Embedding: PCA



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



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

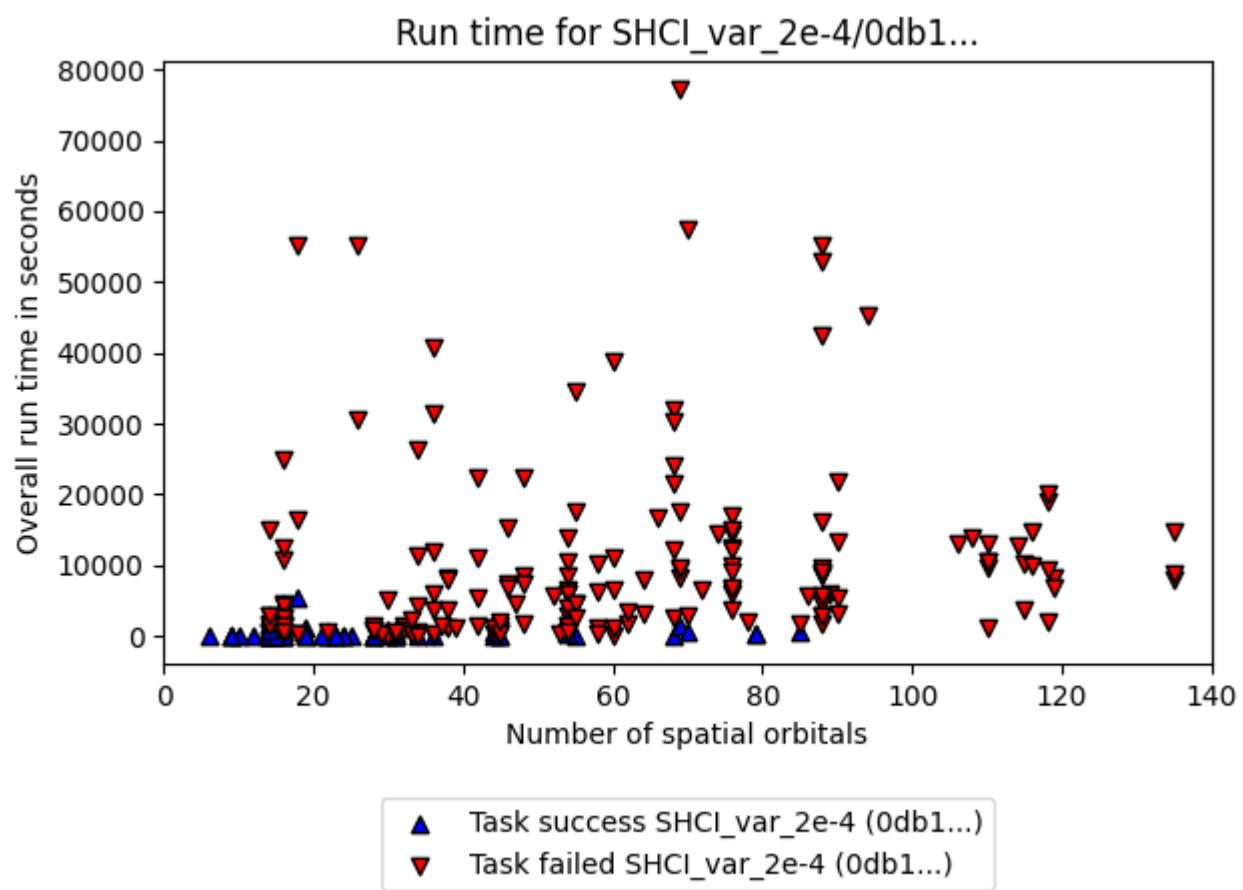


Solver SHCI_var_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a

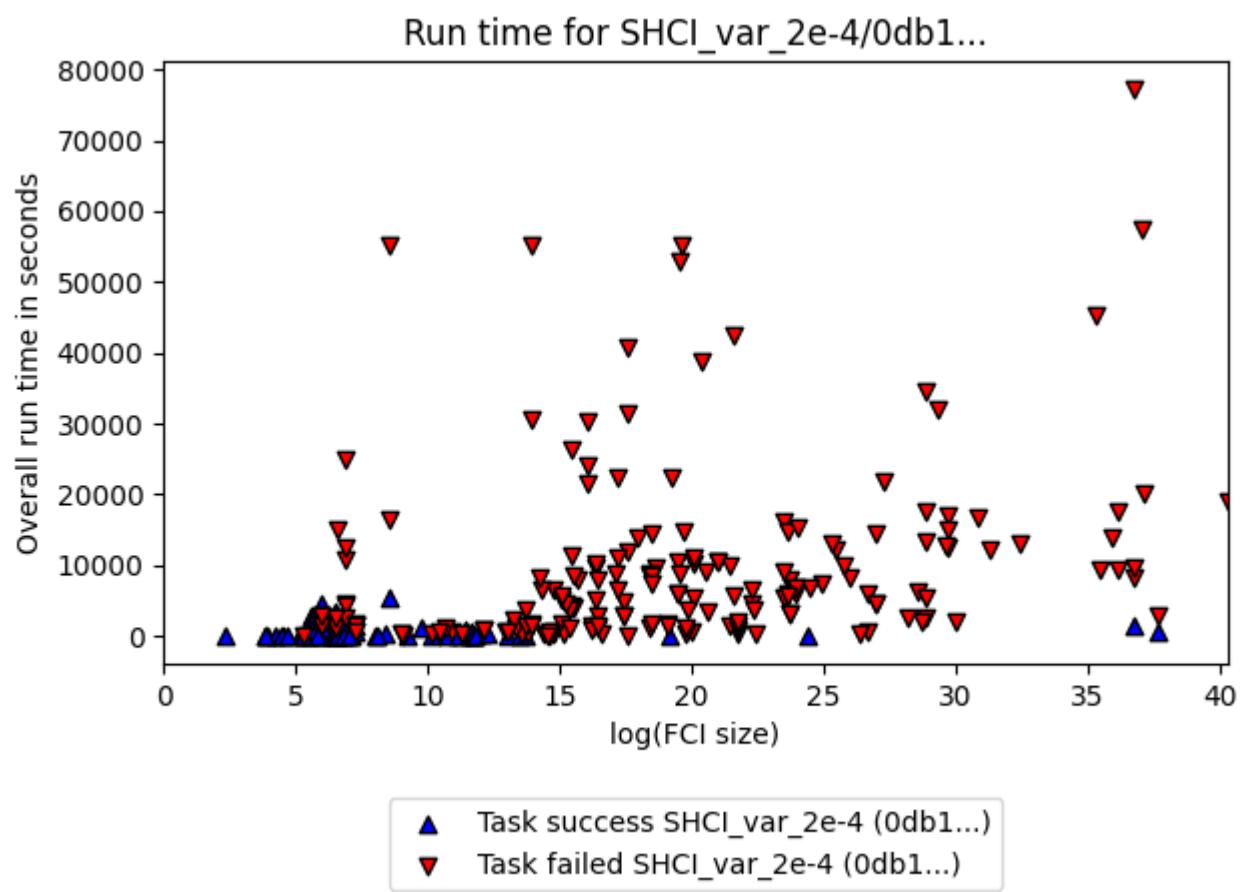
solver_uuid:0db183e3-a86d-491b-9125-599556e37c7a

solver_short_name:SHCI_var_2e-4

compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:SHCI with eps_var 2e-4
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: eaa18840-7921-4dc2-ba8f-dea6bd24ee52
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 13
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 84
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 84
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 0.2602
comment: solvability ratio based on PCA embedding.
f1_score: [0.9681528662420382, 0.9700598802395209]
ml_metrics_calculator_version: 1



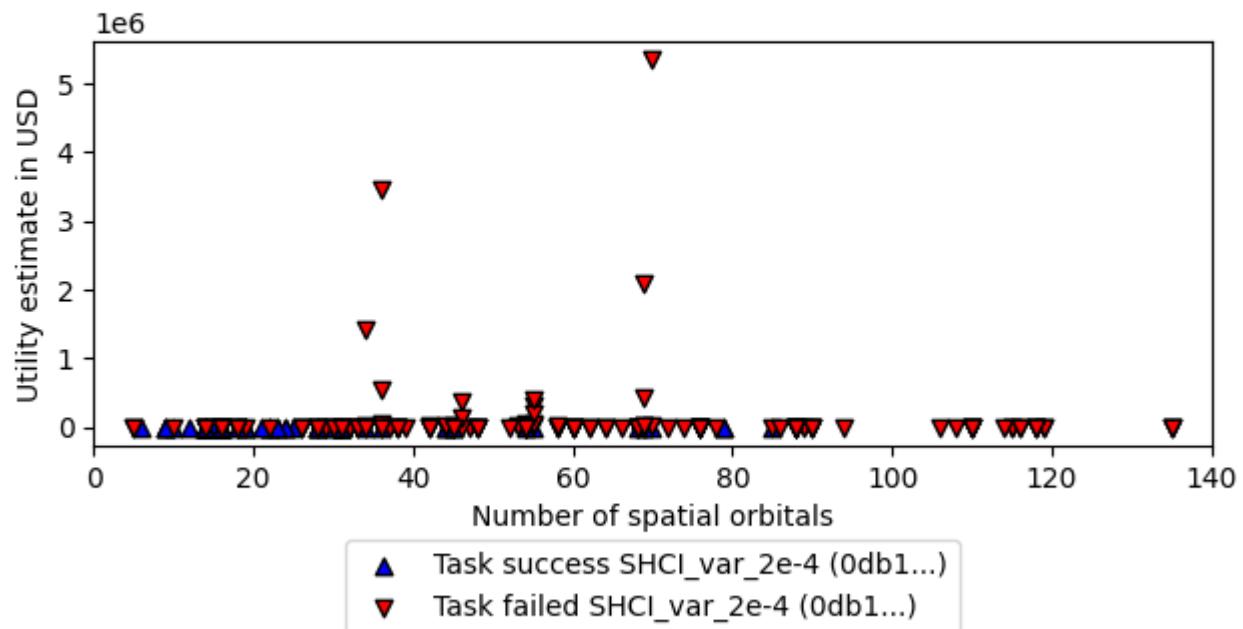
Note: plot only contains attempted tasks.



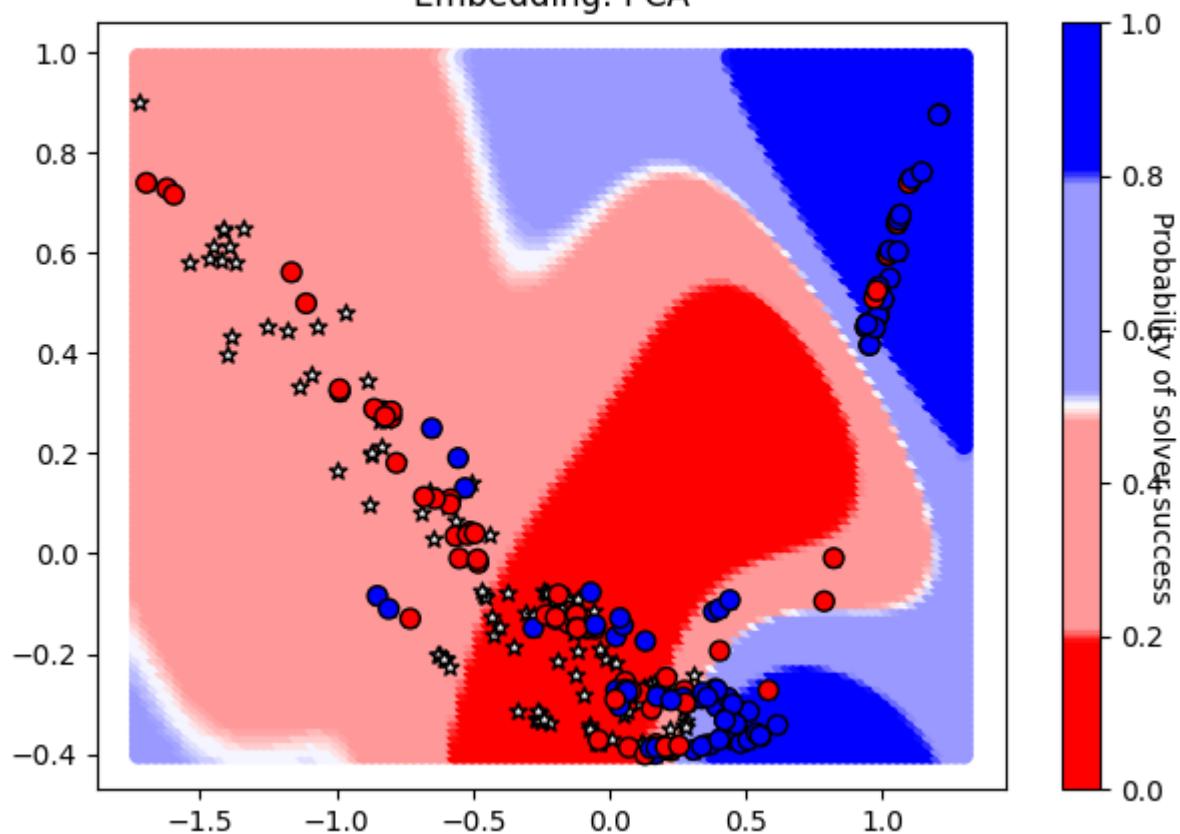
Note: plot only contains attempted tasks.

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

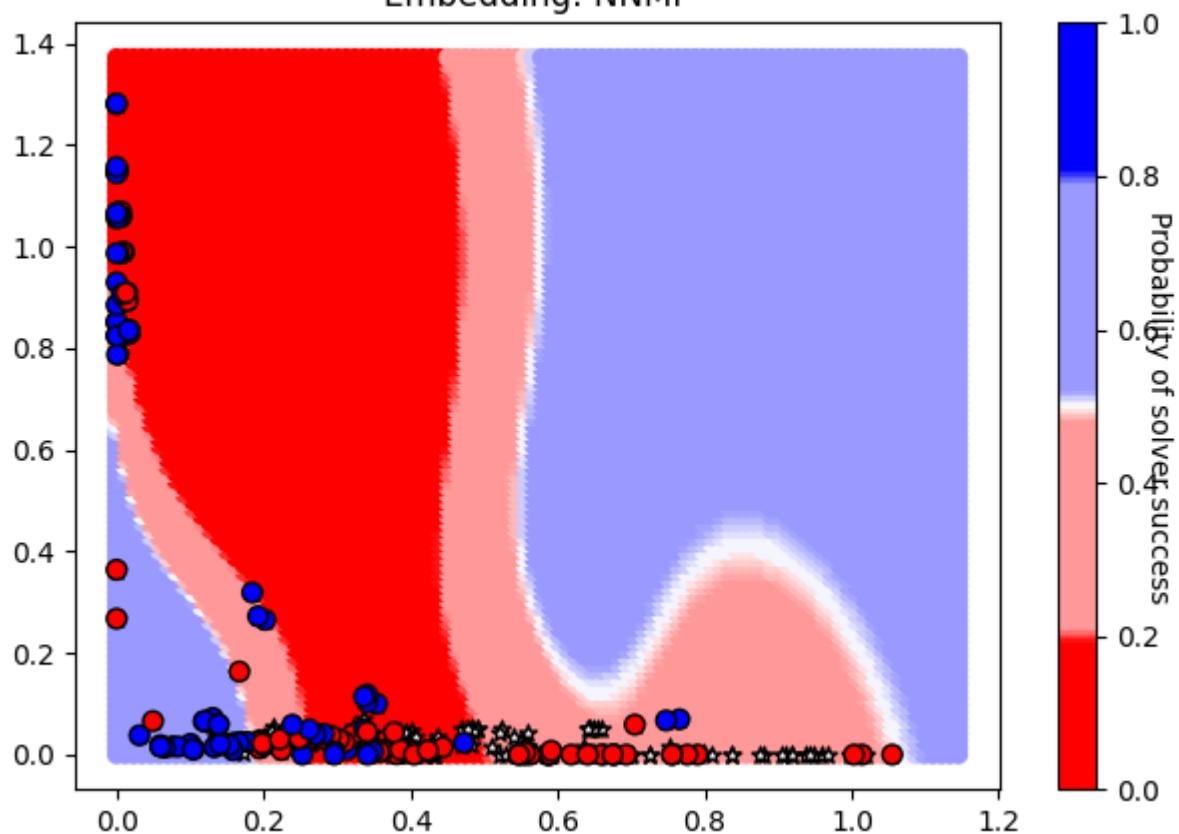
(captured: $\$8.6\text{e+}01/1.5\text{e+}07$, approximately $5.8\text{e-}04\%$)



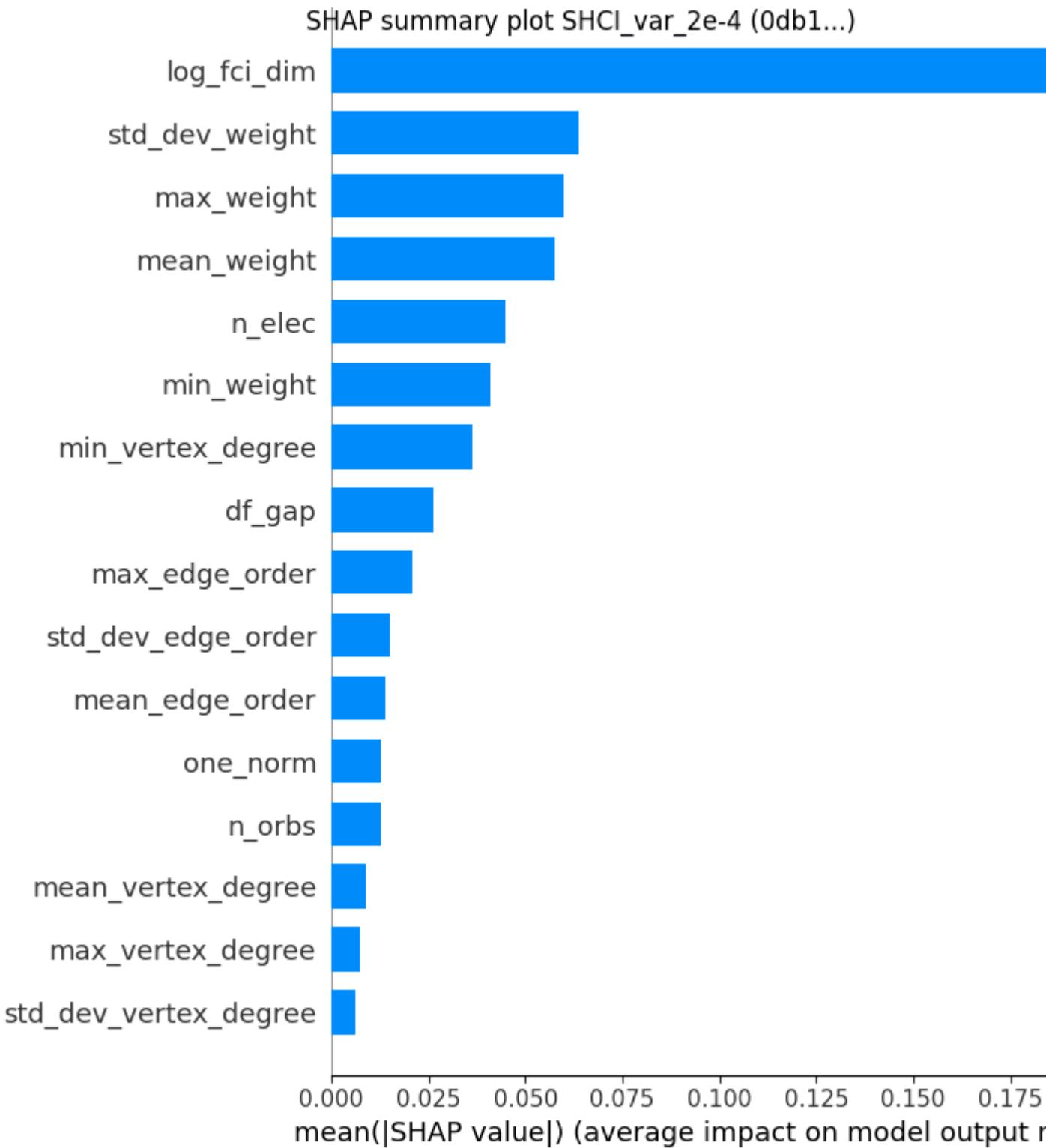
Solver SHCI_var_2e-4 (0db1...)
Embedding: PCA



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



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

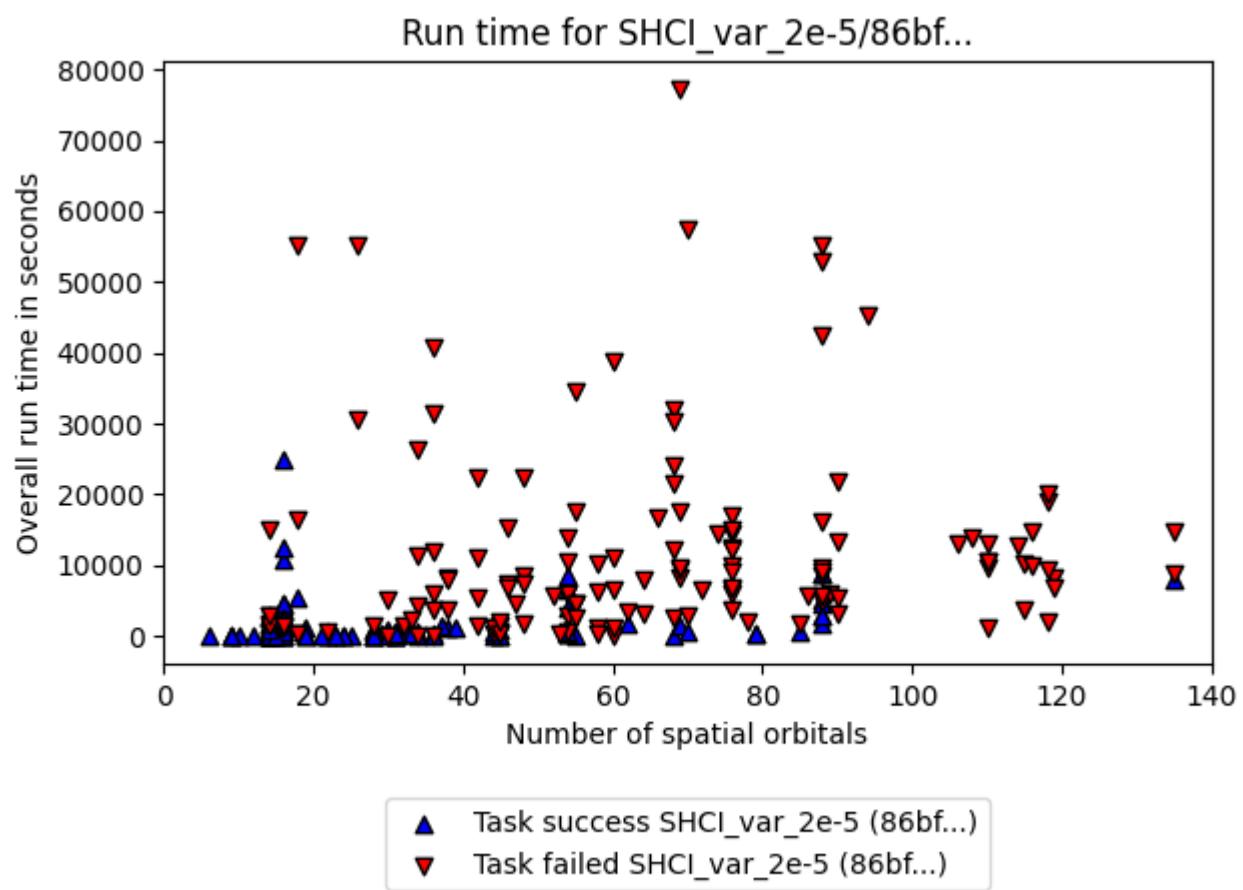


Solver SHCI_var_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688

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

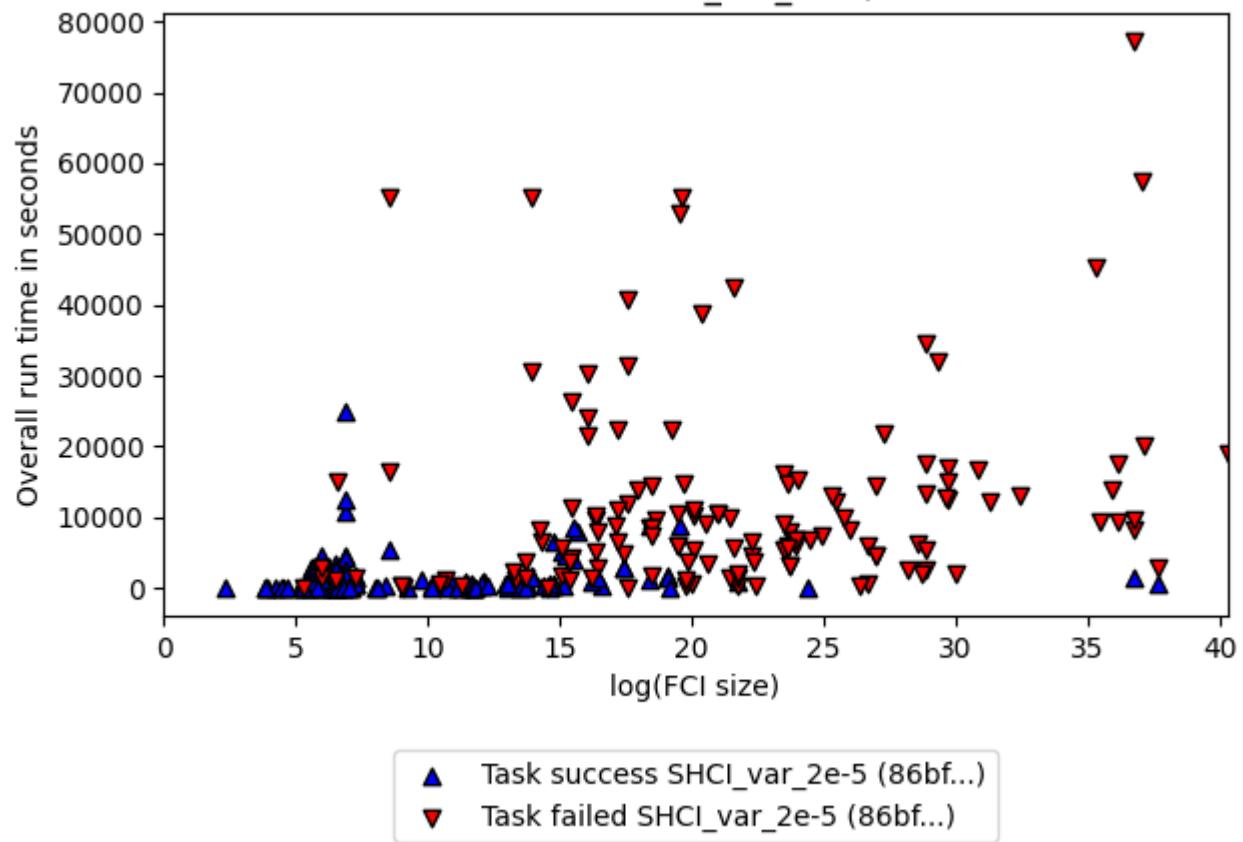
solver_short_name:SHCI_var_2e-5

compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:SHCI with eps_var 2e-5
software.details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance.metrics.uuid: 18643df5-e1cf-4d9d-857a-c75df1b26491
creation.timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 18
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 133
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 133
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 0.5692
comment: solvability ratio based on PCA embedding.
f1_score: [0.833333333333334, 0.9621212121212122]
ml.metrics_calculator_version: 1



Note: plot only contains attempted tasks.

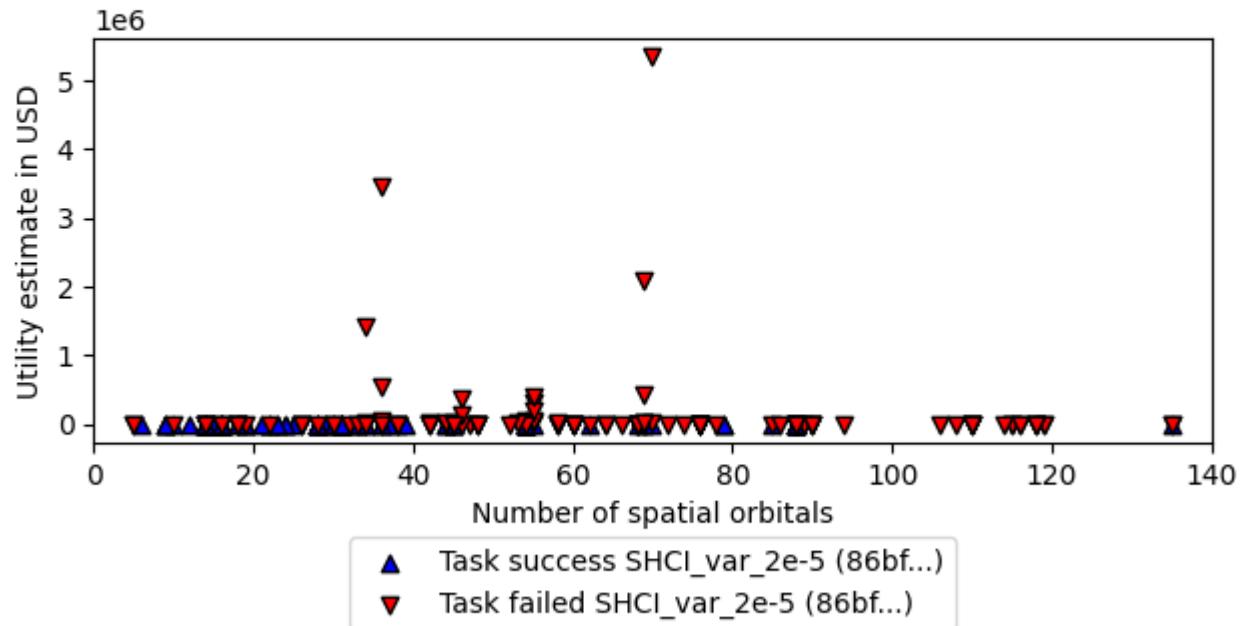
Run time for SHCI_var_2e-5/86bf...



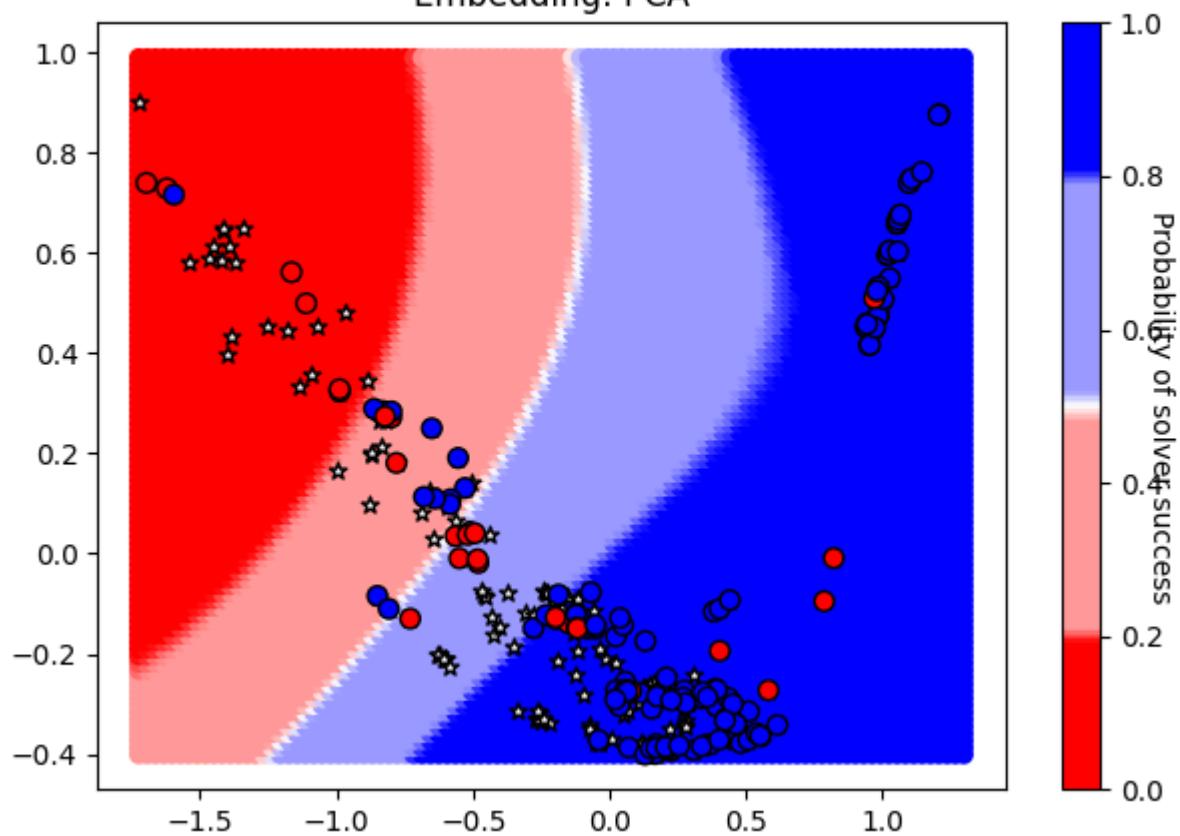
Note: plot only contains attempted tasks.

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

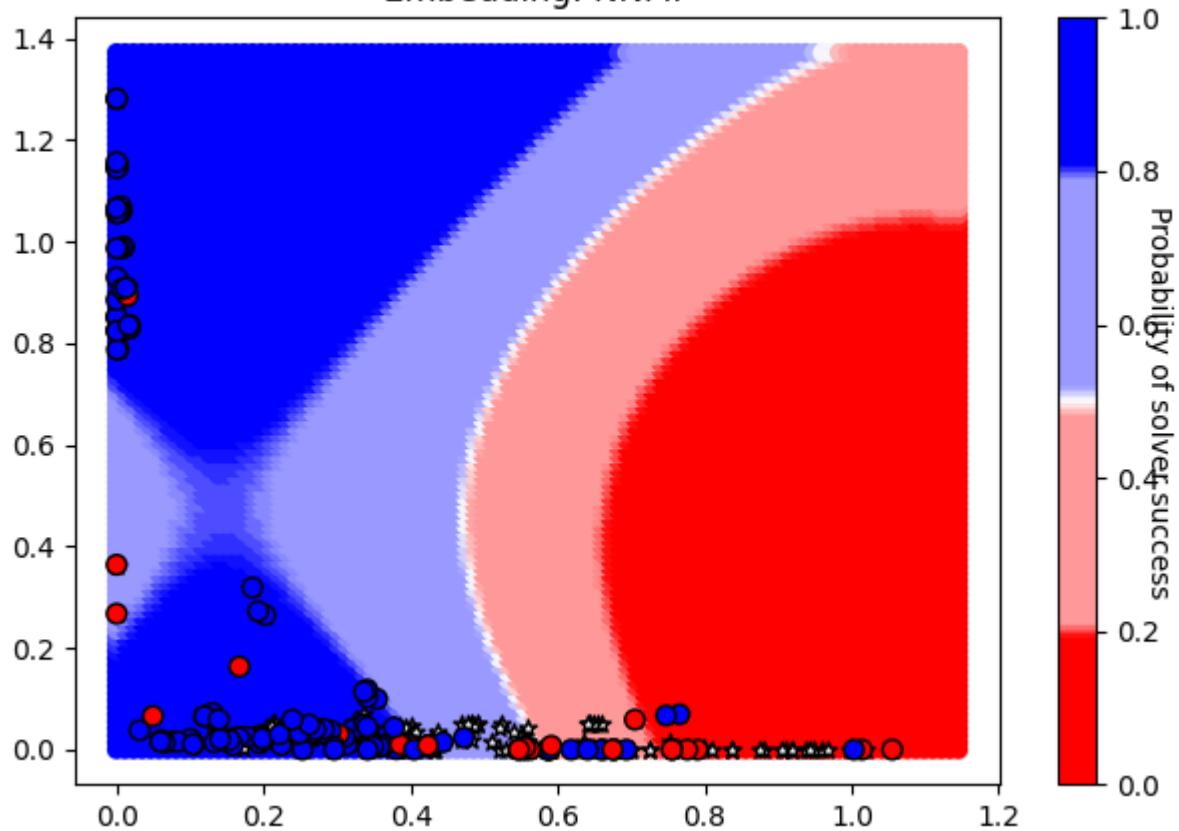
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



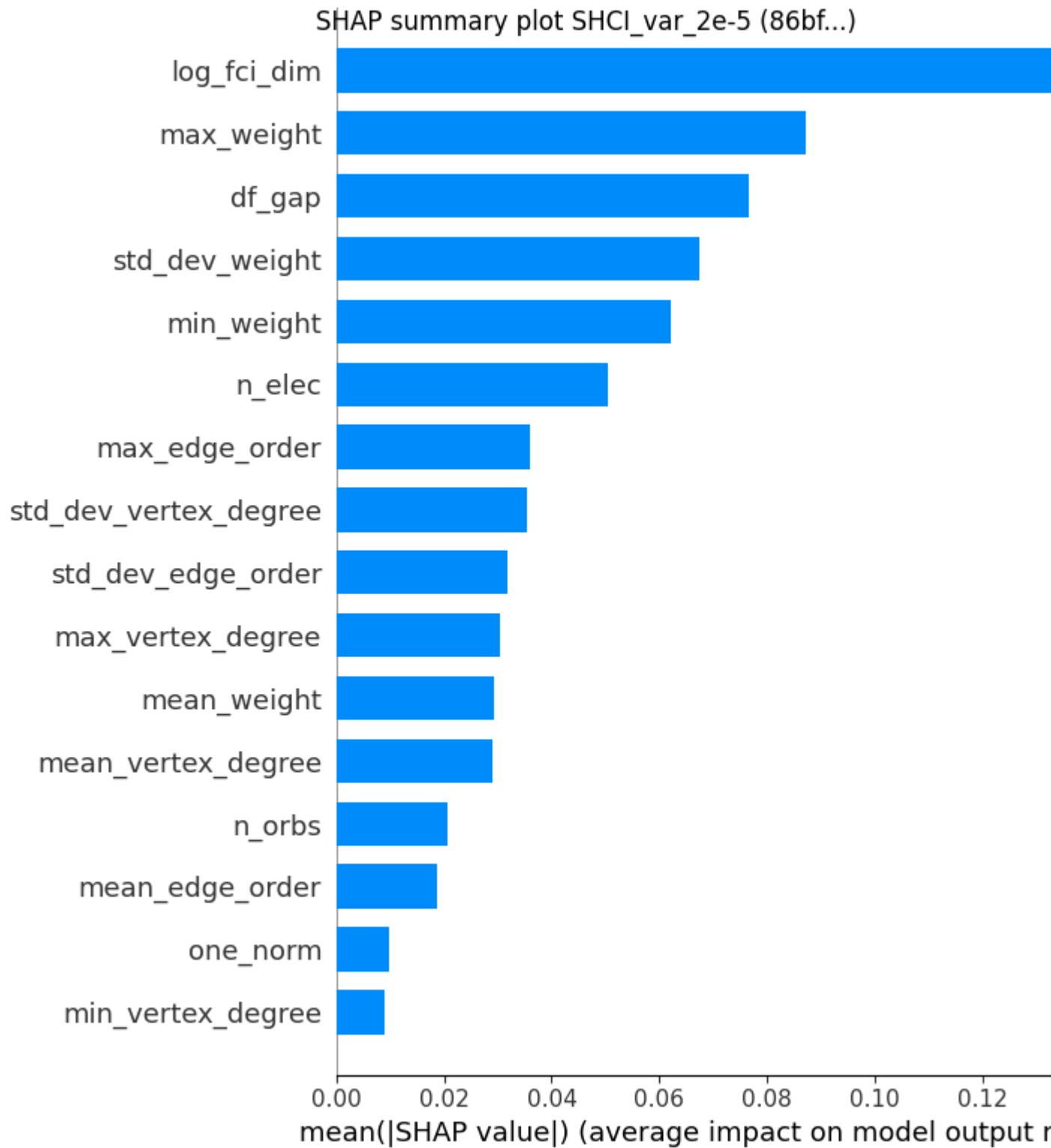
Solver SHCI_var_2e-5 (86bf...)
Embedding: PCA



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



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

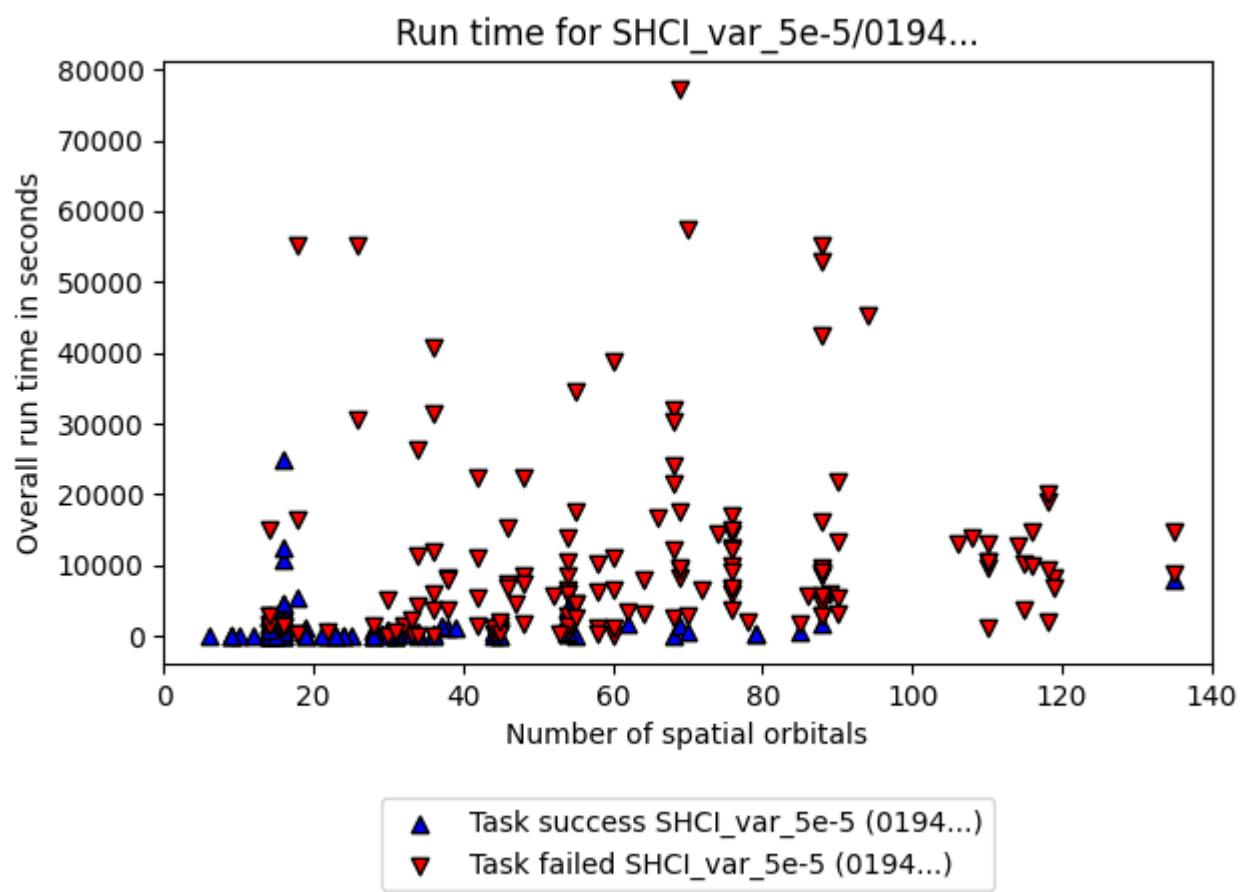


Solver SHCI_var_5e-5, 01949b95-c427-4693-9134-01f47f688c09

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

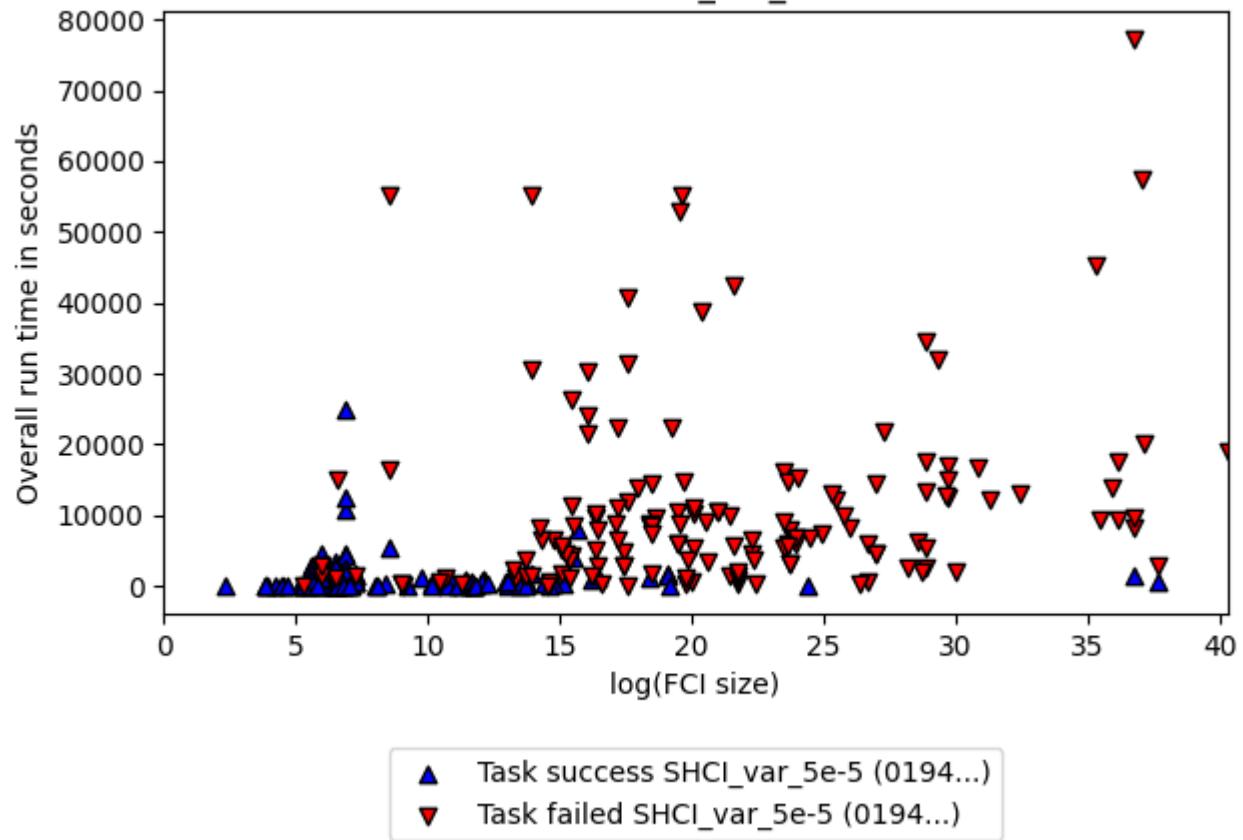
solver_short_name:SHCI_var_5e-5

compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:SHCI with eps_var 5e-5
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).
performance_metrics_uuid: 52133230-0a24-43db-9244-e19d08808c75
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 14
number_of_tasks: 280
number_of_tasks_attempted: 275
number_of_tasks_solved: 120
number_of_tasks_solved_within_run_time_limit: 273
number_of_tasks_solved_within_accuracy_threshold: 120
max_run_time_of_attempted_tasks: 77244.15200000002
sum_of_run_time_of_attempted_tasks: 1863349.633000001
solvability_ratio: 0.5156
comment: solvability ratio based on PCA embedding.
f1_score: [0.8095238095238095, 0.9333333333333333]
ml_metrics_calculator_version: 1



Note: plot only contains attempted tasks.

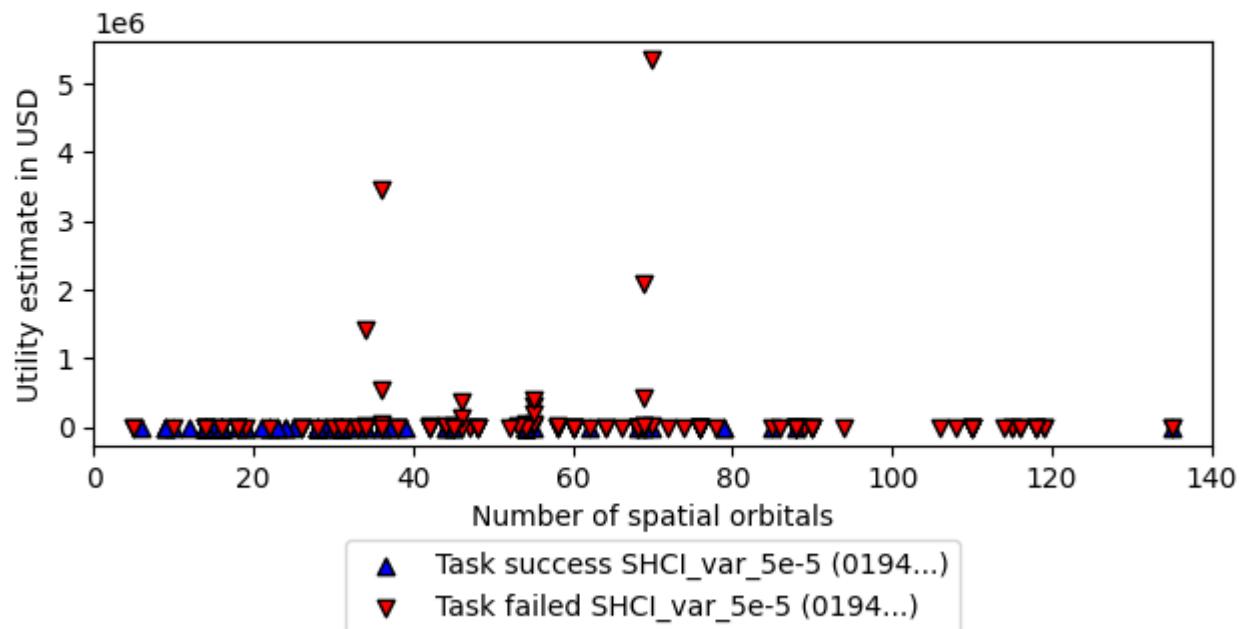
Run time for SHCI_var_5e-5/0194...



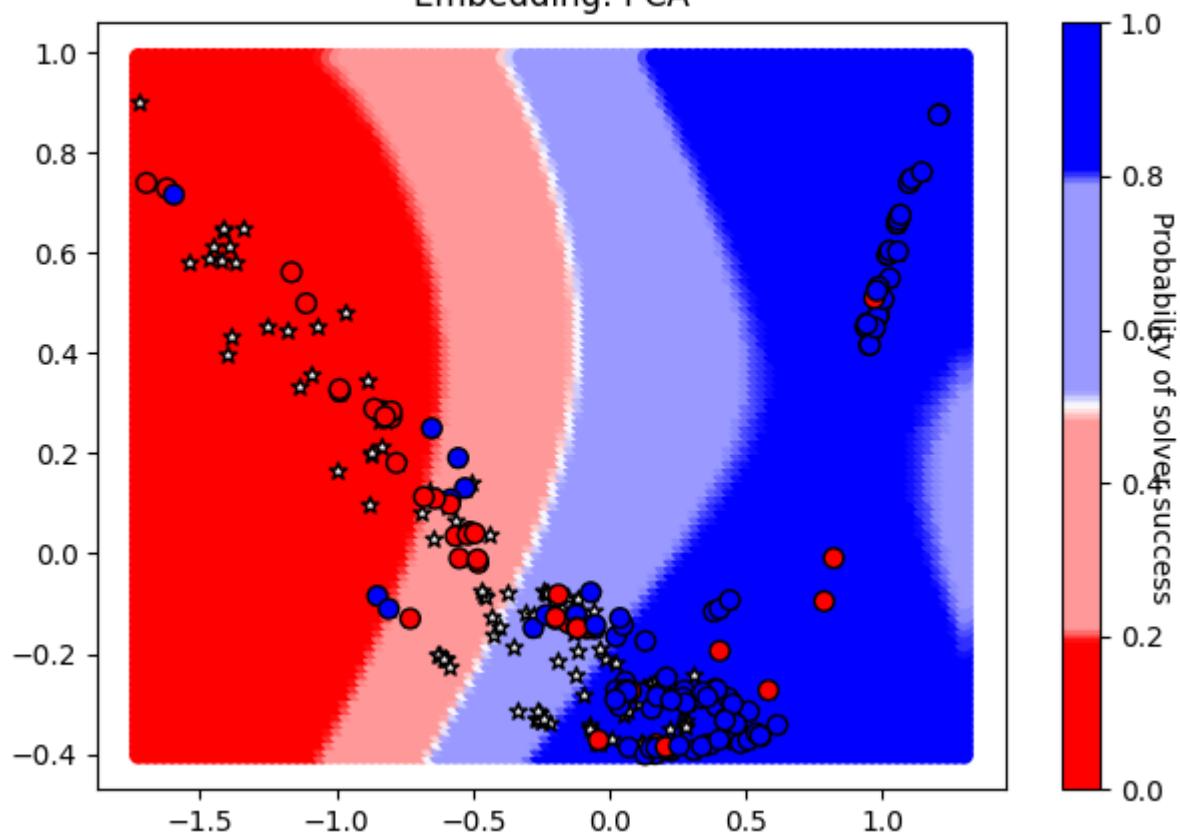
Note: plot only contains attempted tasks.

Utility capture from SHCI_var_5e-5/0194...

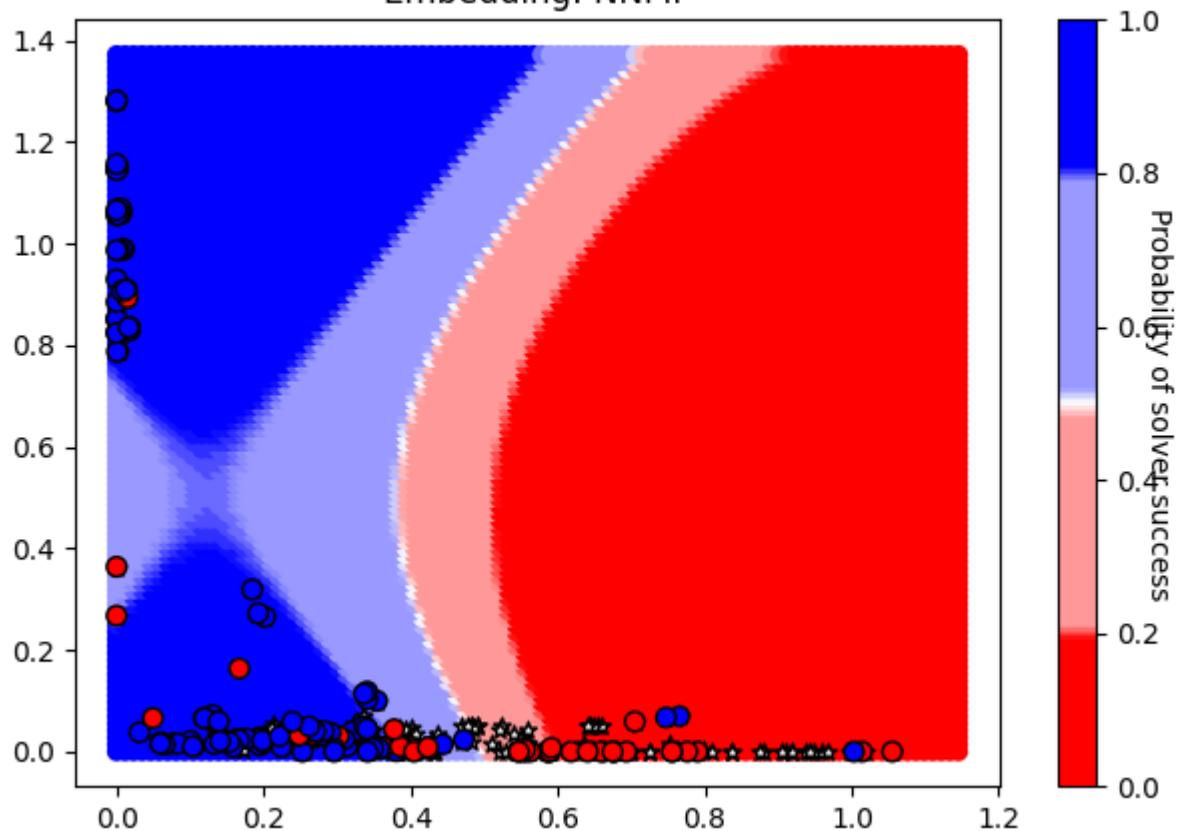
(captured: $\$4.5\text{e+}02/1.5\text{e+}07$, approximately $3.0\text{e-}03\%$)



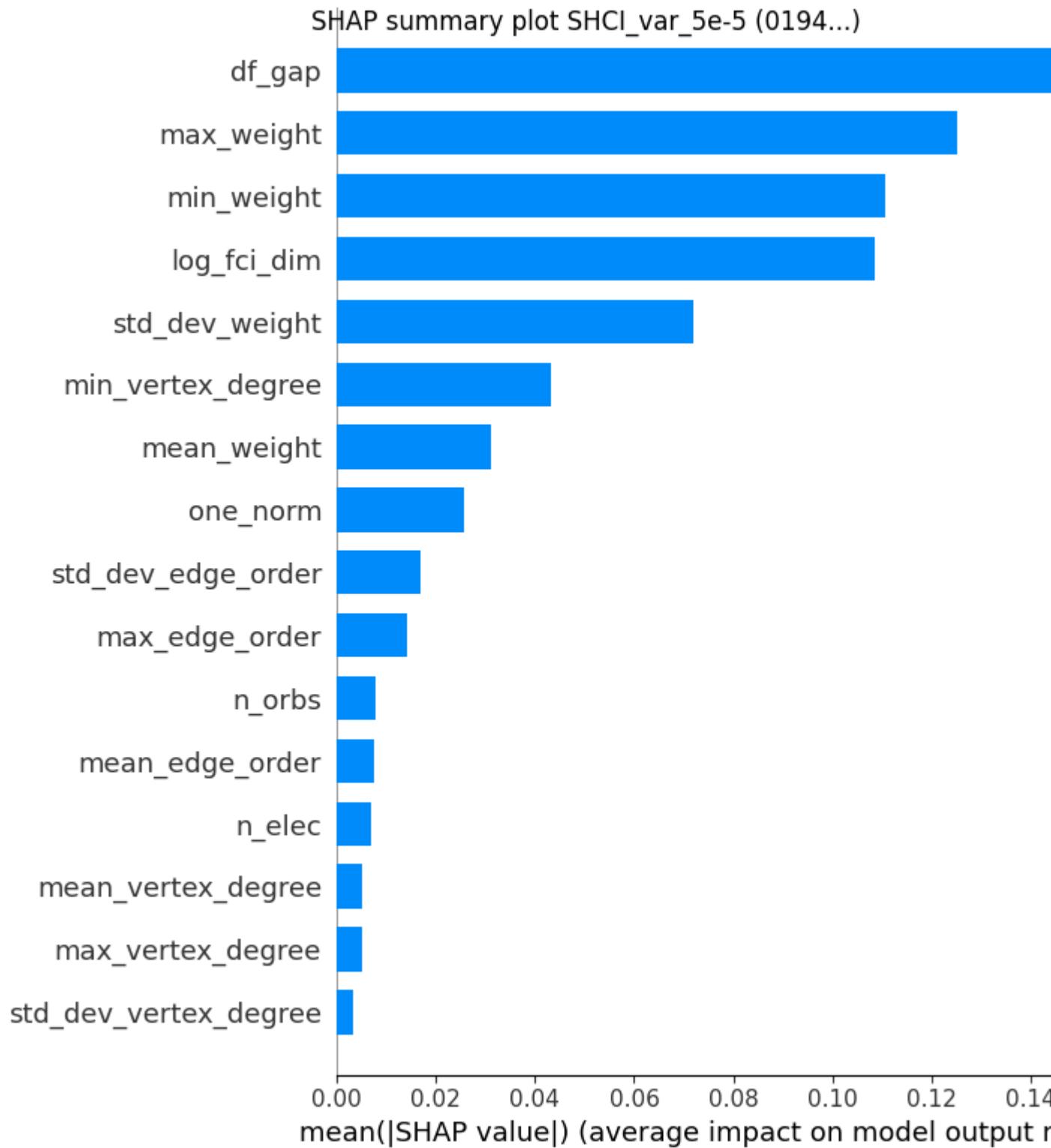
Solver SHCI_var_5e-5 (0194...)
Embedding: PCA



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



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



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

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

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

software_details:[{'software_name': 'pyLIQTR', 'software_version': '1.3.4'}, {'software_name': 'qb-gsee-benchmark', 'software_version': '0.1.0a2.dev193+g879c00d'}, {'software_name': 'Python', 'software_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]'}, {'software_name': 'qualtran', 'software_version': '0.4.0'}]

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

logical_resource_estimate_solution_uuid:e5377ec1-7a7f-4559-8336-548da65ea6e0

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

performance_metrics_uuid: 1b8ba5ef-de6e-44ef-8b9c-54a488aec314

creation_timestamp: 2025-02-19T18:26:13.854054+00:00

number_of_problem_instances: 88

number_of_problem_instances_attempted: 24

number_of_problem_instances_solved: 0

number_of_tasks: 280

number_of_tasks_attempted: 166

number_of_tasks_solved: 0

number_of_tasks_solved_within_run_time_limit: 0

number_of_tasks_solved_within_accuracy_threshold: 166

max_run_time_of_attempted_tasks: 3.667583349758134e+17

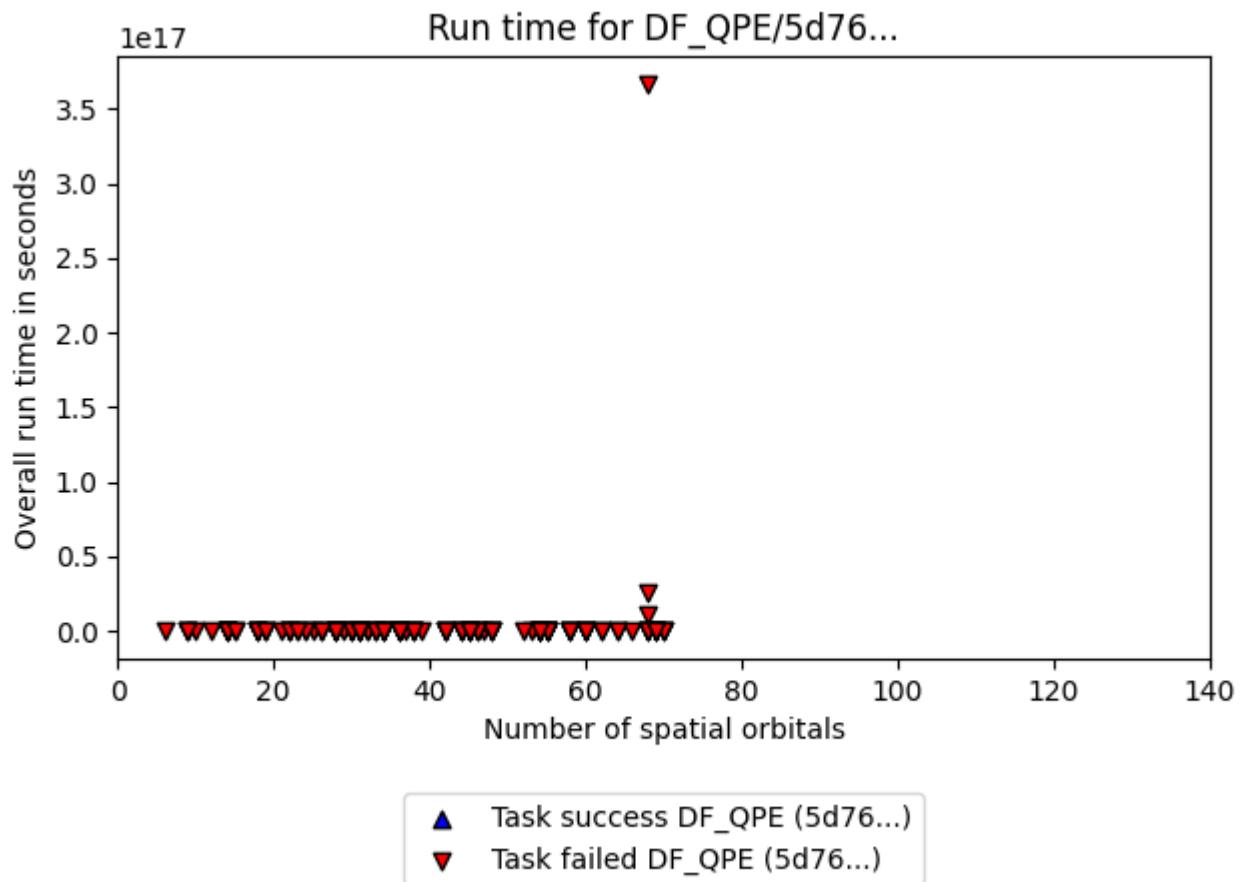
sum_of_run_time_of_attempted_tasks: 4.0384302123797466e+17

solvability_ratio: None

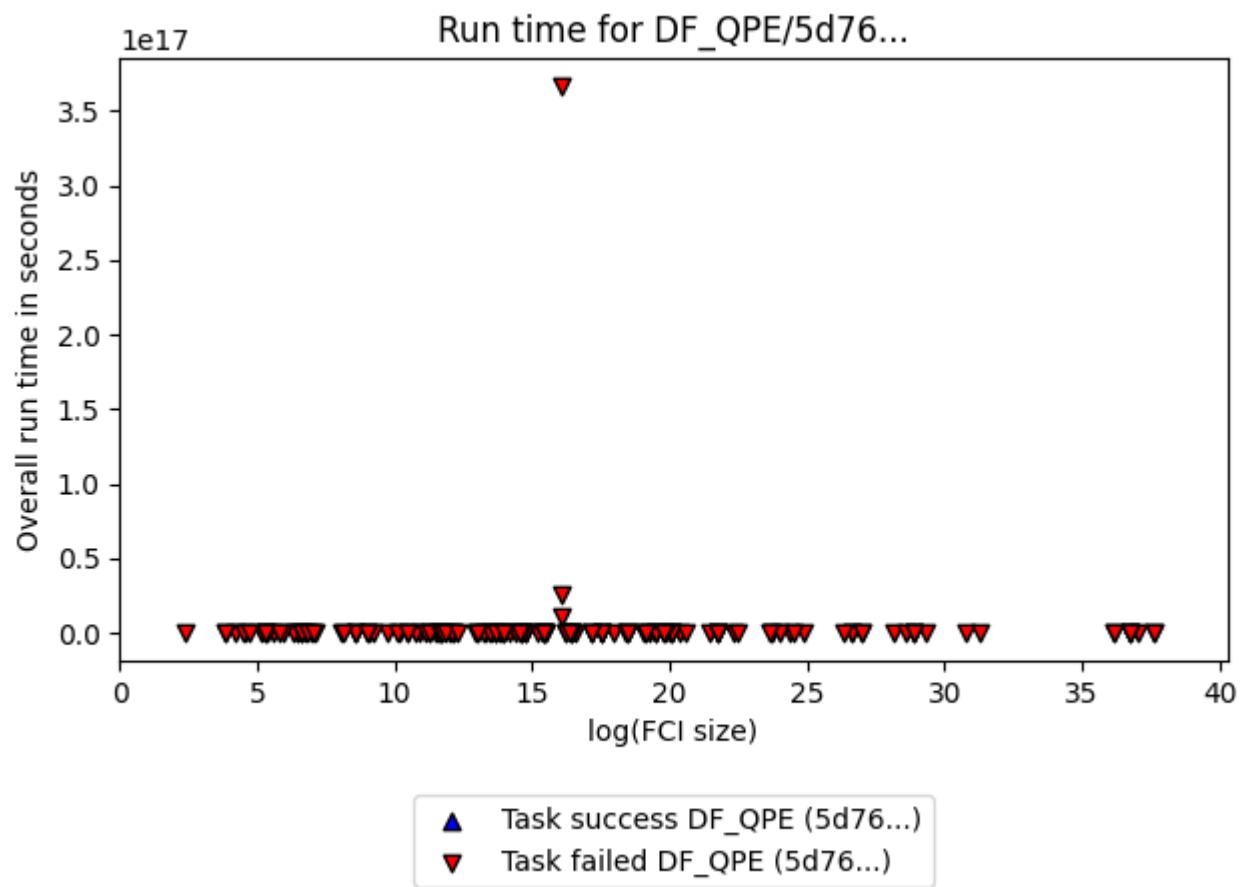
f1_score: None

ml_metrics_calculator_version: 1

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

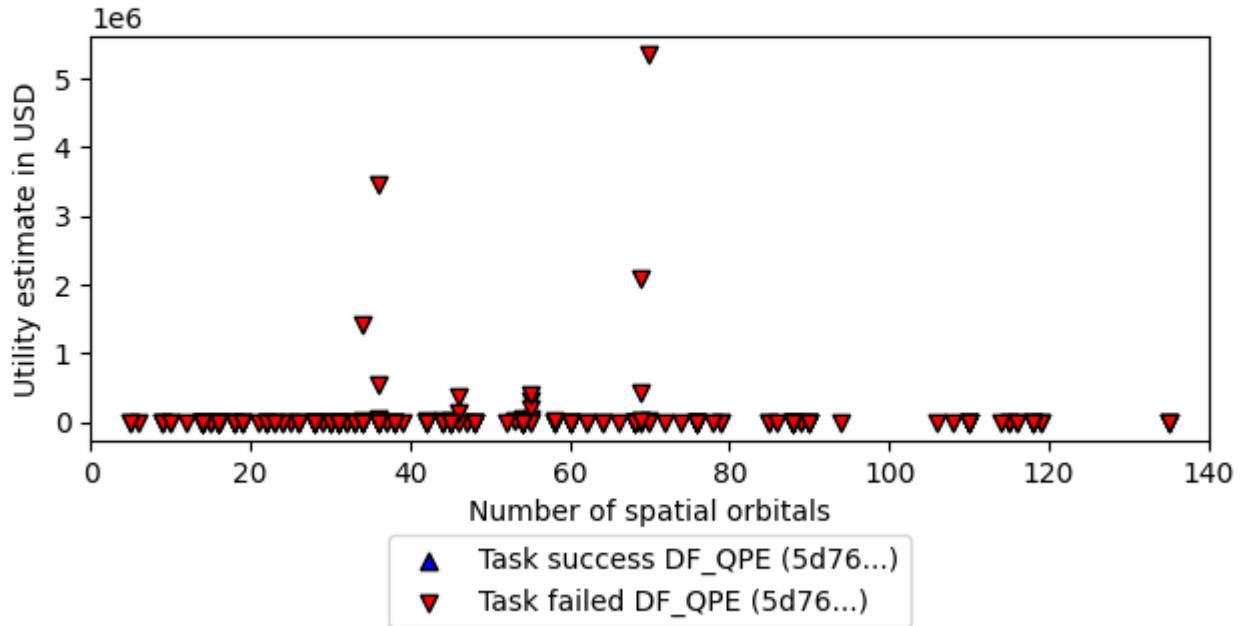


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5d76...
(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 DF_QPE, 5dad4064-cd11-412f-85cb-d722afe3b3de

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by

DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70} }

software_details:[{'software_name': 'pyLIQTR', 'software_version': '1.3.4'}, {'software_name': 'qb-gsee-benchmark', 'software_version': '0.1.0a2.dev193+g879c00d'}, {'software_name': 'Python', 'software_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]'}, {'software_name': 'qualtran', 'software_version': '0.4.0'}]

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

logical_resource_estimate_solution_uuid:e54dd6a9-6481-452a-a6e9-31c8e53cdb75

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

performance_metrics_uuid: e14406a3-3271-4d83-b884-3c3631e8dc17

creation_timestamp: 2025-02-19T18:26:13.854054+00:00

number_of_problem_instances: 88

number_of_problem_instances_attempted: 22

number_of_problem_instances_solved: 0

number_of_tasks: 280

number_of_tasks_attempted: 154

number_of_tasks_solved: 0

number_of_tasks_solved_within_run_time_limit: 0

number_of_tasks_solved_within_accuracy_threshold: 154

max_run_time_of_attempted_tasks: 1394068547267.4111

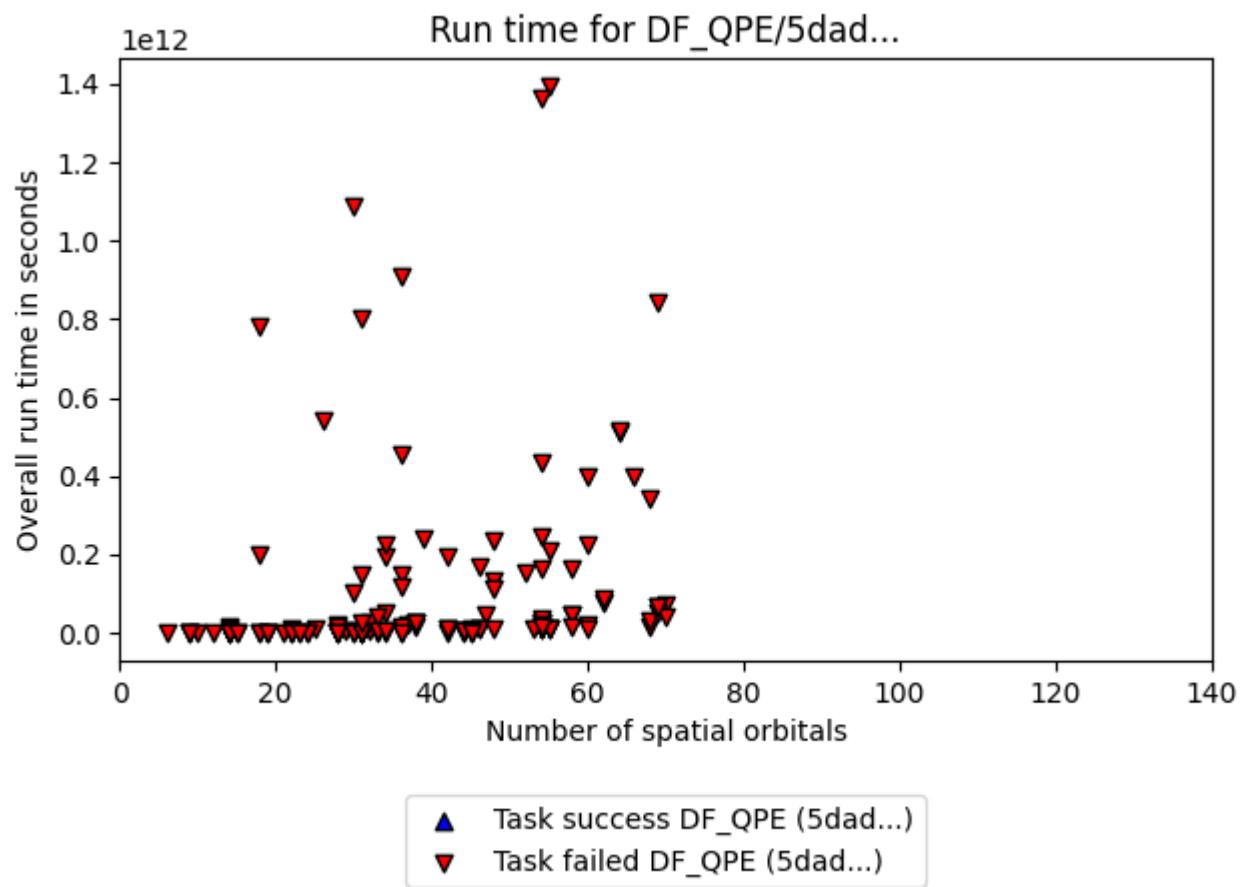
sum_of_run_time_of_attempted_tasks: 15652541022388.93

solvability_ratio: None

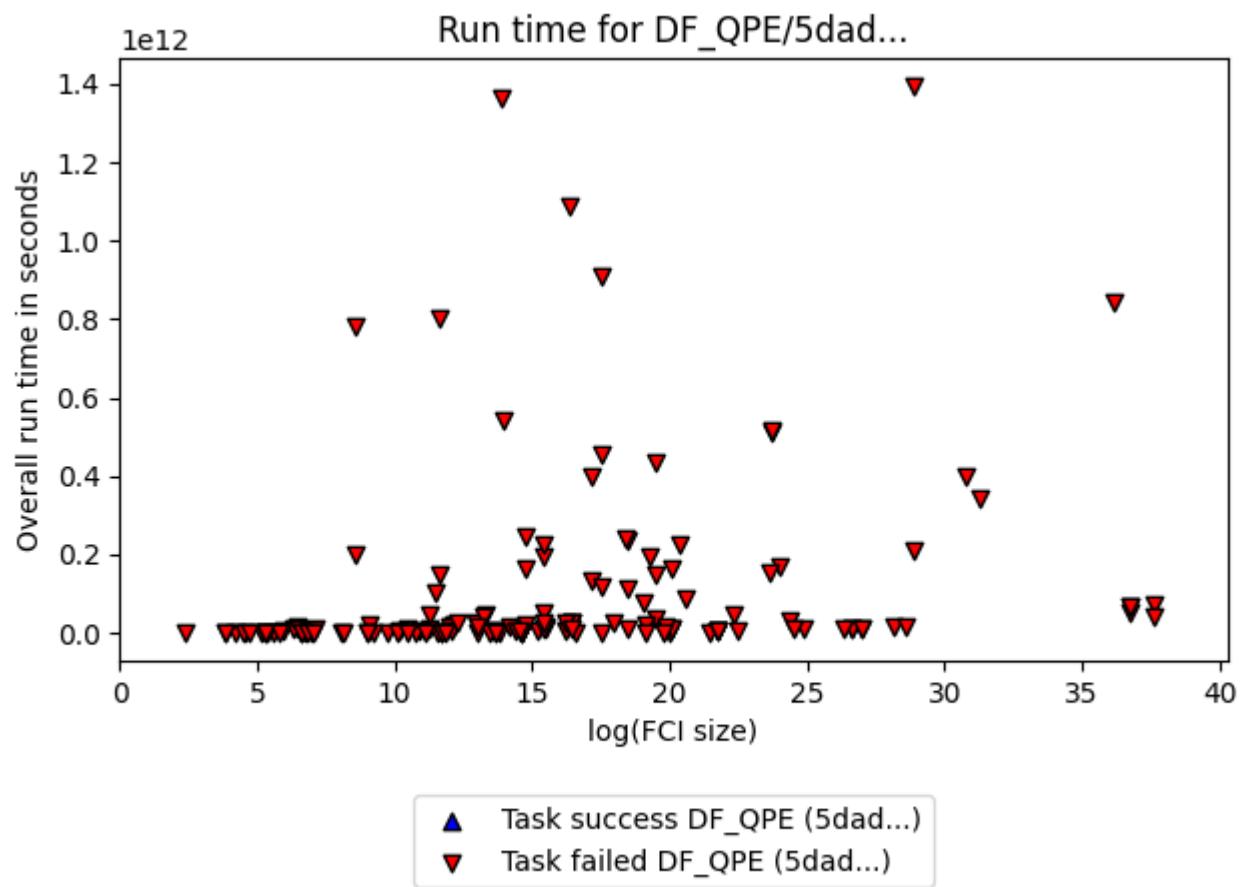
f1_score: None

ml_metrics_calculator_version: 1

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

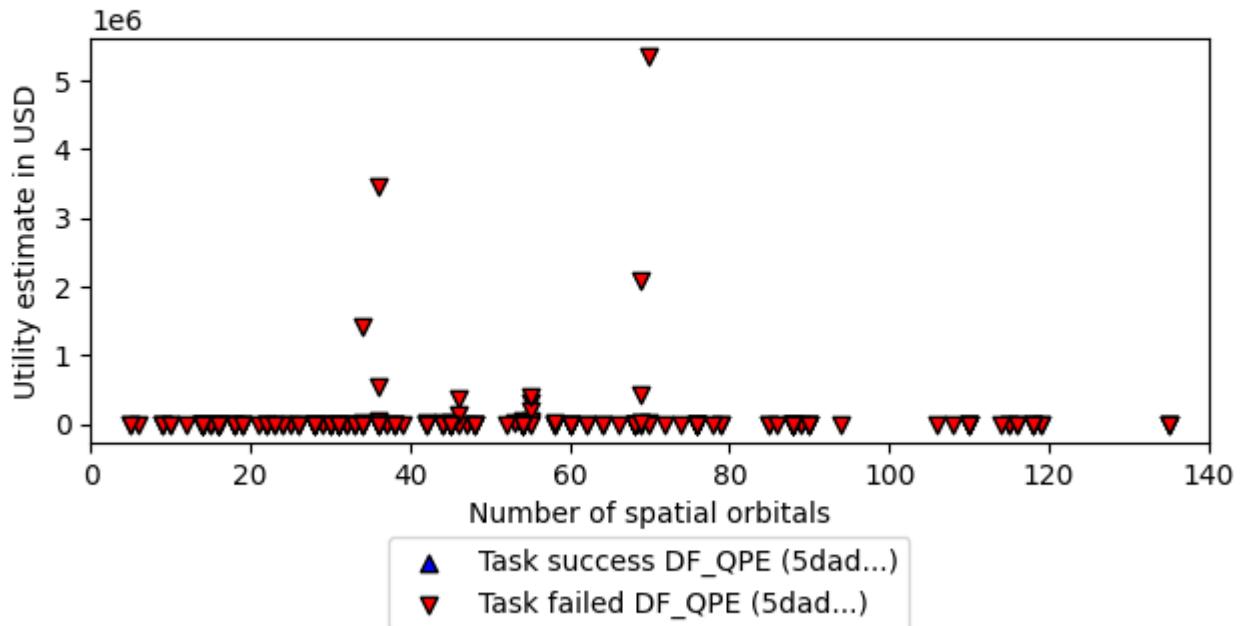


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/5dad...
(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 CISD, 418f060e-496b-4024-8d2d-9b1f8791e76d

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

solver_short_name:CISD

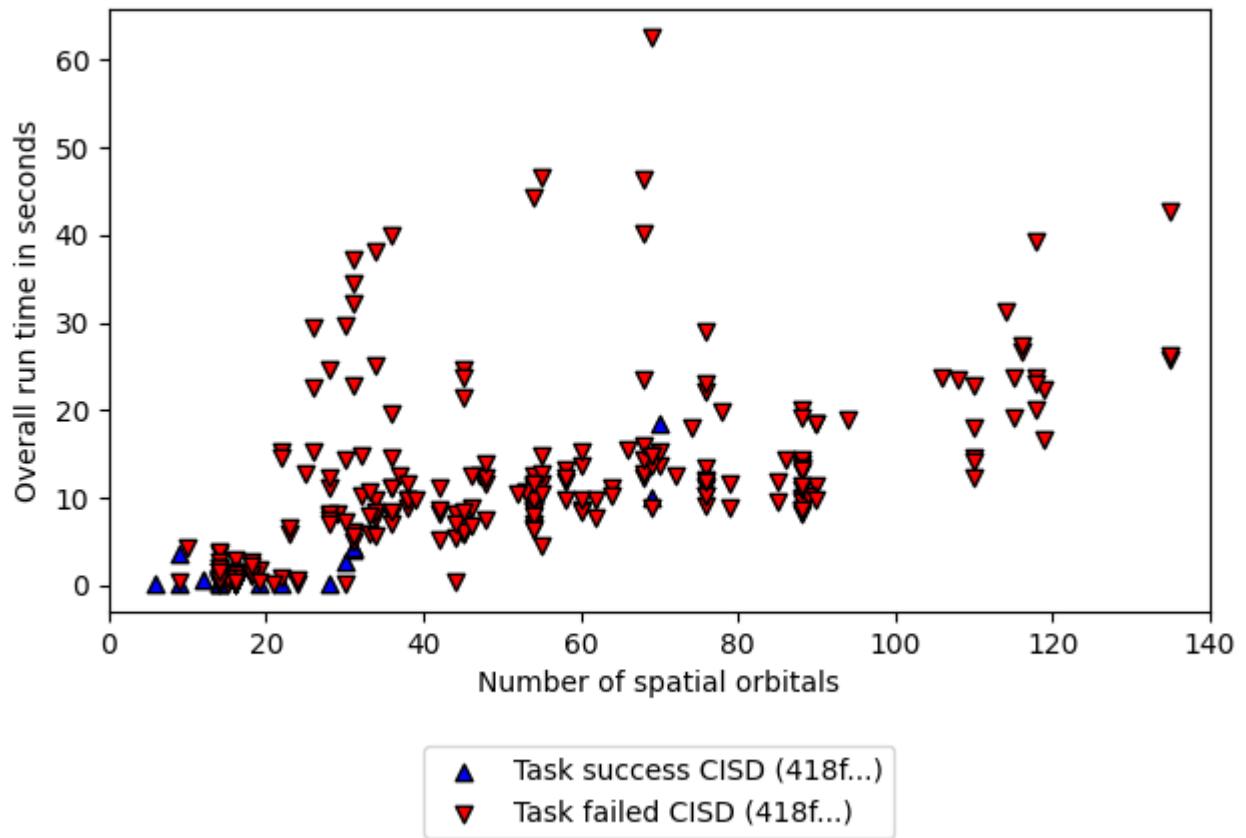
compute.hardware_type:classical_computer

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

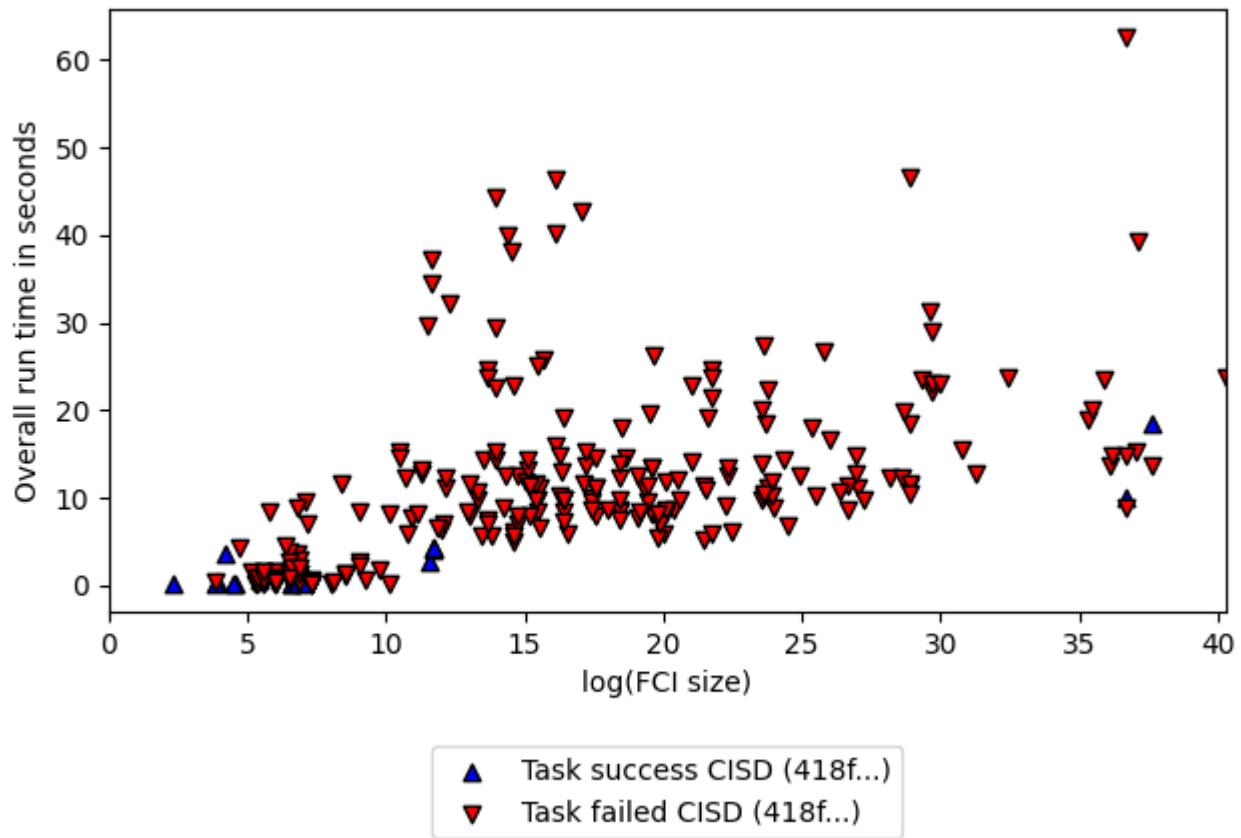
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 7e530c12-a17e-44c1-a57c-432ec044bfa4
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 84
number_of_problem_instances_solved: 9
number_of_tasks: 280
number_of_tasks_attempted: 276
number_of_tasks_solved: 17
number_of_tasks_solved_within_run_time_limit: 276
number_of_tasks_solved_within_accuracy_threshold: 17
max_run_time_of_attempted_tasks: 62.58296537399292
sum_of_run_time_of_attempted_tasks: 2929.870177745819
solvability_ratio: 0.0498
comment: solvability ratio based on PCA embedding.
f1_score: [0.9752650176678446, 0.8292682926829268]
ml_metrics_calculator_version: 1

Run time for CISD/418f...



Note: plot only contains attempted tasks.

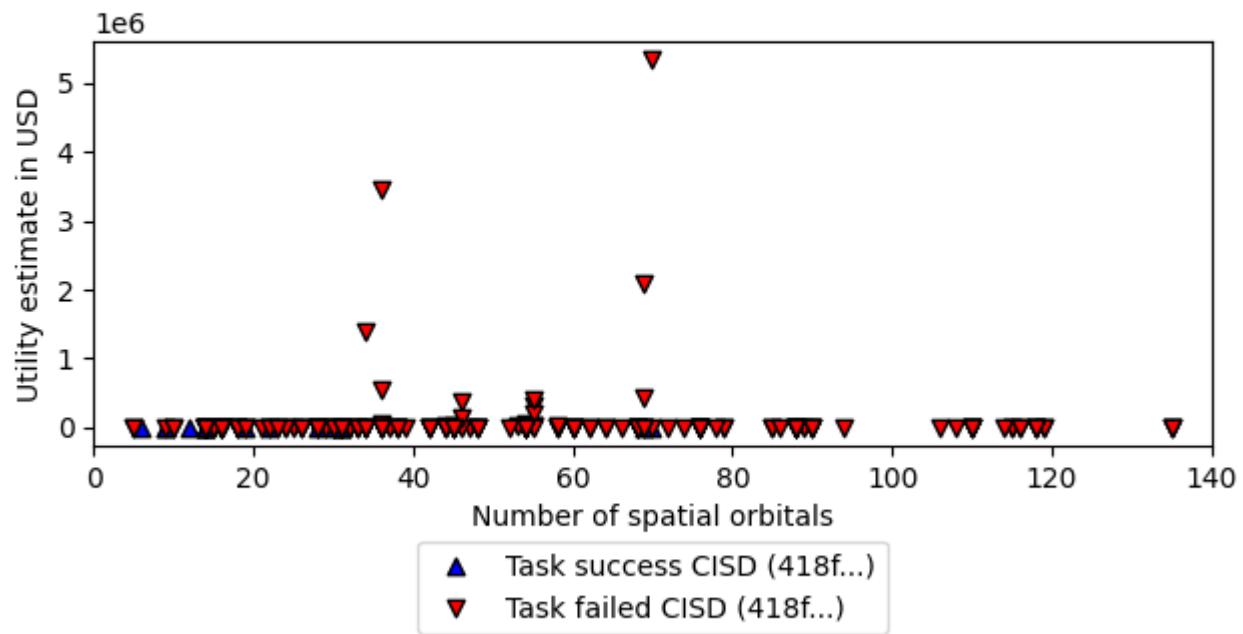
Run time for CISD/418f...



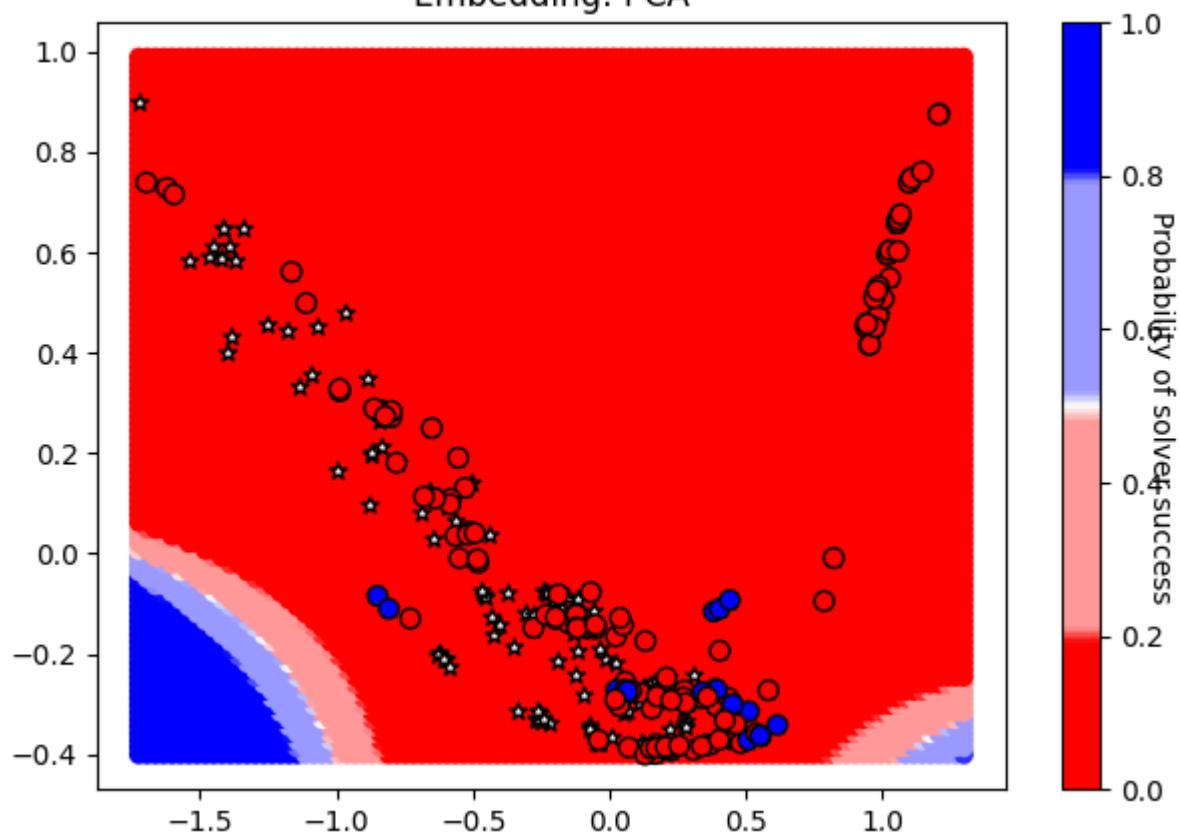
Note: plot only contains attempted tasks.

Utility capture from CISD/418f...

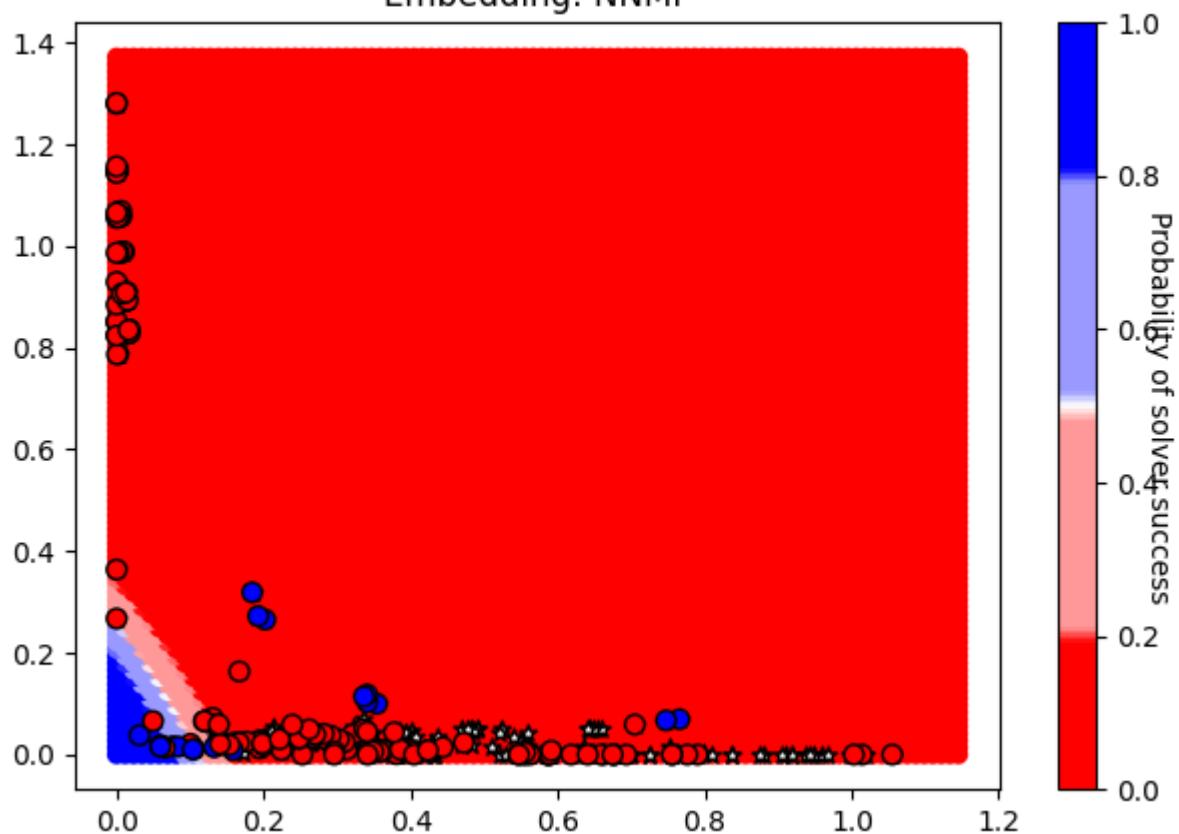
(captured: \$4.8e-03/1.5e+07, approximately 3.2e-08%)



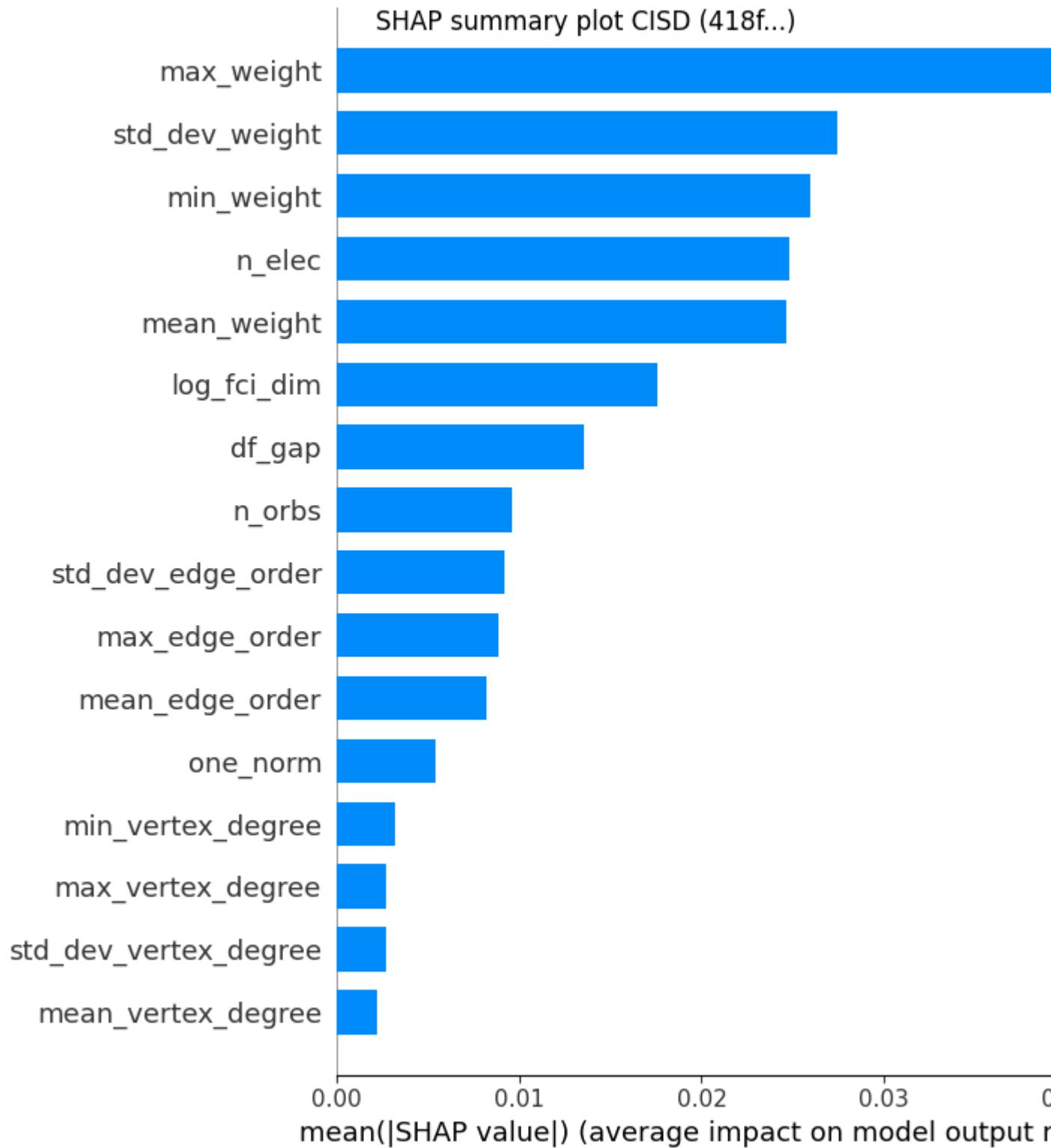
Solver CISD (418f...)
Embedding: PCA



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



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



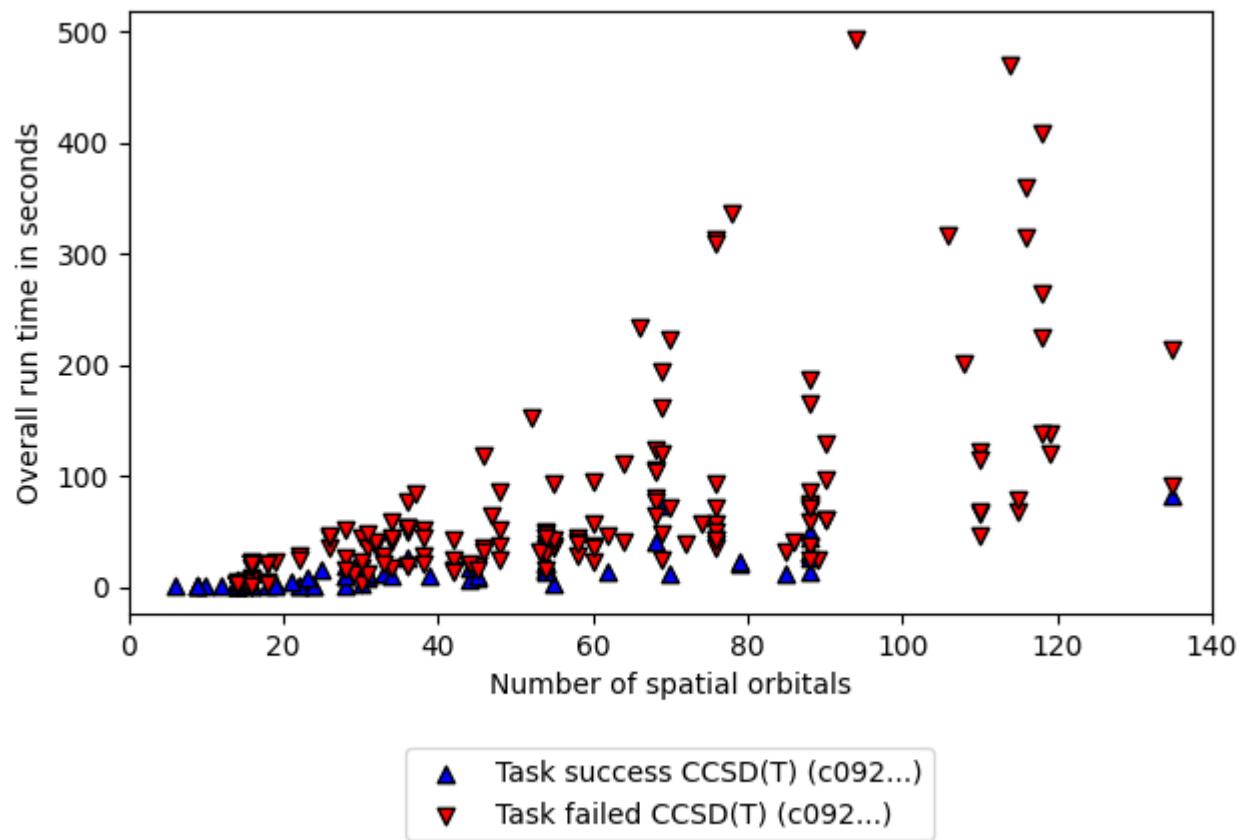
Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878

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

solver_short_name:CCSD(T)

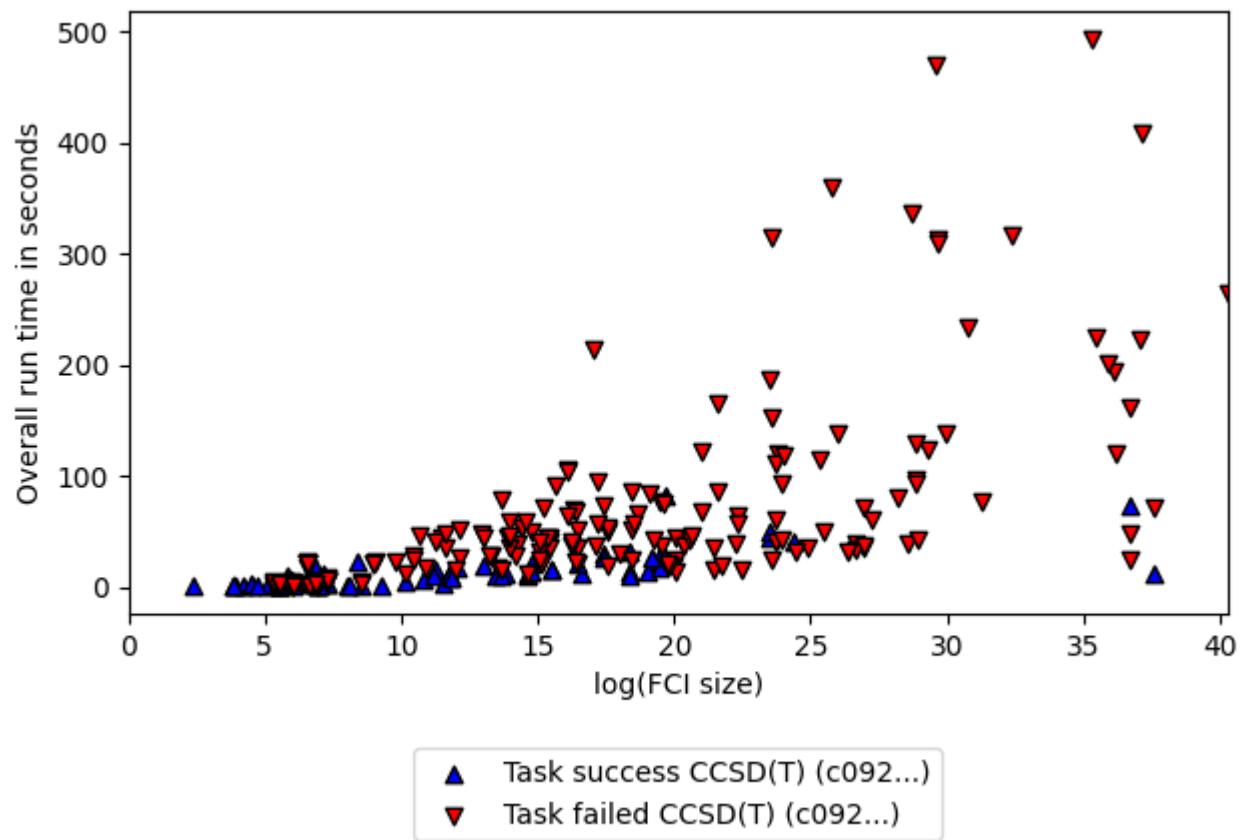
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD(T)
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 862a9612-50aa-4ad5-b803-96c220651957
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 79
number_of_problem_instances_solved: 19
number_of_tasks: 280
number_of_tasks_attempted: 264
number_of_tasks_solved: 71
number_of_tasks_solved_within_run_time_limit: 264
number_of_tasks_solved_within_accuracy_threshold: 71
max_run_time_of_attempted_tasks: 493.4080808162689
sum_of_run_time_of_attempted_tasks: 13199.317583084106
solvability_ratio: 0.2424
comment: solvability ratio based on PCA embedding.
f1_score: [0.9239766081871345, 0.9150326797385621]
ml_metrics_calculator_version: 1

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



Note: plot only contains attempted tasks.

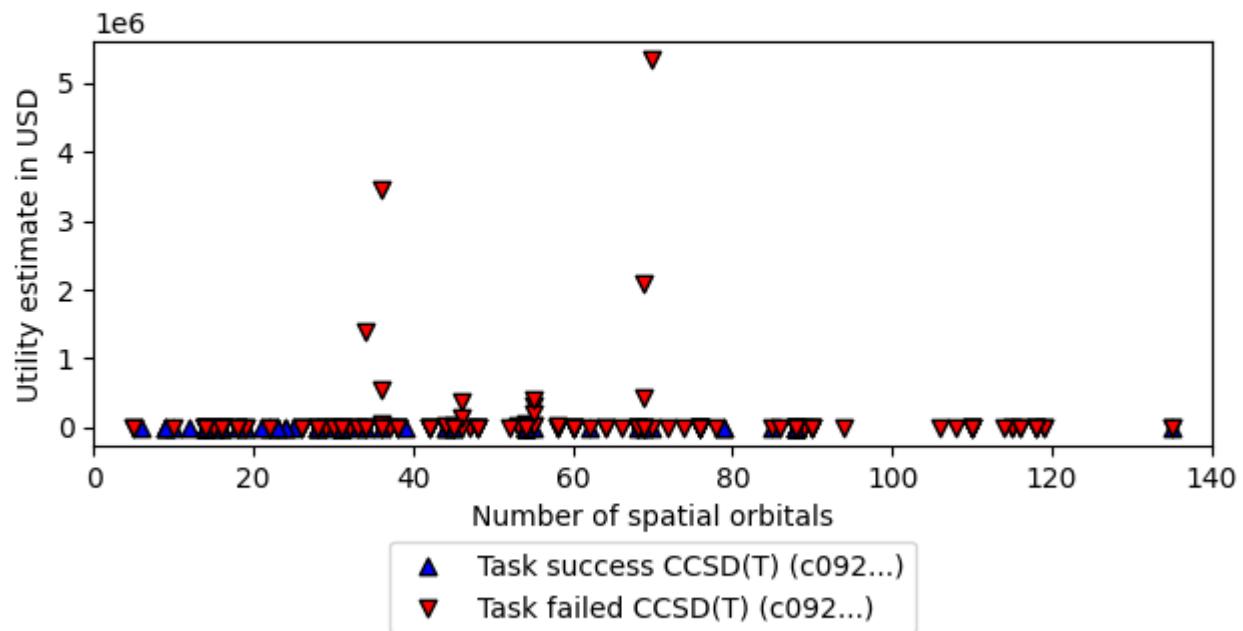
Run time for CCSD(T)/c092...



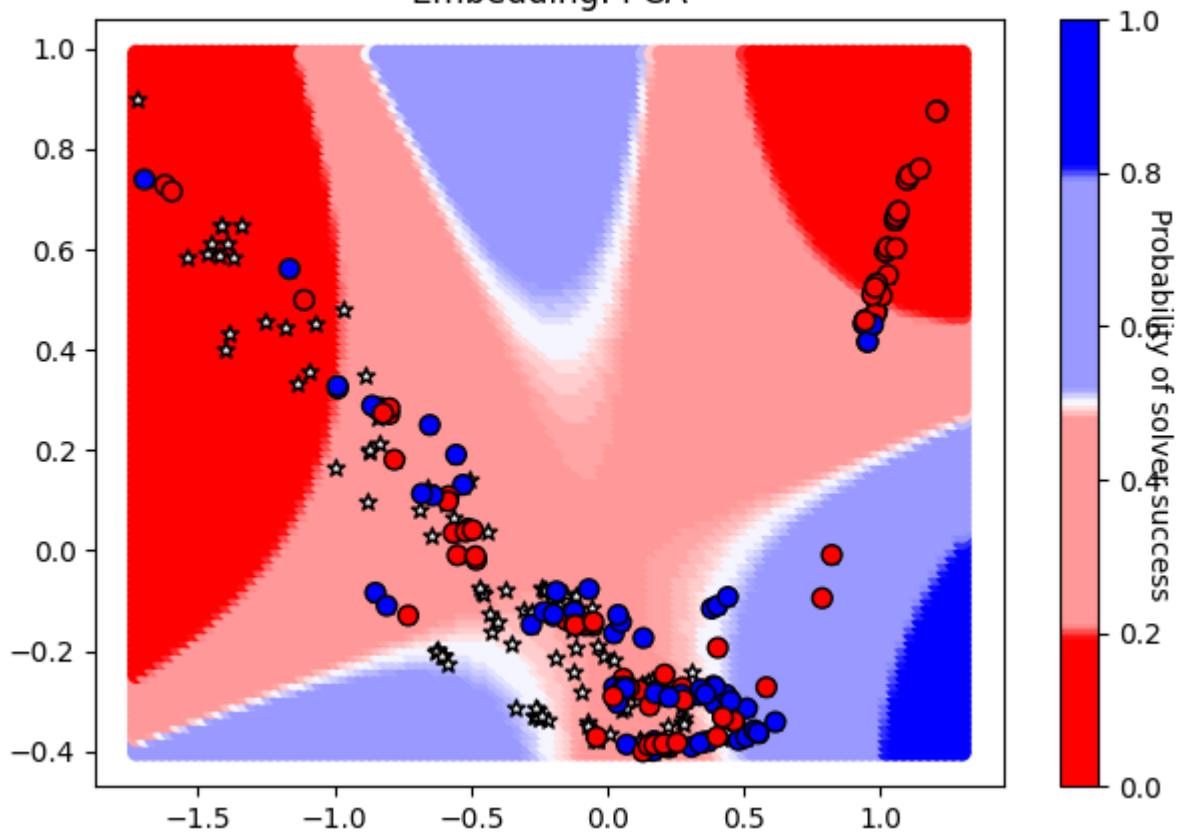
Note: plot only contains attempted tasks.

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

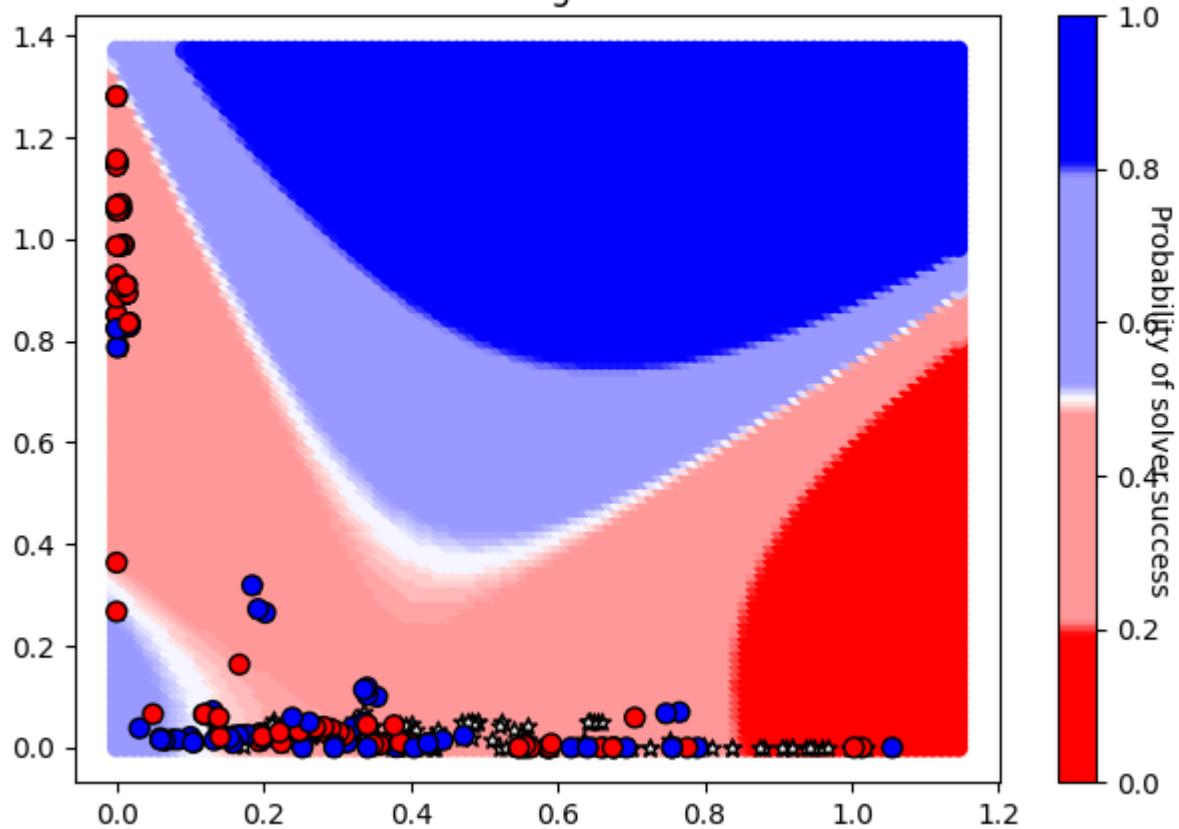
(captured: $\$1.8e+02/1.5e+07$, approximately $1.2e-03\%$)



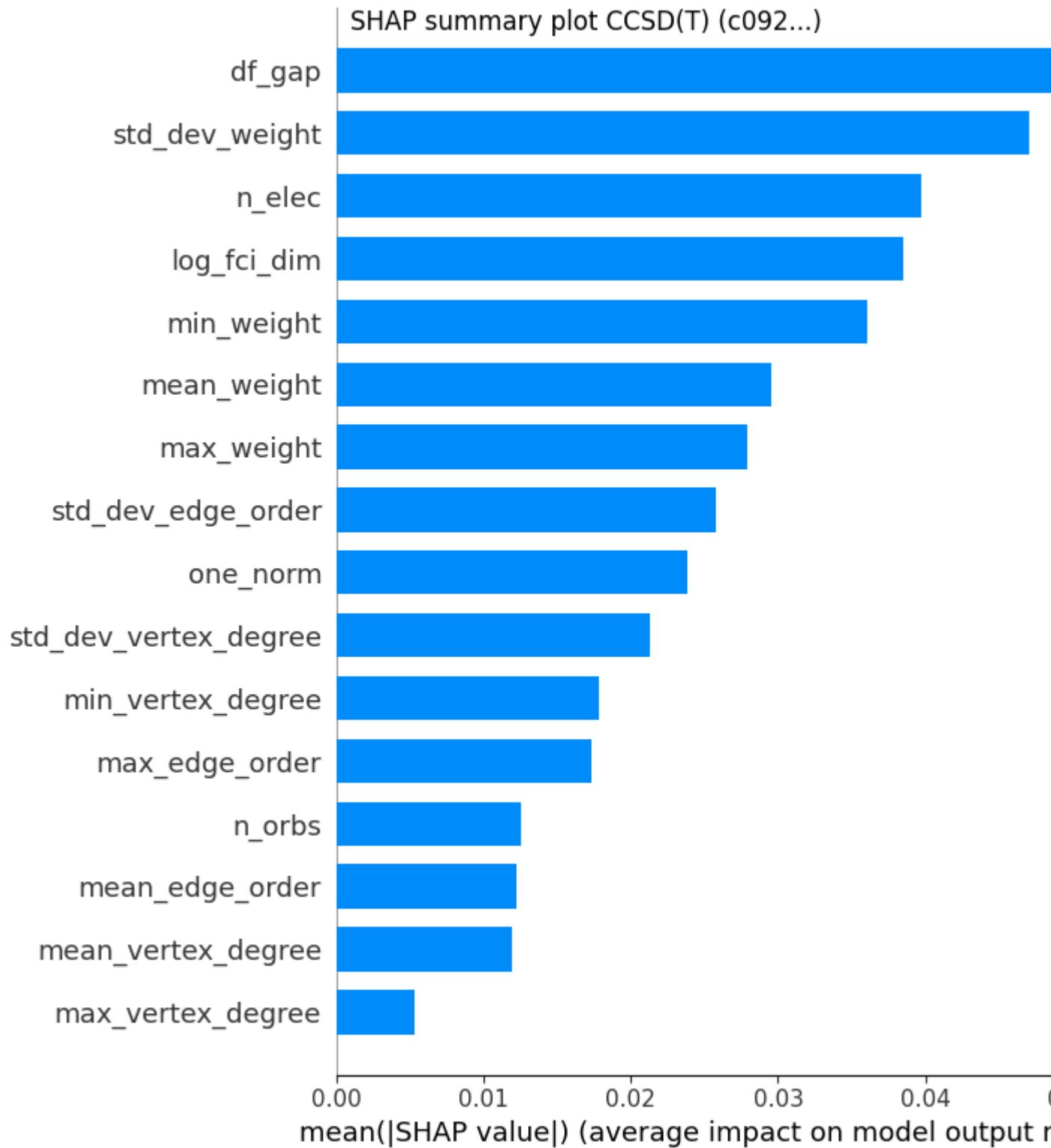
Solver CCSD(T) (c092...)
Embedding: PCA



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



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



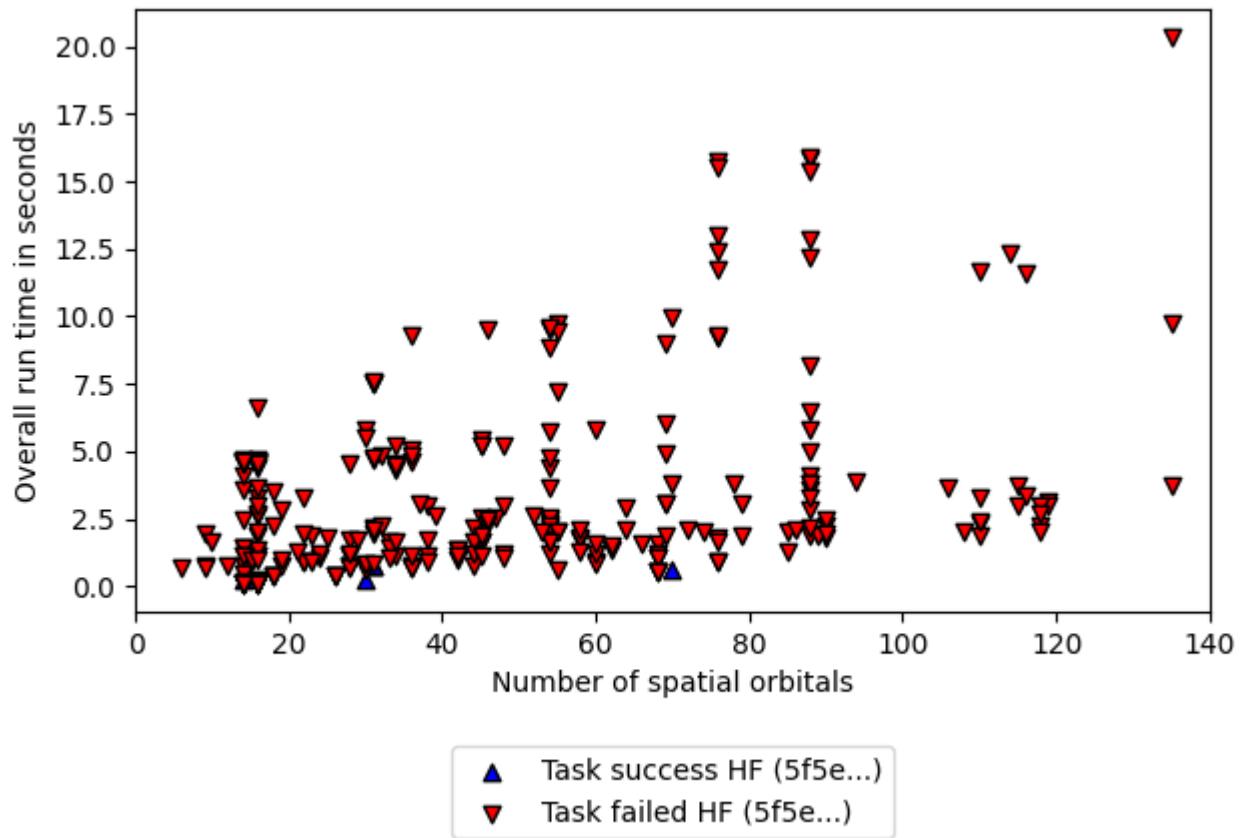
Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

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

solver_short_name:HF

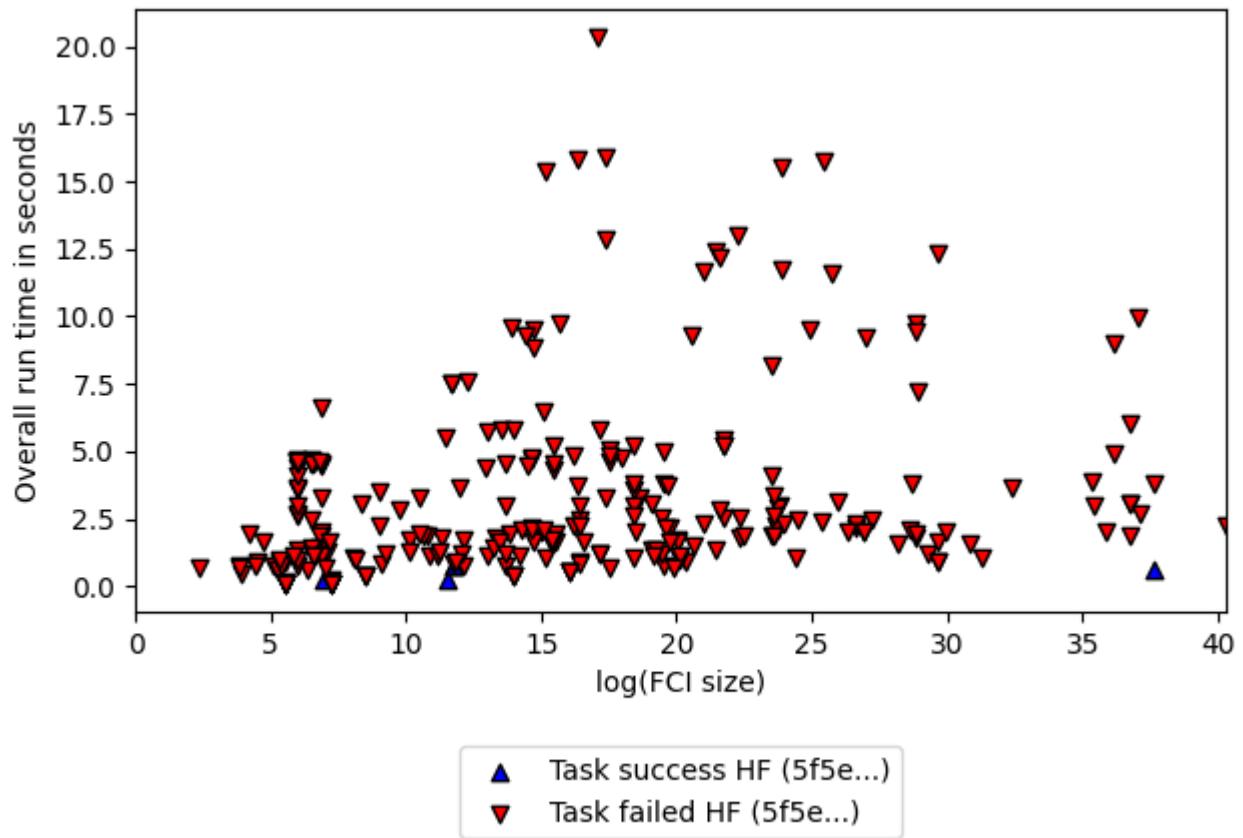
compute.hardware_type:classical_computer
classical.hardware.details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm.details:Hartree Fock
software.details:pyscf (<https://github.com/pyscf/pyscf>).
performance.metrics.uuid: 0f5ad36d-f43c-4ffa-b65c-b29f35773a8a
creation.timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 84
number_of_problem_instances_solved: 5
number_of_tasks: 280
number_of_tasks_attempted: 276
number_of_tasks_solved: 5
number_of_tasks_solved_within_run_time_limit: 276
number_of_tasks_solved_within_accuracy_threshold: 5
max_run_time_of_attempted_tasks: 20.338801622390747
sum_of_run_time_of_attempted_tasks: 906.4860525131226
solvability_ratio: 0.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.9870967741935484, 0.7142857142857143]
ml.metrics_calculator_version: 1

Run time for HF/5f5e...



Note: plot only contains attempted tasks.

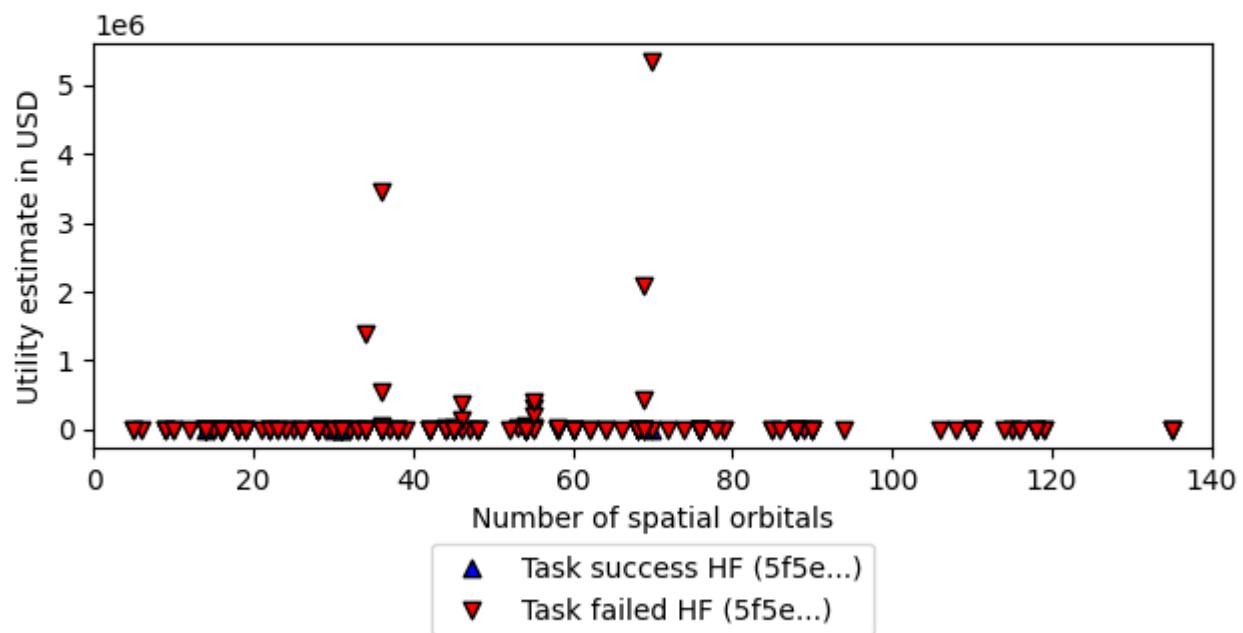
Run time for HF/5f5e...



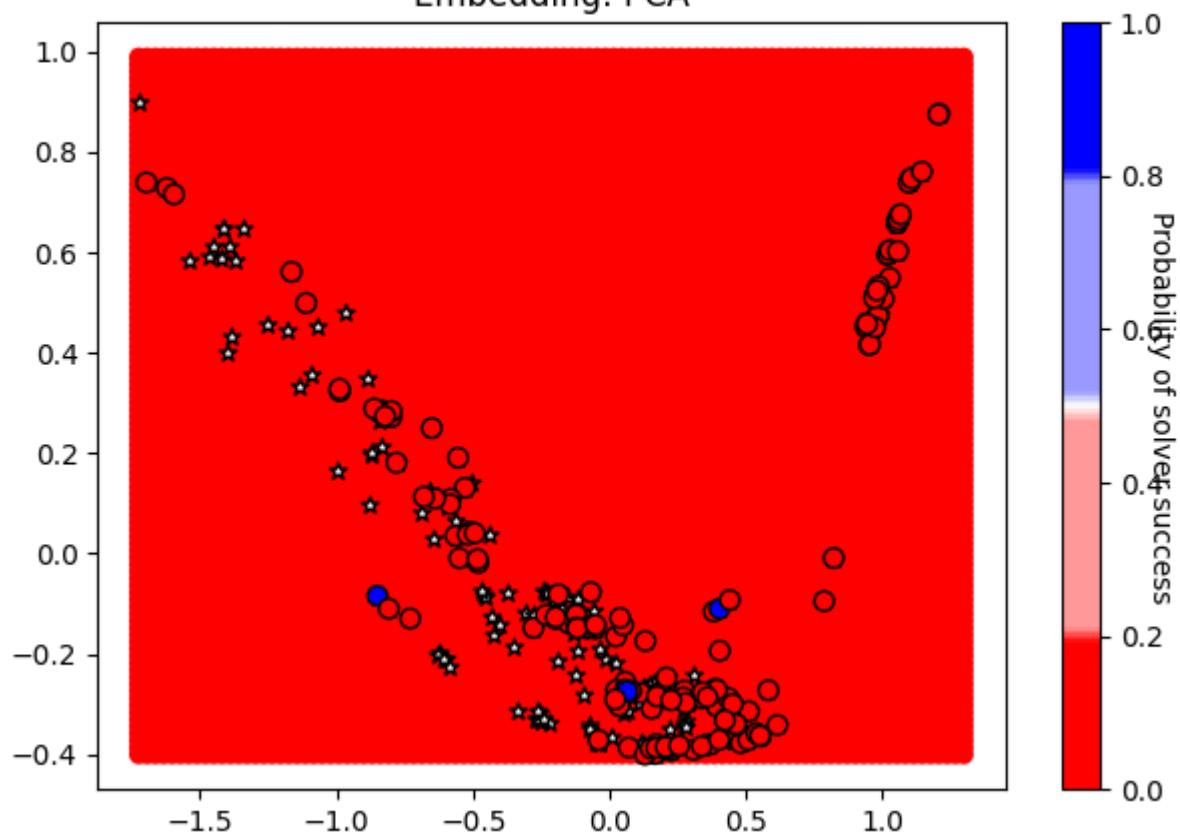
Note: plot only contains attempted tasks.

Utility capture from HF/5f5e...

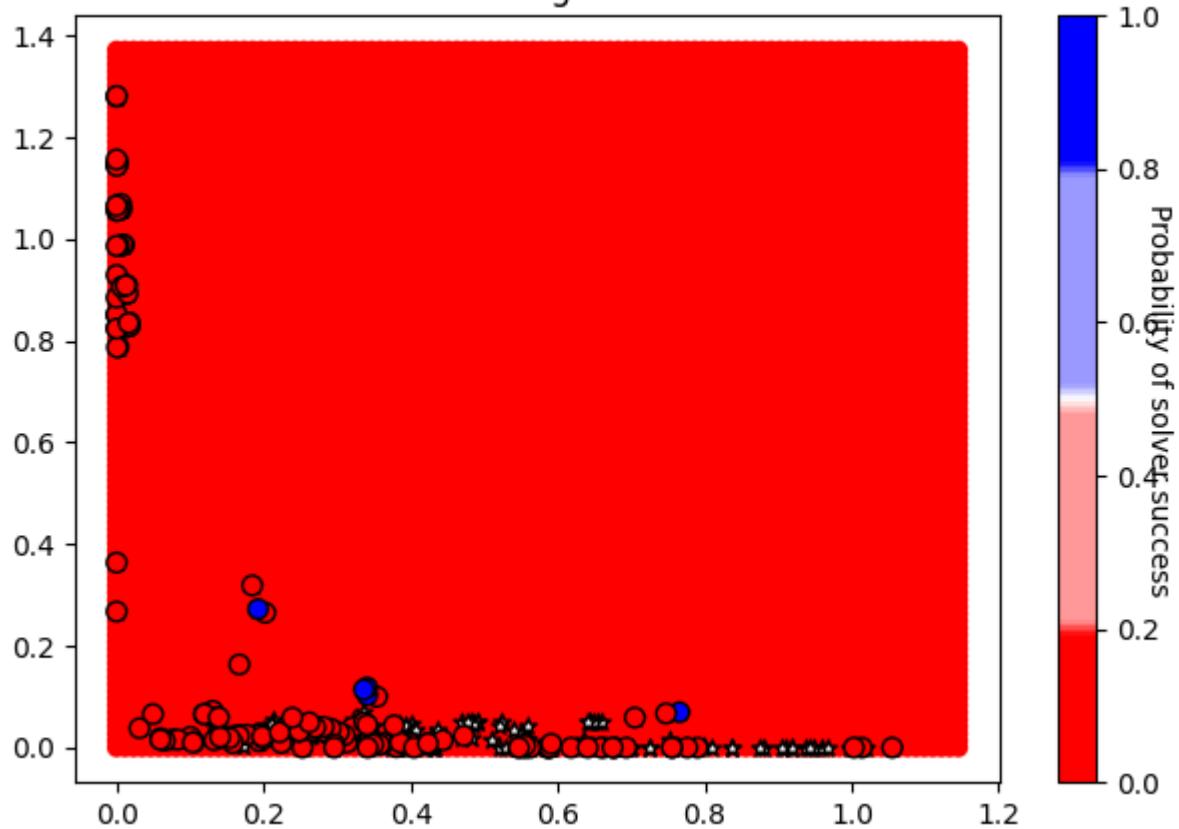
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



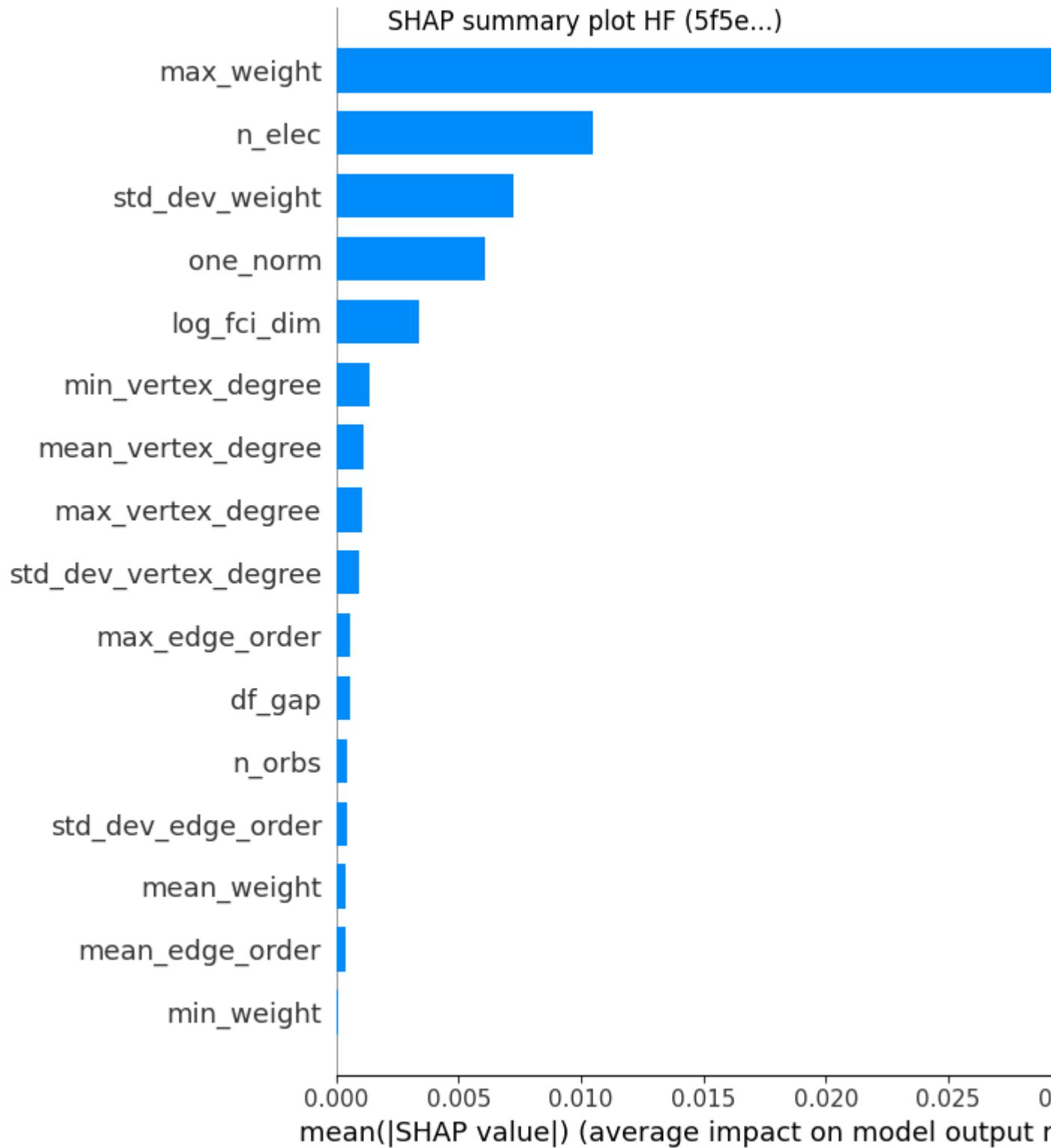
Solver HF (5f5e...)
Embedding: PCA



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



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



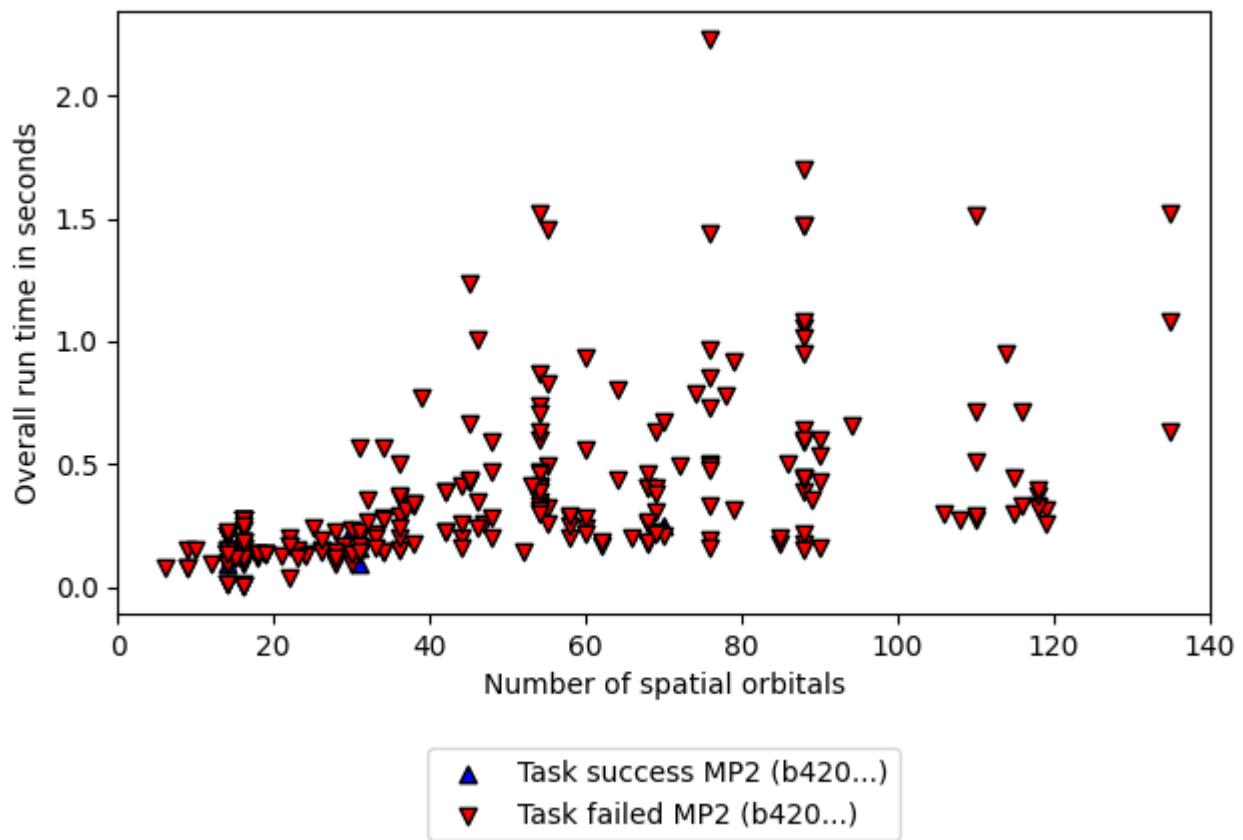
Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aecd2

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

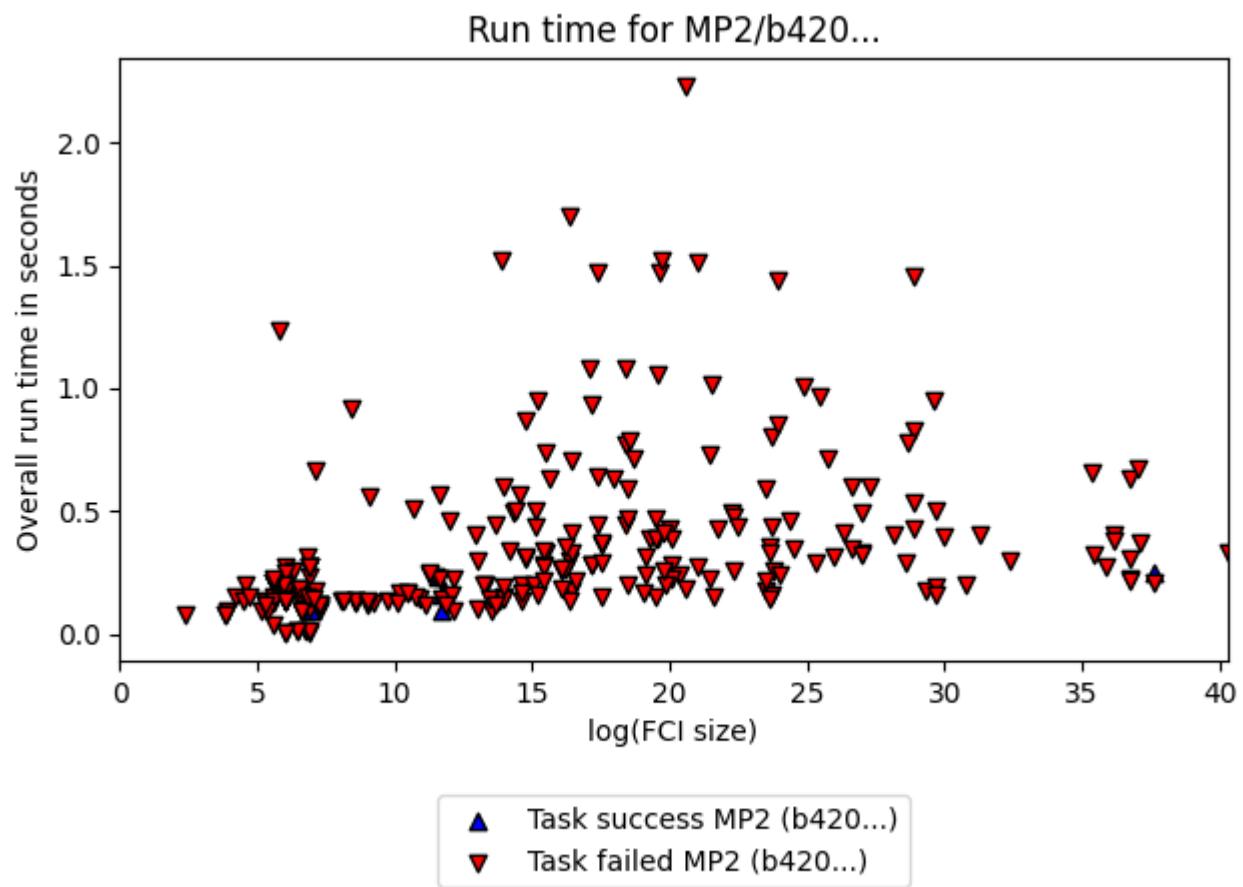
solver_short_name:MP2

compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:MP2
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 0fe19268-d797-46f3-997d-841eb8ed2e78
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 81
number_of_problem_instances_solved: 5
number_of_tasks: 280
number_of_tasks_attempted: 268
number_of_tasks_solved: 5
number_of_tasks_solved_within_run_time_limit: 268
number_of_tasks_solved_within_accuracy_threshold: 5
max_run_time_of_attempted_tasks: 2.230440139770508
sum_of_run_time_of_attempted_tasks: 94.7442626953125
solvability_ratio: 0.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.9870967741935484, 0.7142857142857143]
ml_metrics_calculator_version: 1

Run time for MP2/b420...



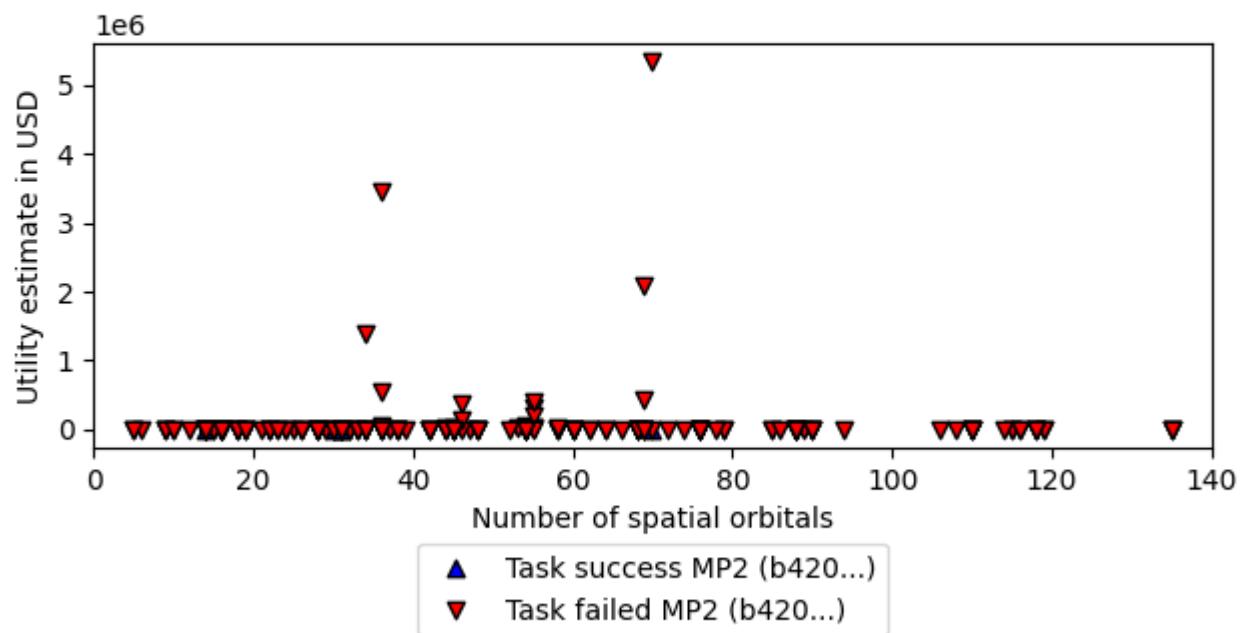
Note: plot only contains attempted tasks.



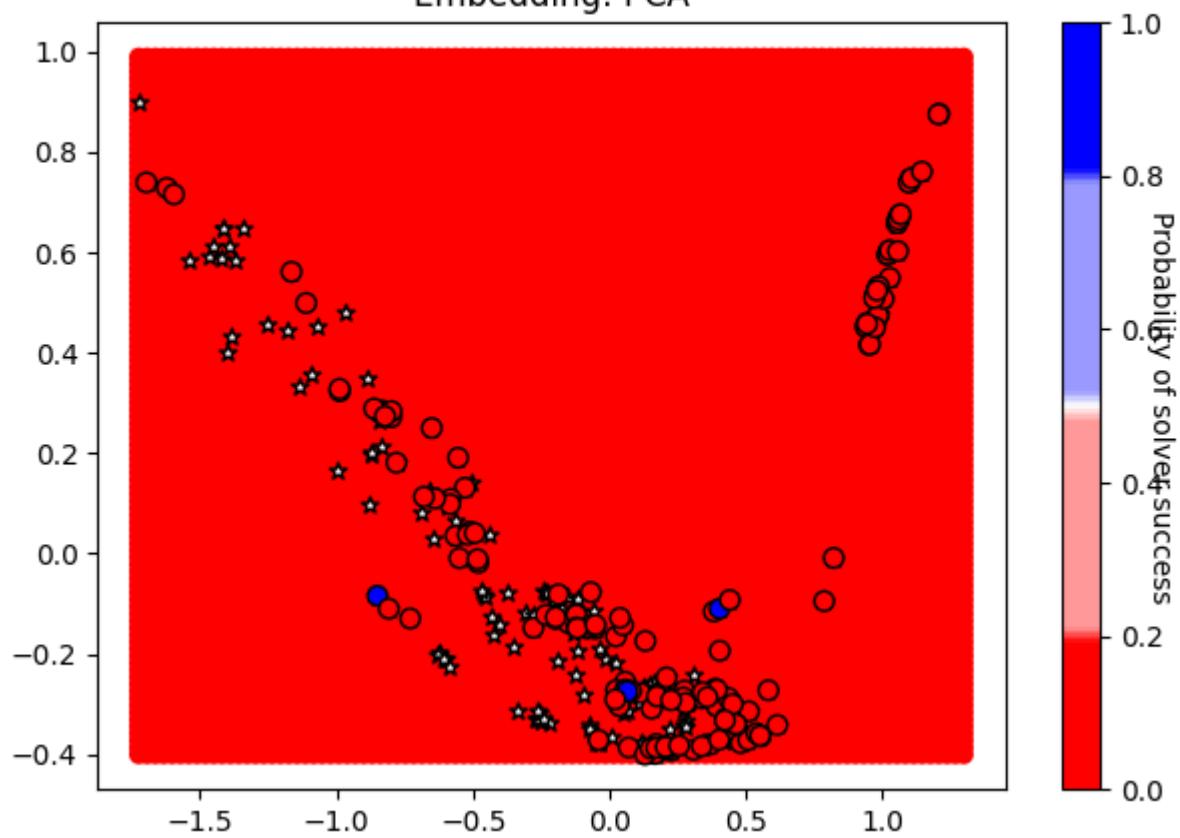
Note: plot only contains attempted tasks.

Utility capture from MP2/b420...

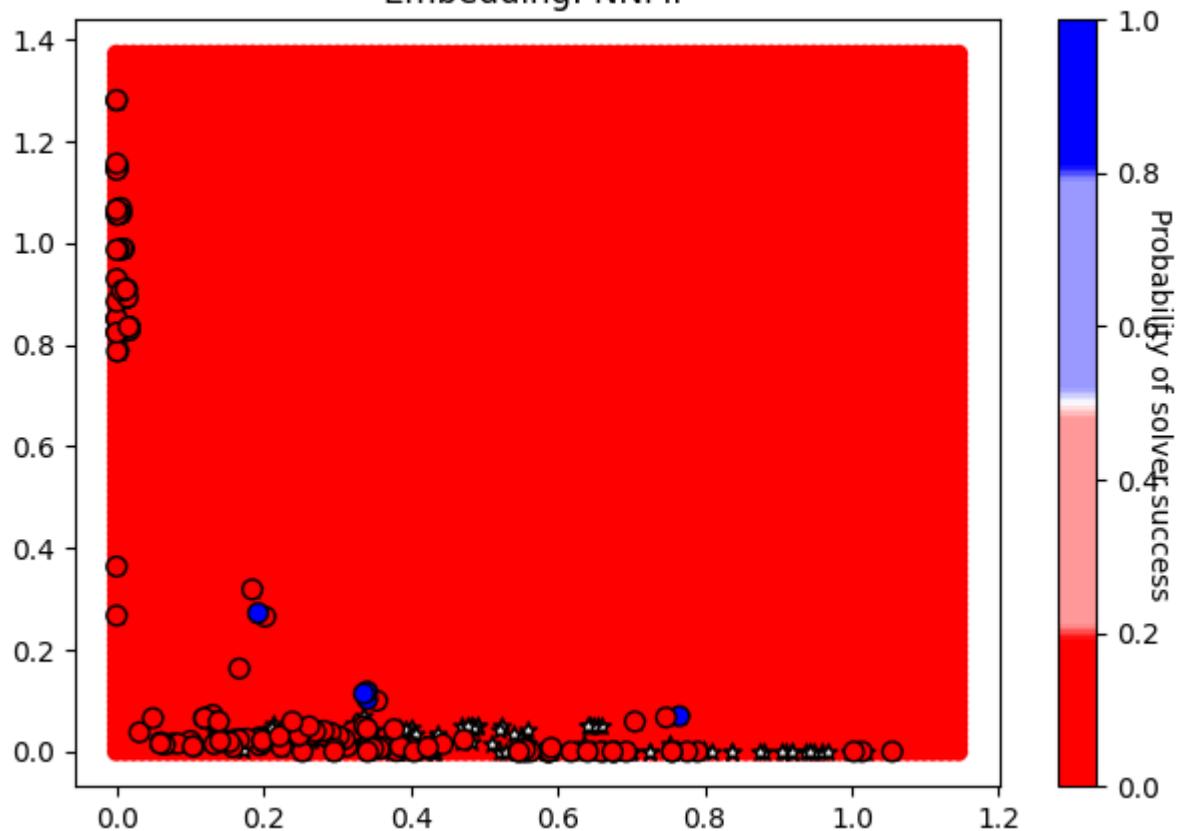
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



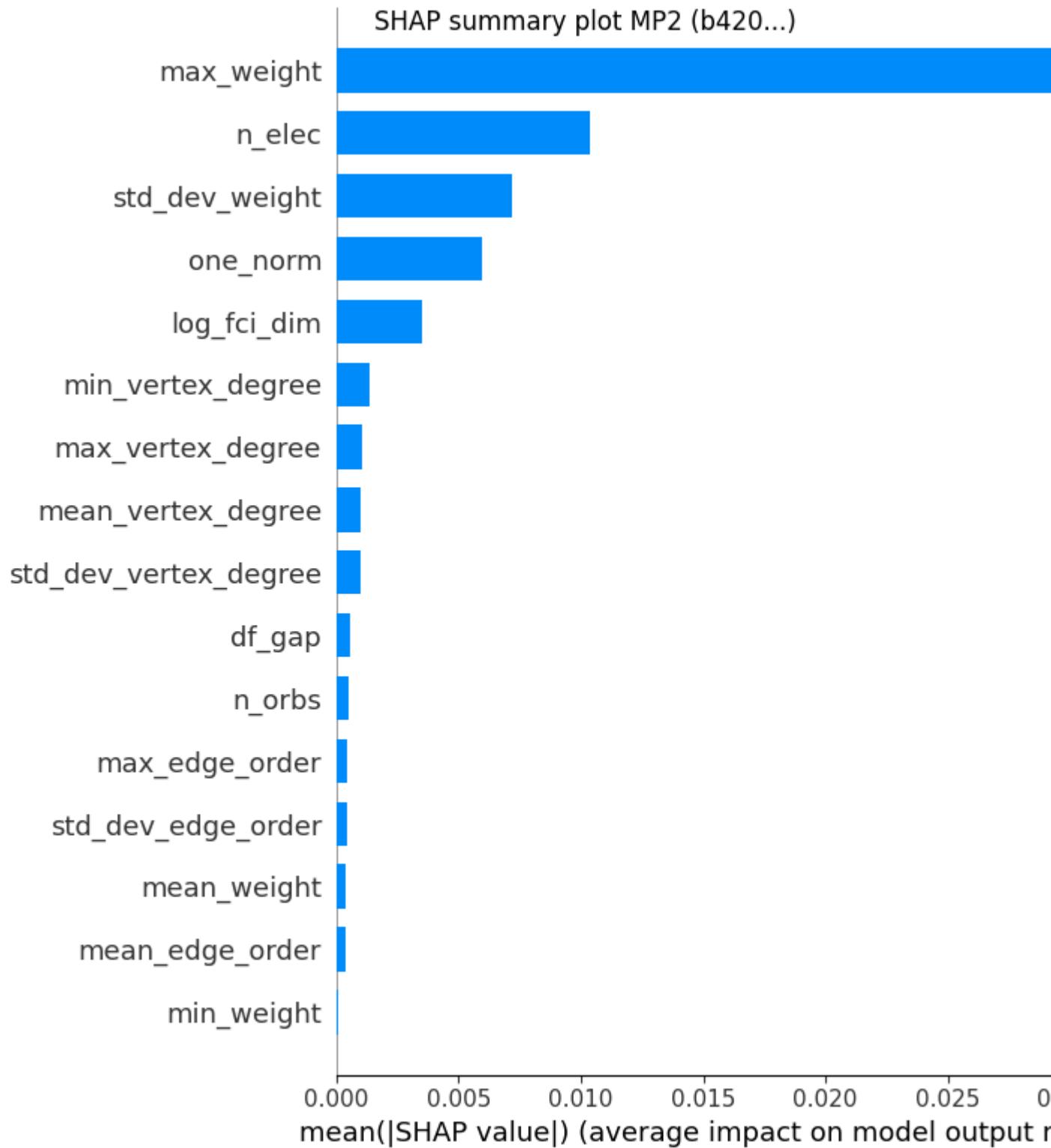
Solver MP2 (b420...)
Embedding: PCA



Solver MP2 (b420...)
Embedding: NNMF



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



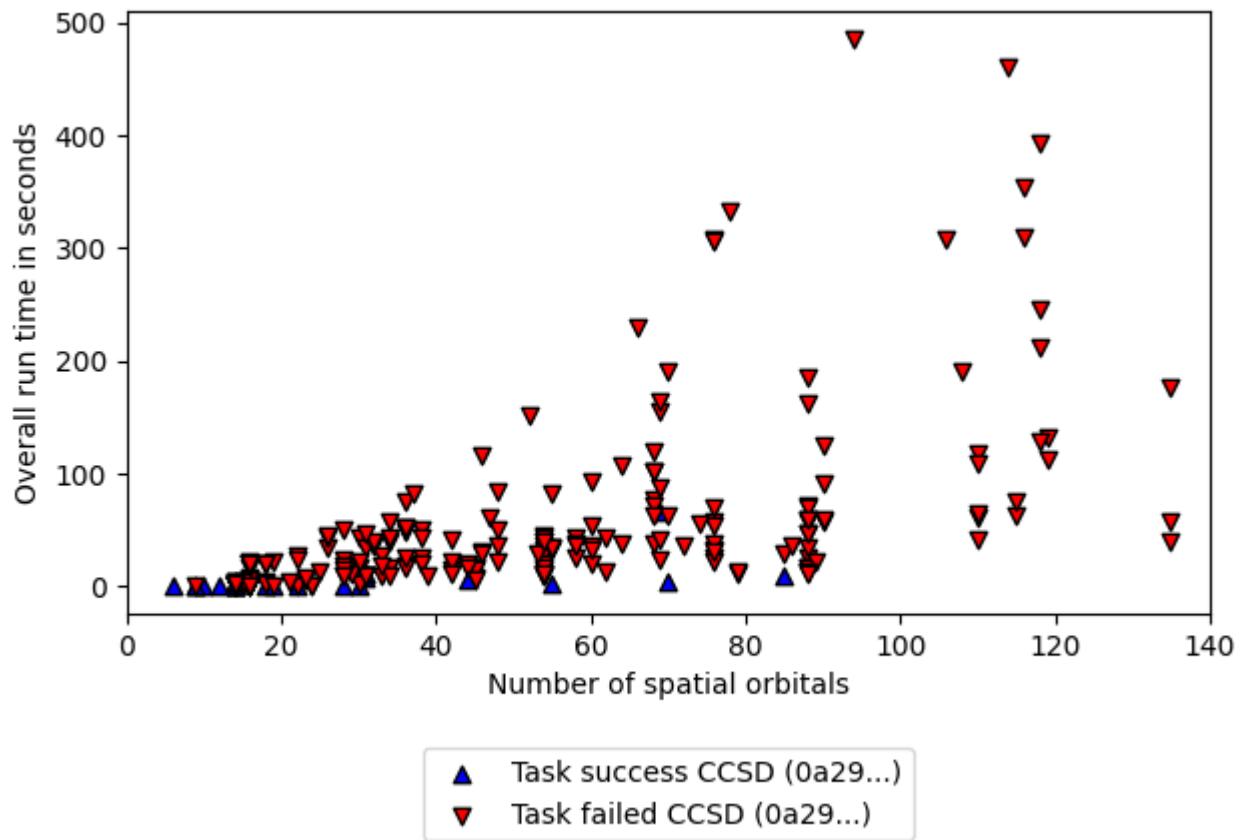
Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

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

solver_short_name:CCSD

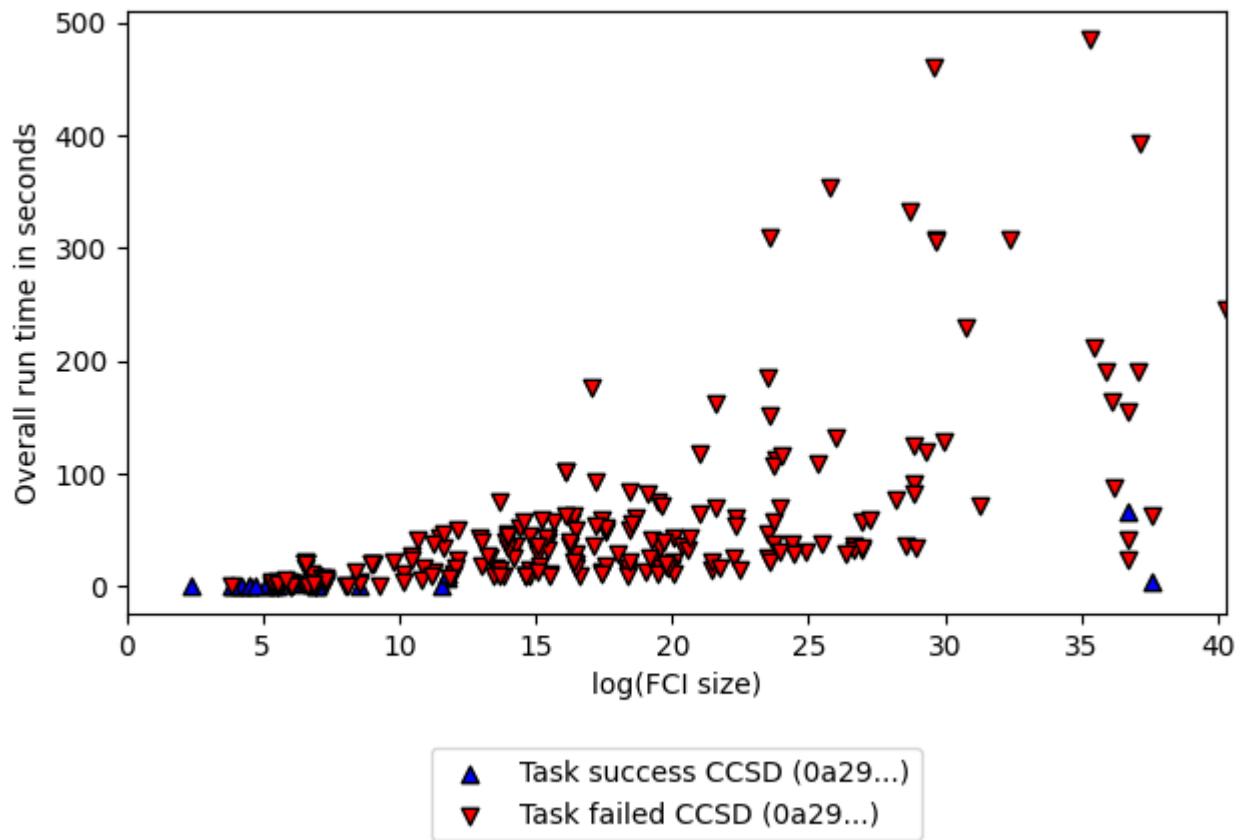
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 99cc28f3-fd40-4dd6-9eef-fd8f7da170e1
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 79
number_of_problem_instances_solved: 10
number_of_tasks: 280
number_of_tasks_attempted: 264
number_of_tasks_solved: 24
number_of_tasks_solved_within_run_time_limit: 264
number_of_tasks_solved_within_accuracy_threshold: 24
max_run_time_of_attempted_tasks: 485.1982181072235
sum_of_run_time_of_attempted_tasks: 12252.72845697403
solvability_ratio: 0.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.9852941176470589, 0.9230769230769231]
ml_metrics_calculator_version: 1

Run time for CCSD/0a29...



Note: plot only contains attempted tasks.

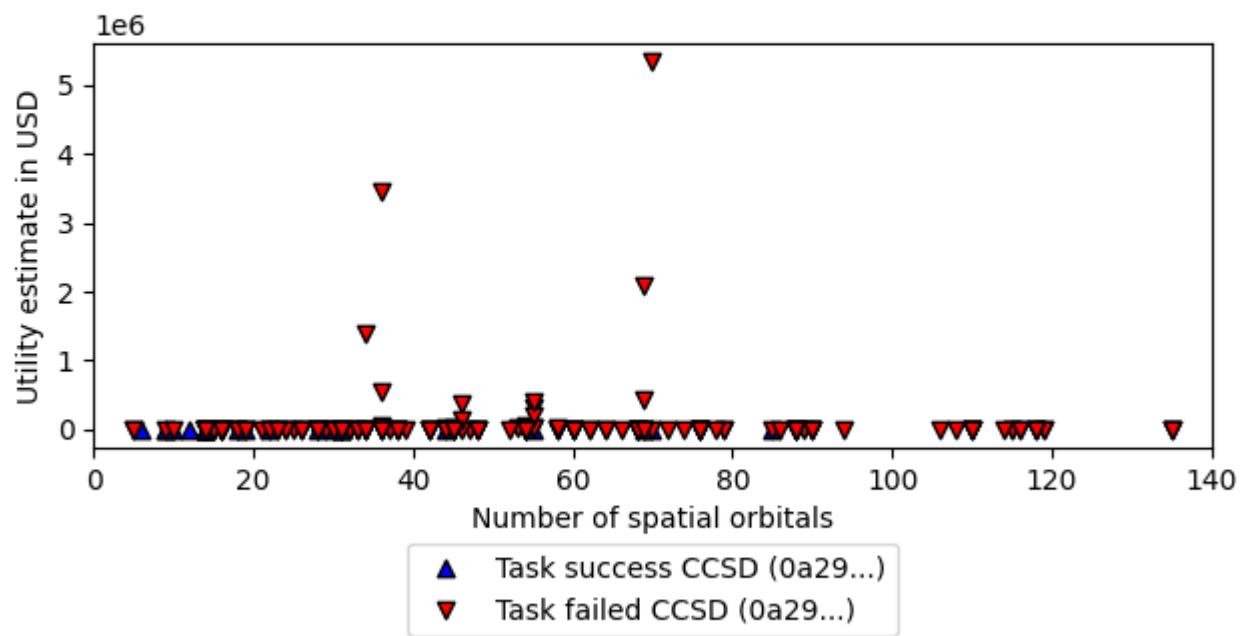
Run time for CCSD/0a29...



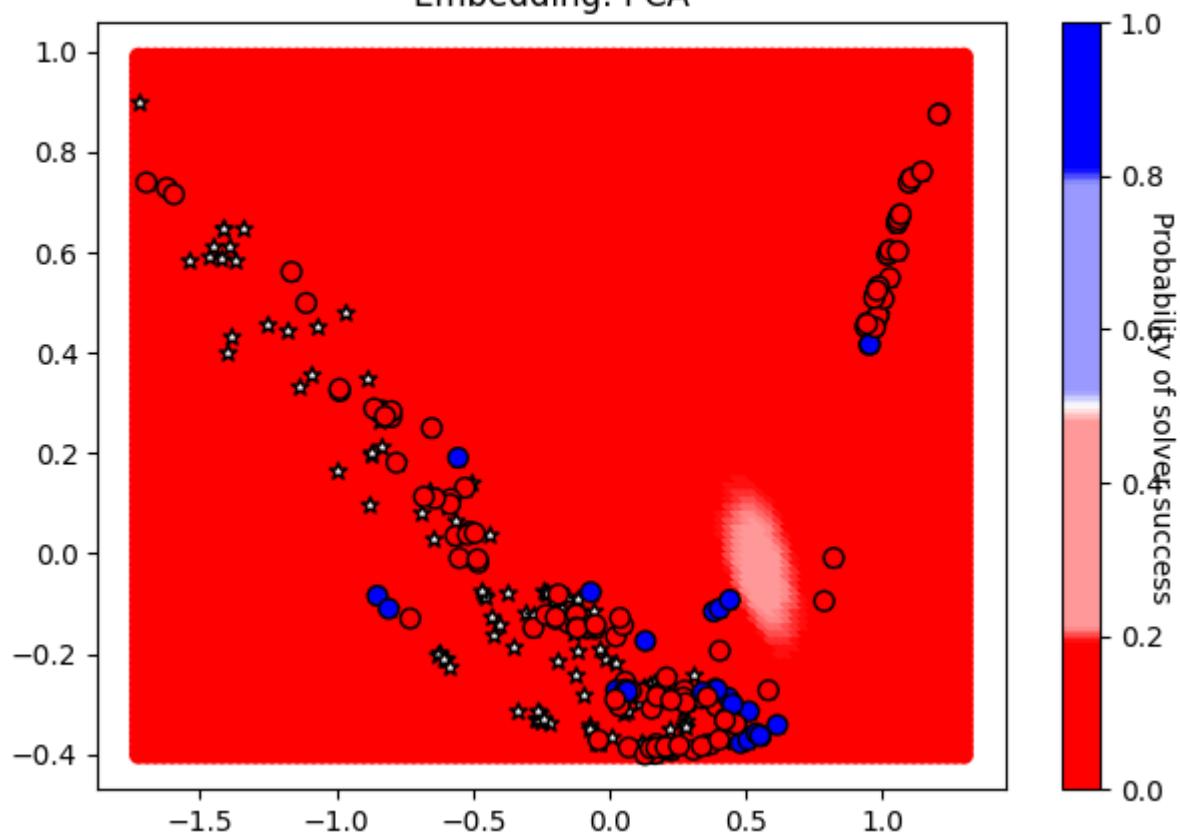
Note: plot only contains attempted tasks.

Utility capture from CCSD/0a29...

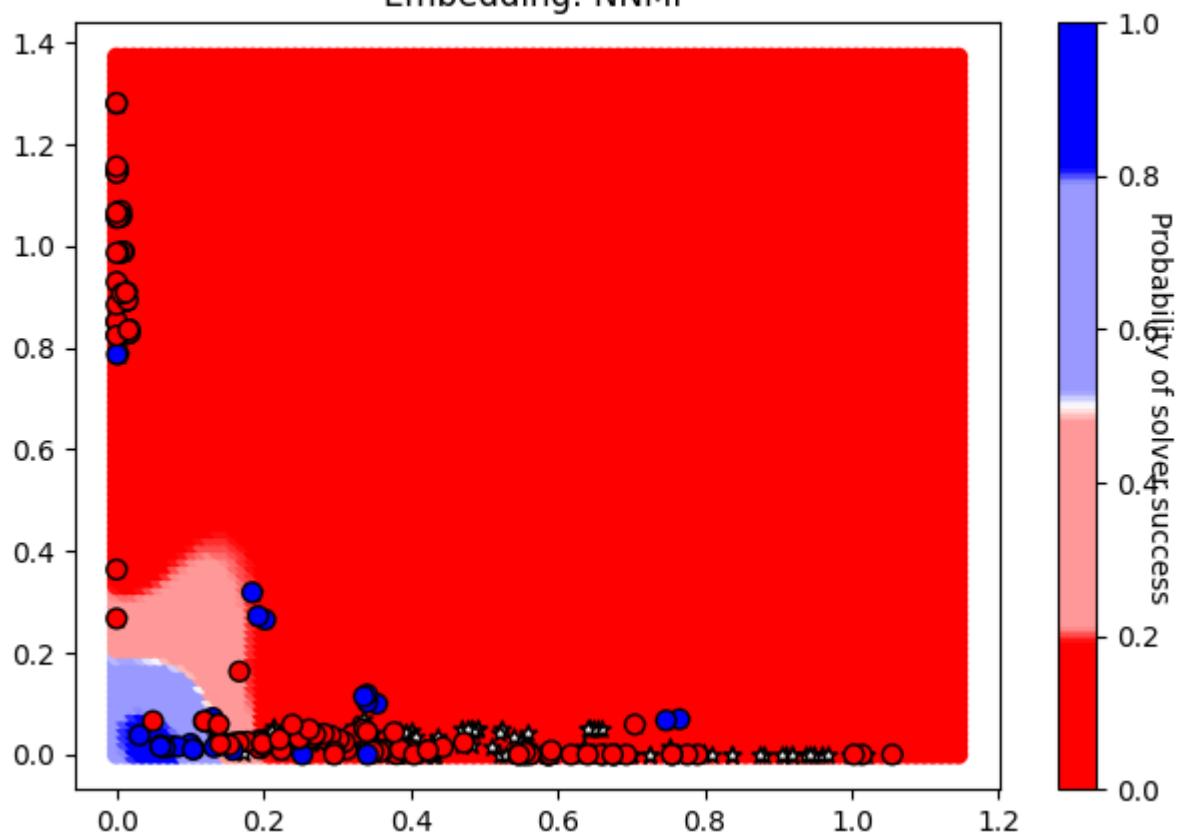
(captured: \$2.1e-02/1.5e+07, approximately 1.4e-07%)



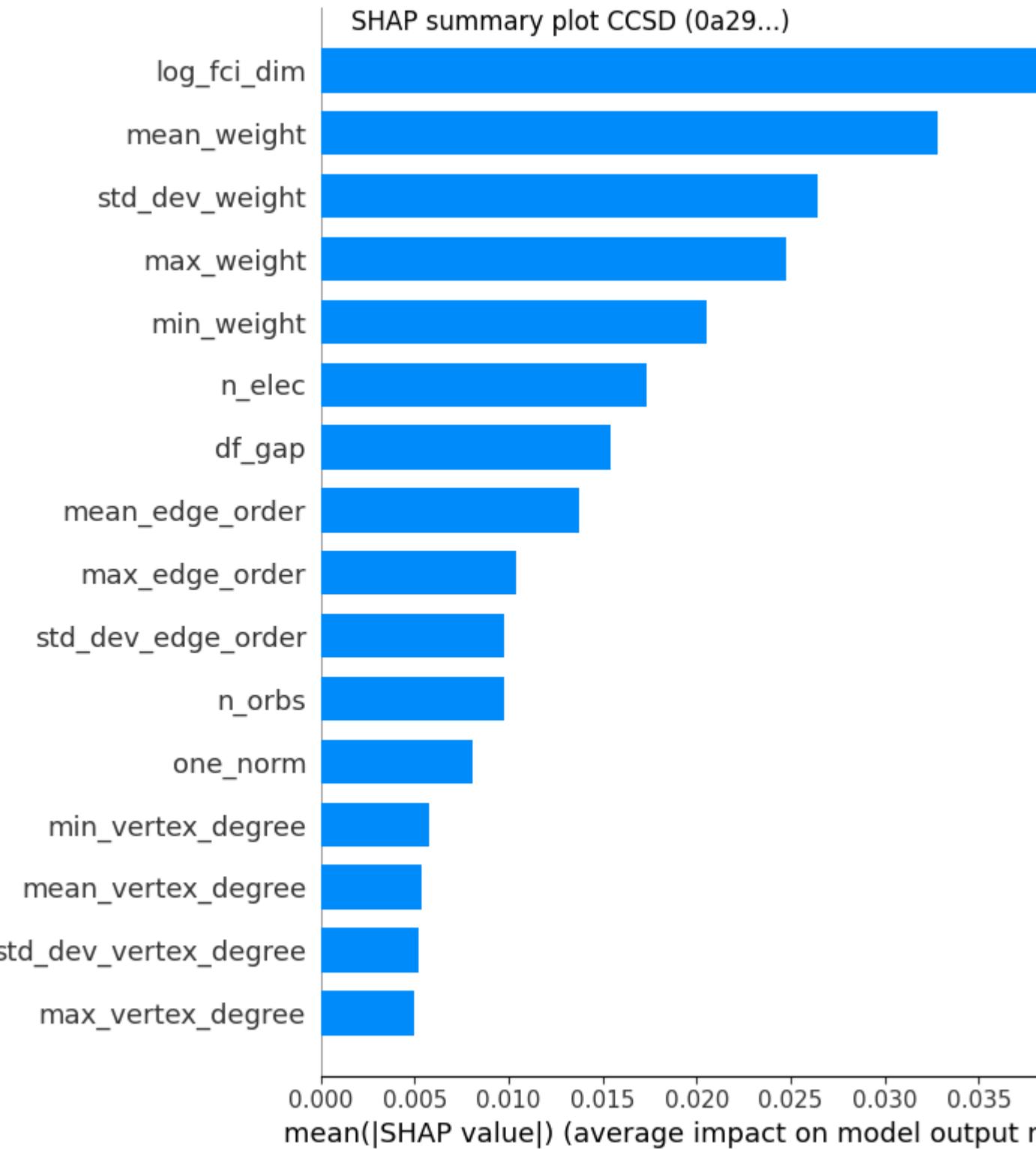
Solver CCSD (0a29...)
Embedding: PCA



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



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

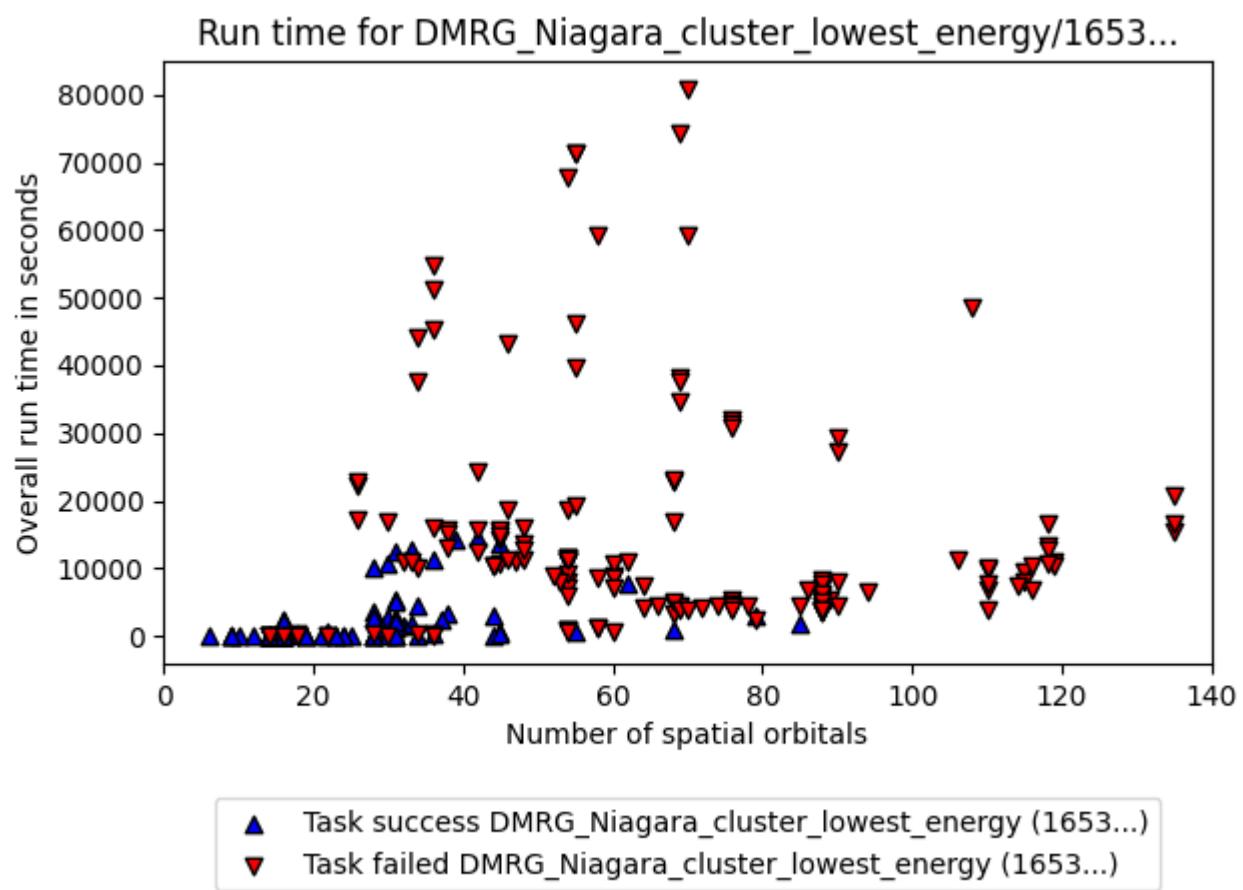


Solver DMRG_Niagara_cluster_lowest_energy, 16537433-9f4c-4eae-a65d-787dc3b35b59

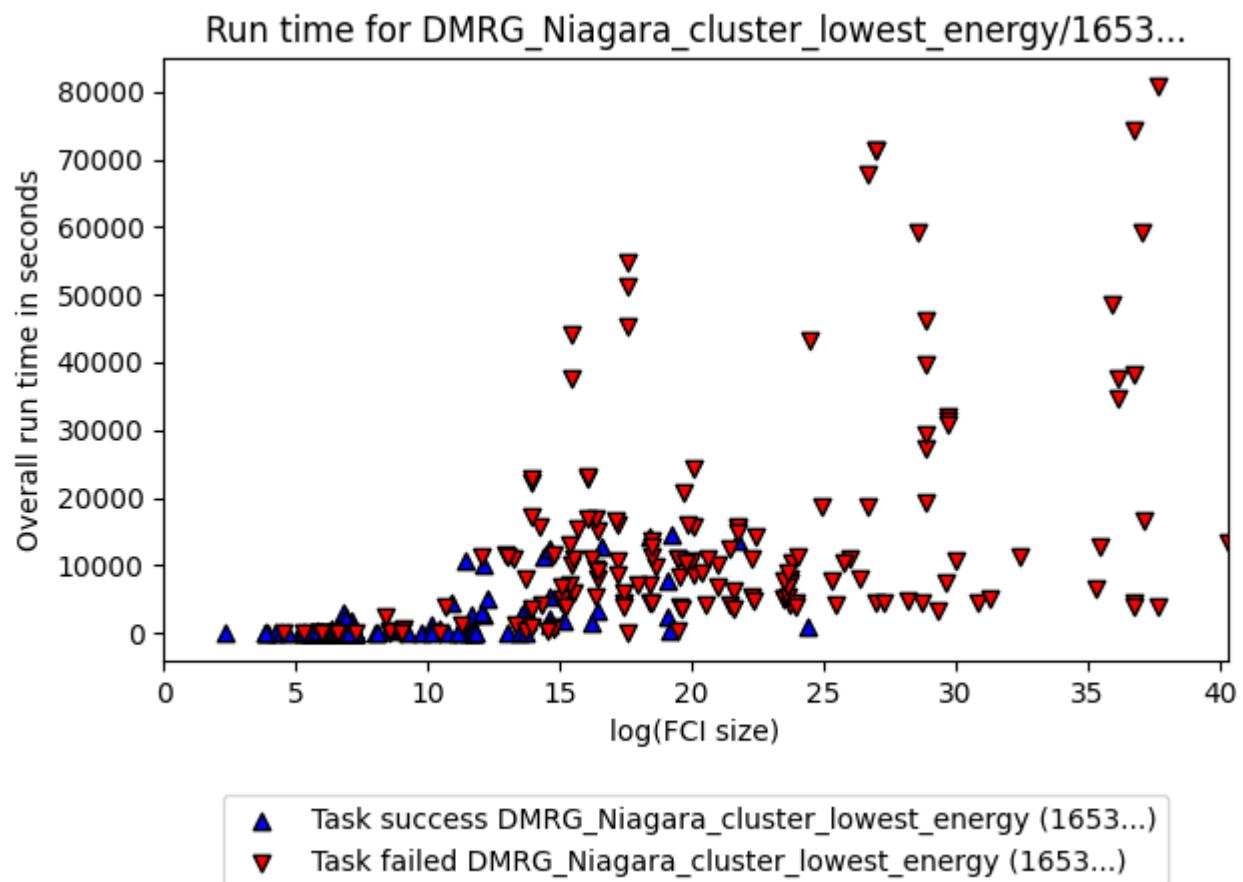
solver_uuid:16537433-9f4c-4eae-a65d-787dc3b35b59

solver_short_name:DMRG_Niagara_cluster_lowest_energy

compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'Niagara Cluster, Compute Canada', 'cpu_description': '40 Intel "Skylake" cores at 2.4 GHz or 40 Intel "CascadeLake" cores at 2.5 GHz', 'ram_available_gb': '202 GB (188 GiB)', 'clock_speed': '2.4 GHz or 2.5 GHz', 'total_num_cores': 40}
algorithm_details:DMRG with the lowest variational energy obtained so far.
software_details:Block2 v0.5.3rc16 with dmrghandler, commit version d603fdc6409fc194a416aa3a519362d5d91790d9 or later.
performance_metrics_uuid: ec7c30bb-7176-4860-8aab-823e8e7d72bd
creation_timestamp: 2025-02-19T18:26:13.854054+00:00
number_of_problem_instances: 88
number_of_problem_instances_attempted: 84
number_of_problem_instances_solved: 9
number_of_tasks: 280
number_of_tasks_attempted: 276
number_of_tasks_solved: 112
number_of_tasks_solved_within_run_time_limit: 276
number_of_tasks_solved_within_accuracy_threshold: 112
max_run_time_of_attempted_tasks: 80820.729907066
sum_of_run_time_of_attempted_tasks: 2471726.9051446947
solvability_ratio: 0.6263
comment: solvability ratio based on PCA embedding.
f1_score: [0.9183673469387755, 0.9646017699115044]
ml_metrics_calculator_version: 1



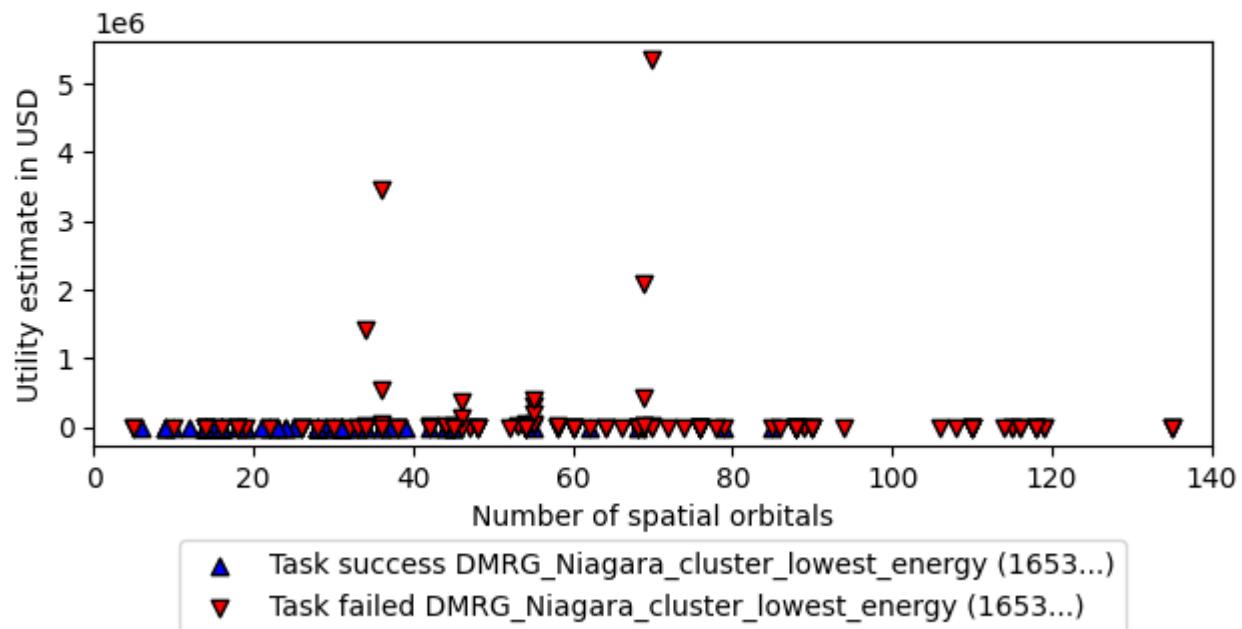
Note: plot only contains attempted tasks.



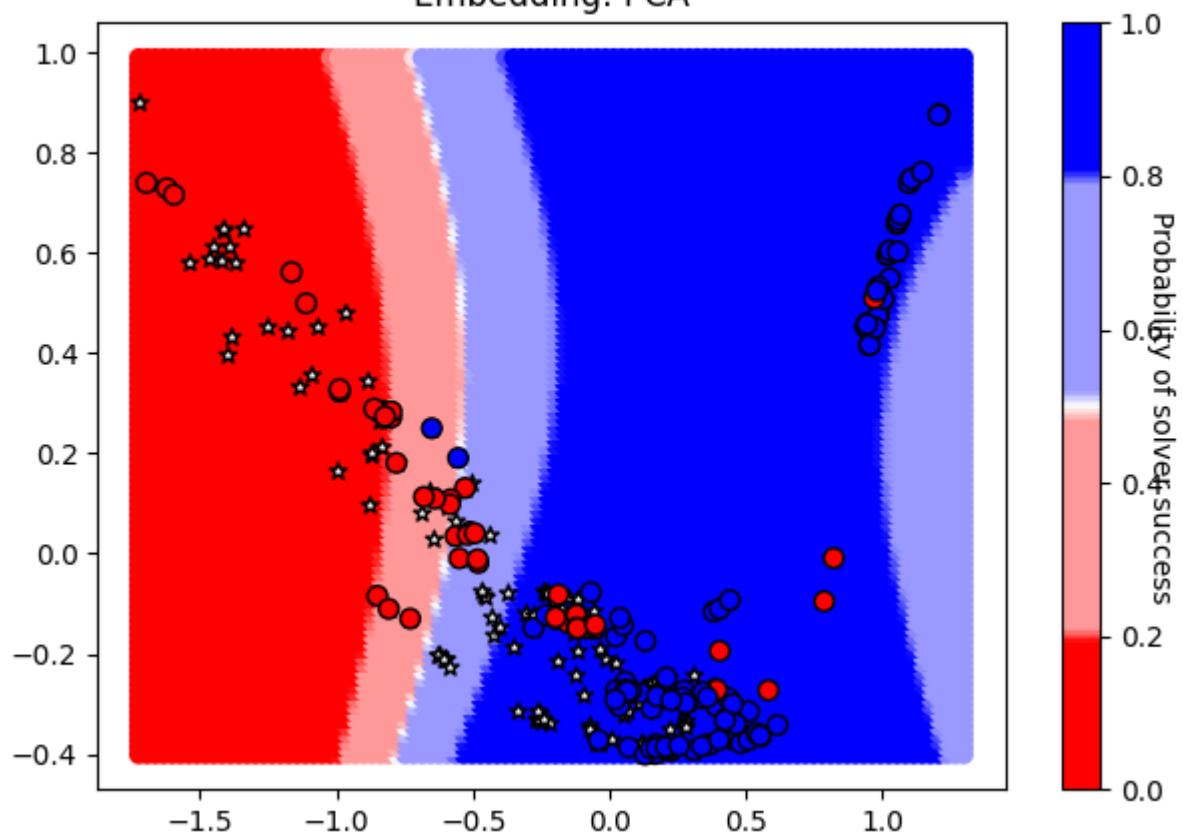
Note: plot only contains attempted tasks.

Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..

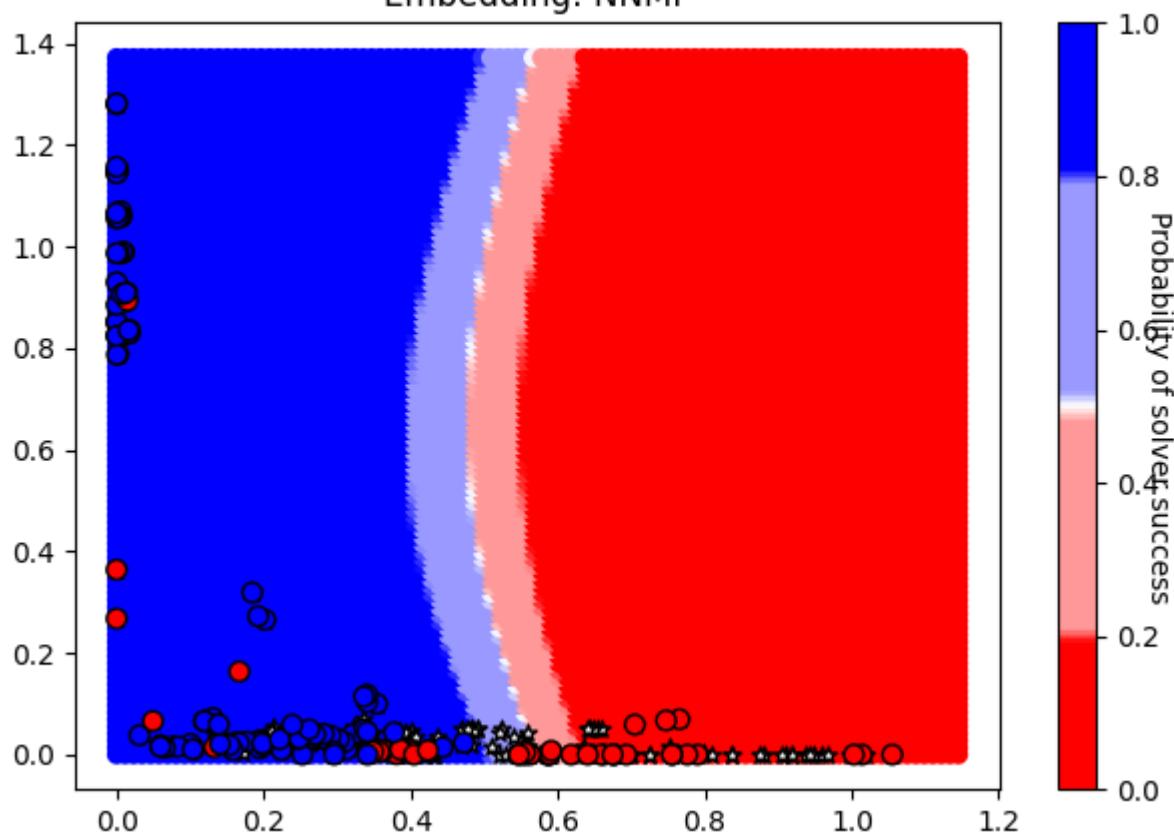
(captured: \$8.0e+02/1.5e+07, approximately 5.3e-03%)



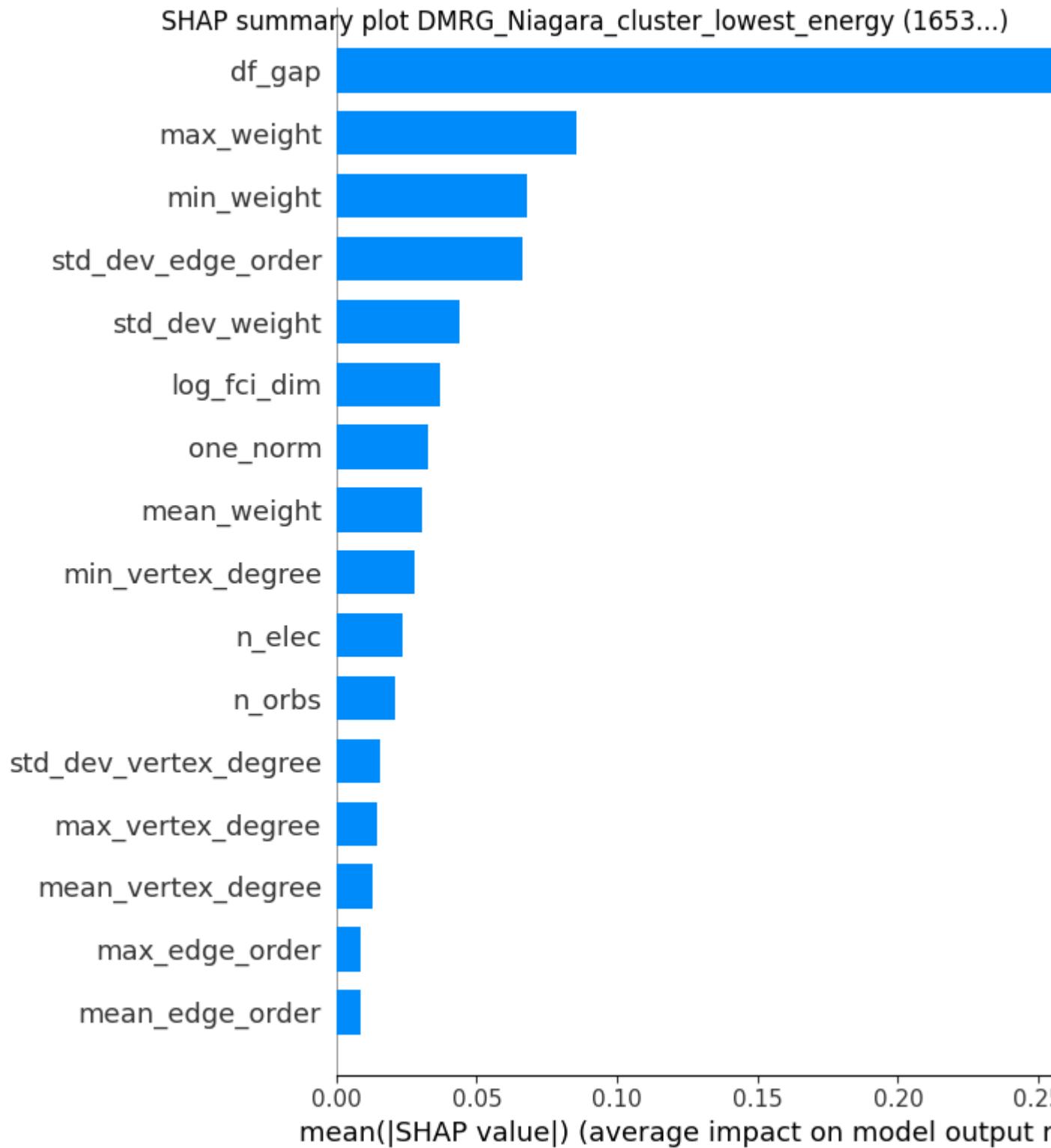
Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: PCA



Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: NMF



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



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

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

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

software_details:[{'software_name': 'benchq', 'software_version': '0.7.1.dev10+g80b8279.d20250116'}, {'software_name': 'openfermion', 'software_version': '1.6.1'}, {'software_name': 'Python', 'software_version': '3.11.5 (main, Sep 11 2023, 08:31:25) [Clang 14.0.6]'}, {'software_name': 'benchq', 'software_version': '0.7.1.dev10+g80b8279.d20250116'}]

quantum_hardware_details:{'quantum_hardware_description': 'Superconducting hardware model based on that described in https://arxiv.org/abs/2011.03494, but with Litinski factories (Quantum 3, 205 (2019)).', 'quantum_hardware_parameters': {'num_factories': 4, 'physical_error_rate': 0.001, 'cycle_time_microseconds': 1}}

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

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

performance_metrics_uuid: e6ebd73e-ec25-4320-a917-e2faddf1c9db

creation_timestamp: 2025-02-19T18:26:13.854054+00:00

number_of_problem_instances: 88

number_of_problem_instances_attempted: 3

number_of_problem_instances_solved: 0

number_of_tasks: 280

number_of_tasks_attempted: 23

number_of_tasks_solved: 0

number_of_tasks_solved_within_run_time_limit: 0

number_of_tasks_solved_within_accuracy_threshold: 23

max_run_time_of_attempted_tasks: 441362513808.82544

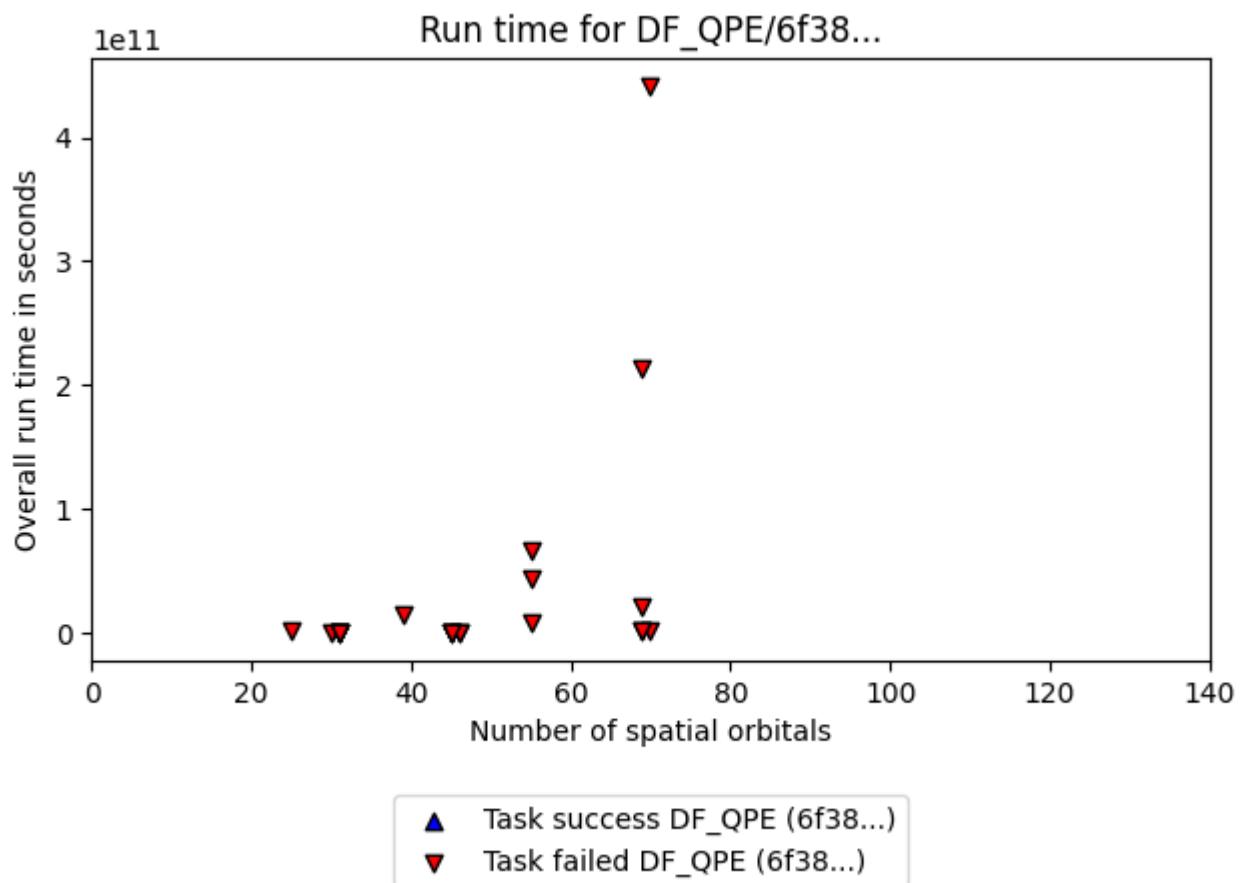
sum_of_run_time_of_attempted_tasks: 819346667619.2955

solvability_ratio: None

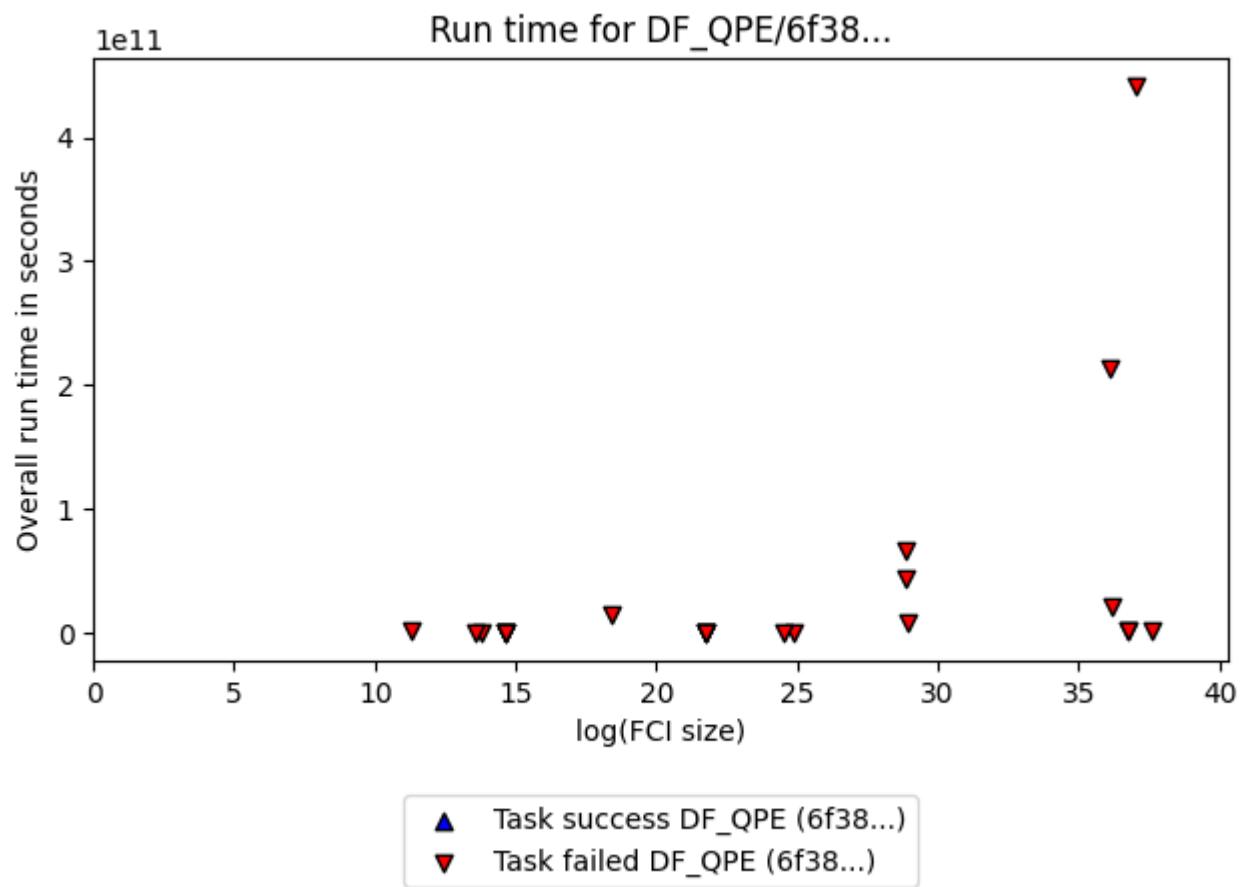
f1_score: None

ml_metrics_calculator_version: 1

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

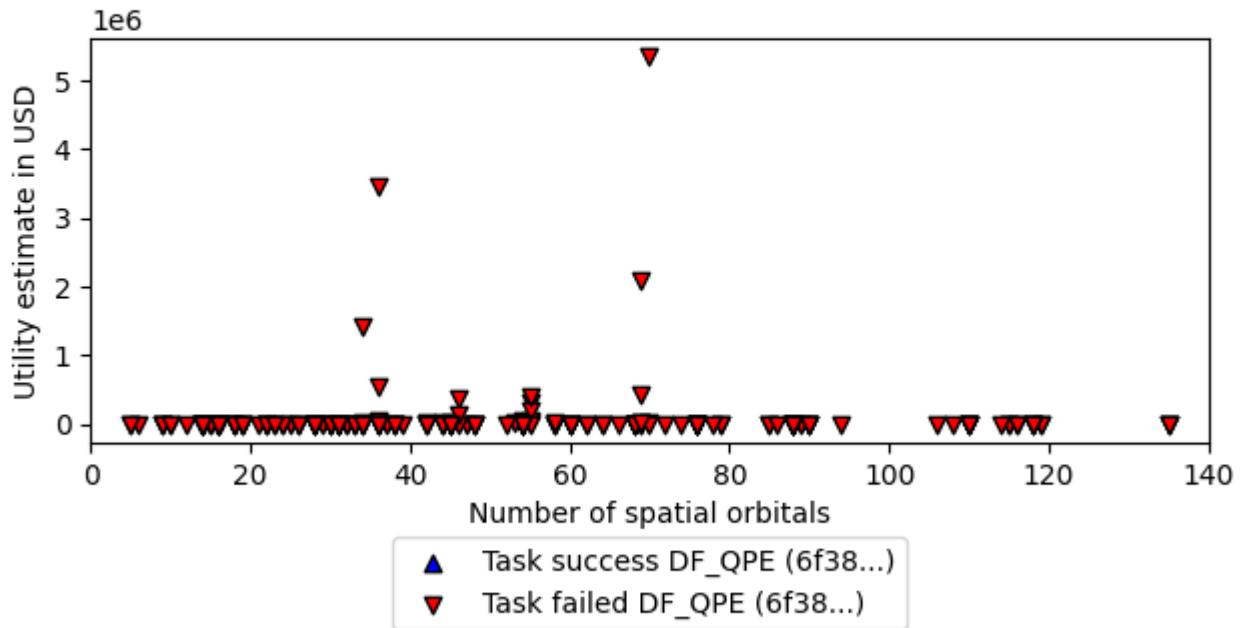


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/6f38...
(captured: \$0.0e+00/1.5e+07, approximately 0.0e+00%)



Solver PCA plot

Solver NNMF plot

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

SHAP summary plot

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

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

algorithm_details:{'algorithm_description': 'Double factorized QPE resource estimates based on methodology of arXiv:2406.06335. Note that the truncation error is not included in the error bounds and that the SCF compute time is not included in the preprocessing time. Ground-state overlap is taken to be that estimated for the dominant CSF as estimated by

DMRG and that this DMRG runtime is not included in the classical compute costs.', 'algorithm_parameters': {'overlap_csv': 'overlaps.csv', 'sf_threshold': 1e-12, 'df_threshold': 0.001, 'max_orbitals': 70} }

software_details:[{'software_name': 'pyLIQTR', 'software_version': '1.3.4'}, {'software_name': 'qb-gsee-benchmark', 'software_version': '0.1.0a2.dev193+g879c00d'}, {'software_name': 'Python', 'software_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]'}, {'software_name': 'qualtran', 'software_version': '0.4.0'}]

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

logical_resource_estimate_solution_uuid:98855a22-d8cf-42a7-9a18-35f99e820882

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

performance_metrics_uuid: fec0829e-be72-4e83-8a3b-d55c8cef4348

creation_timestamp: 2025-02-19T18:26:13.854054+00:00

number_of_problem_instances: 88

number_of_problem_instances_attempted: 24

number_of_problem_instances_solved: 0

number_of_tasks: 280

number_of_tasks_attempted: 166

number_of_tasks_solved: 1

number_of_tasks_solved_within_run_time_limit: 1

number_of_tasks_solved_within_accuracy_threshold: 166

max_run_time_of_attempted_tasks: 3.667583349758435e+16

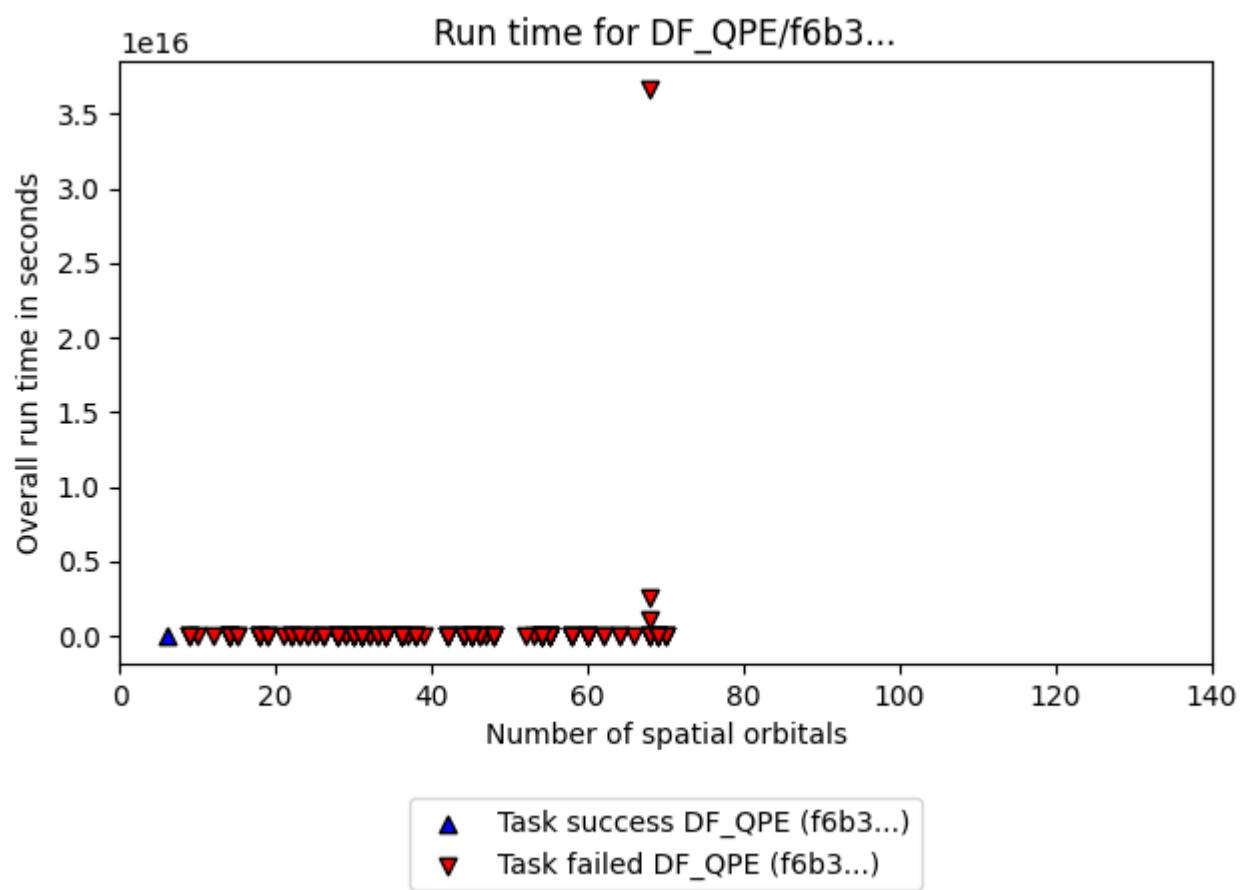
sum_of_run_time_of_attempted_tasks: 4.03843021239543e+16

solvability_ratio: None

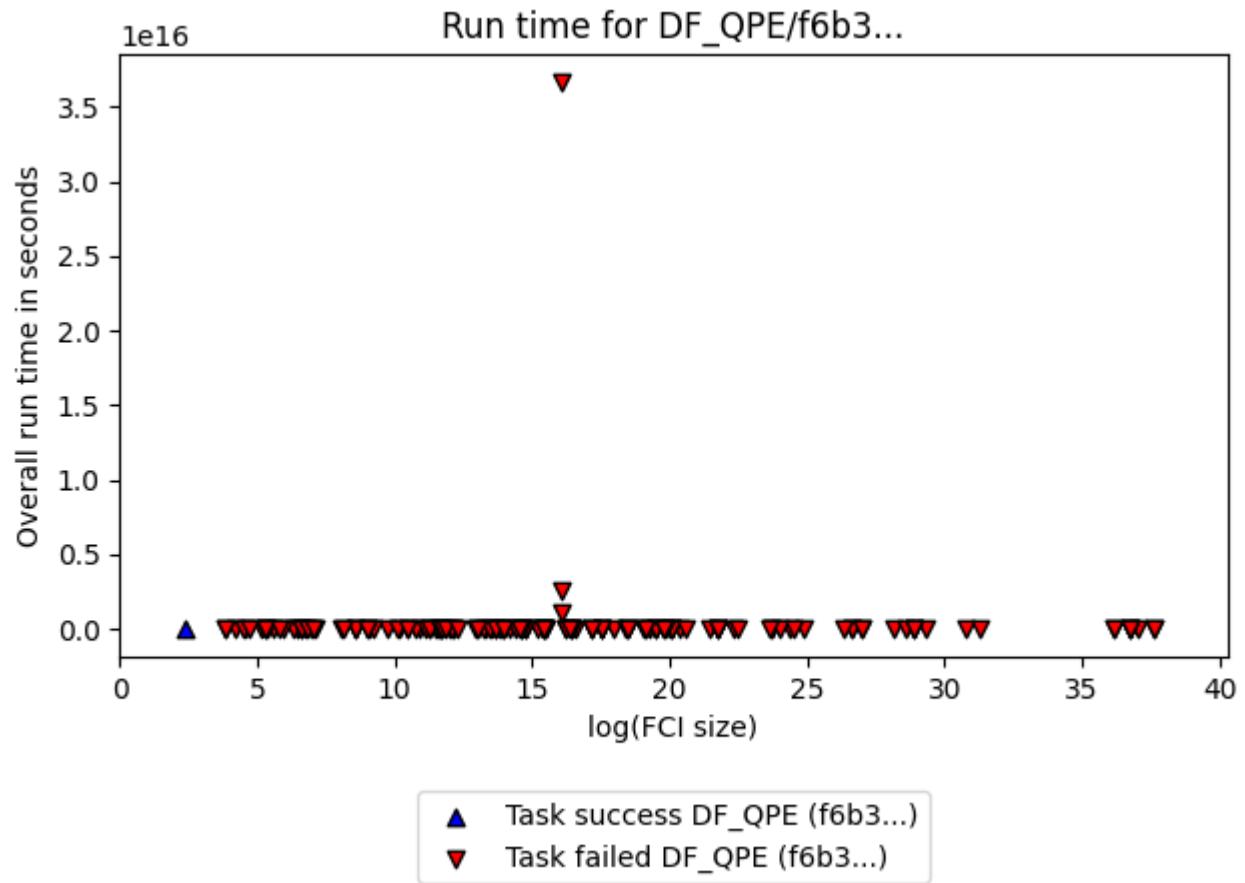
f1_score: None

ml_metrics_calculator_version: 1

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

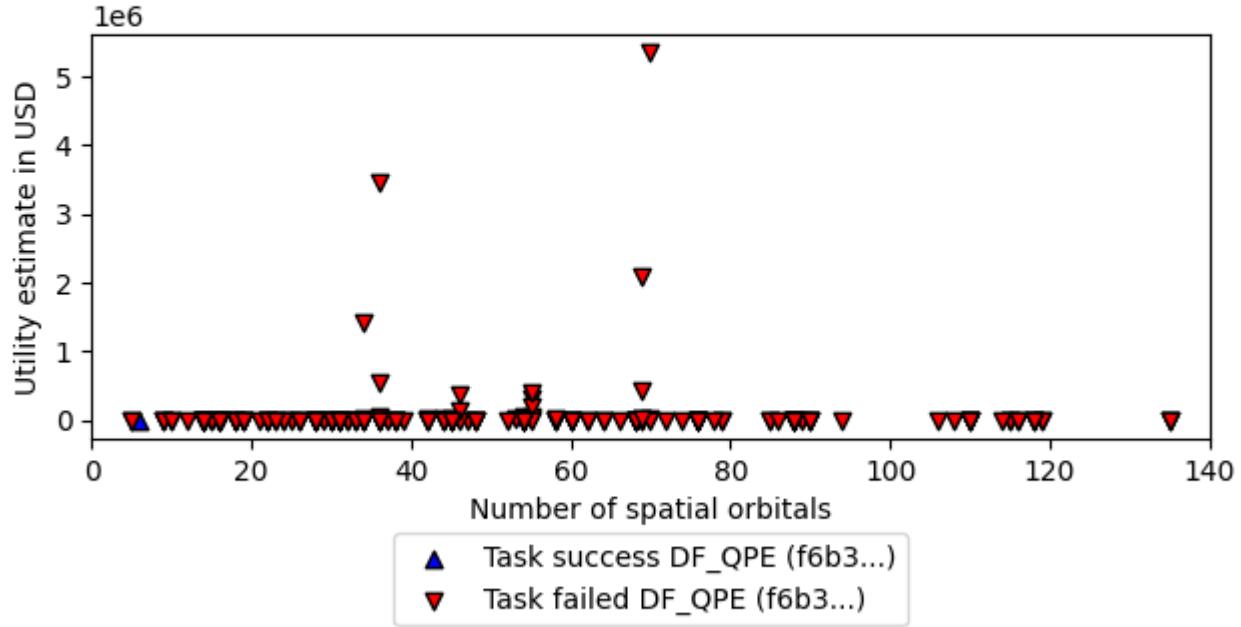


Note: plot only contains attempted tasks.



Note: plot only contains attempted tasks.

Utility capture from DF_QPE/f6b3...
(captured: \$2.5e-04/1.5e+07, approximately 1.7e-09%)



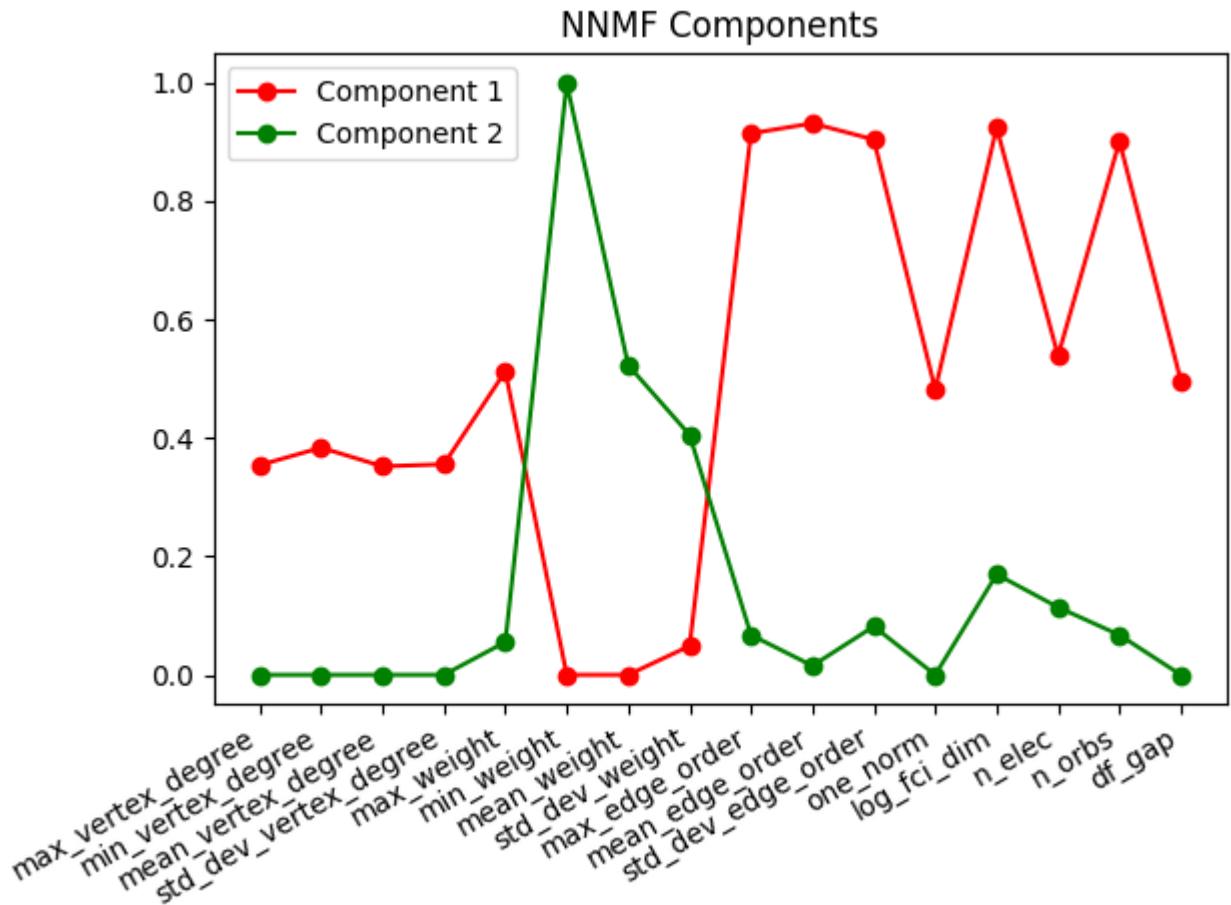
Solver PCA plot

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

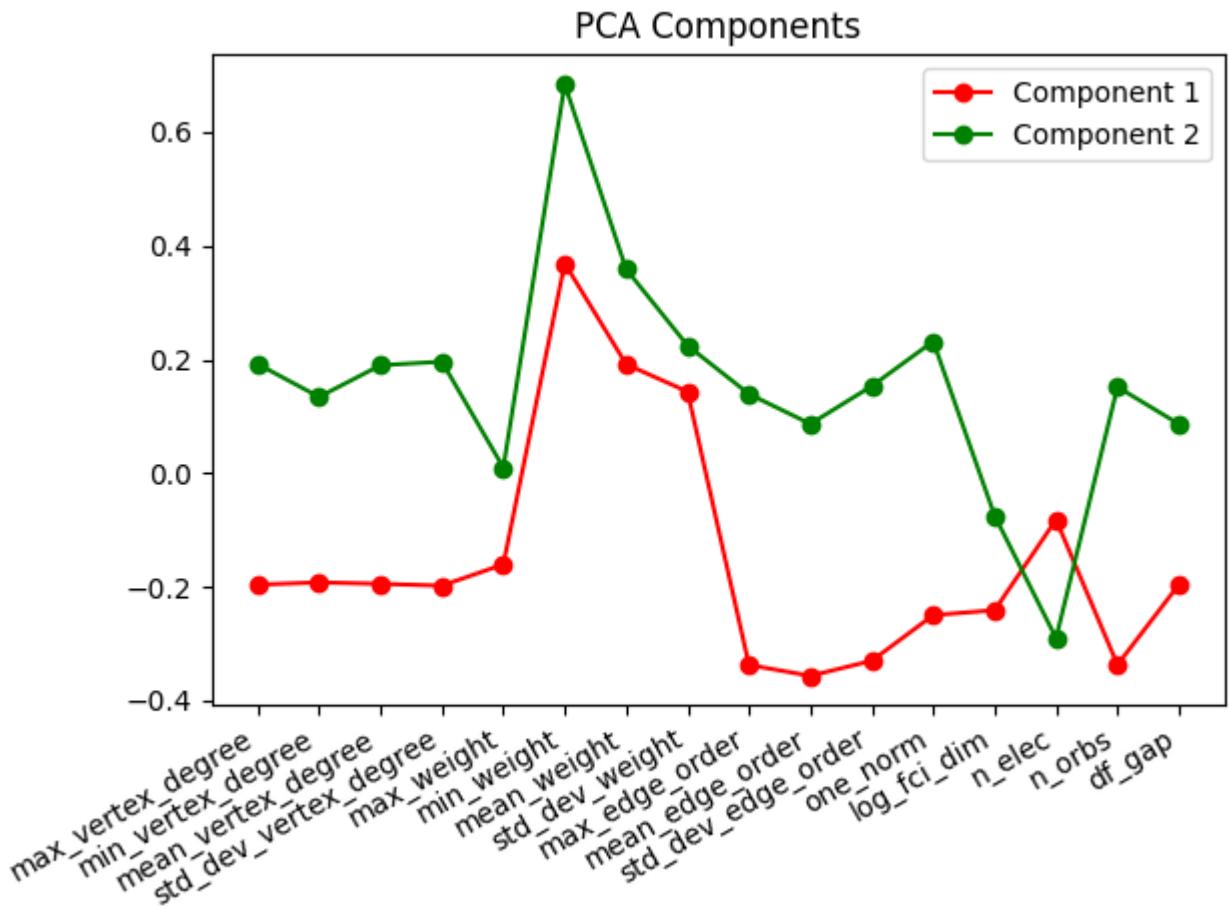
ML Feature Analysis



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: [0.35399743 0.3835676 0.3520002 0.35554304
0.51256815 0.0 0.04877227 0.91405015 0.93106994 0.90369122
0.48147271 0.92382446 0.53848377 0.90084819 0.49628833]

NNMF Component 2: [0. 0. 0. 0. 0.05545497 0.99860891 0.5229628
0.40516152 0.06735171 0.01538102 0.08181161 0. 0.16970458 0.1141114
0.06725901 0.]

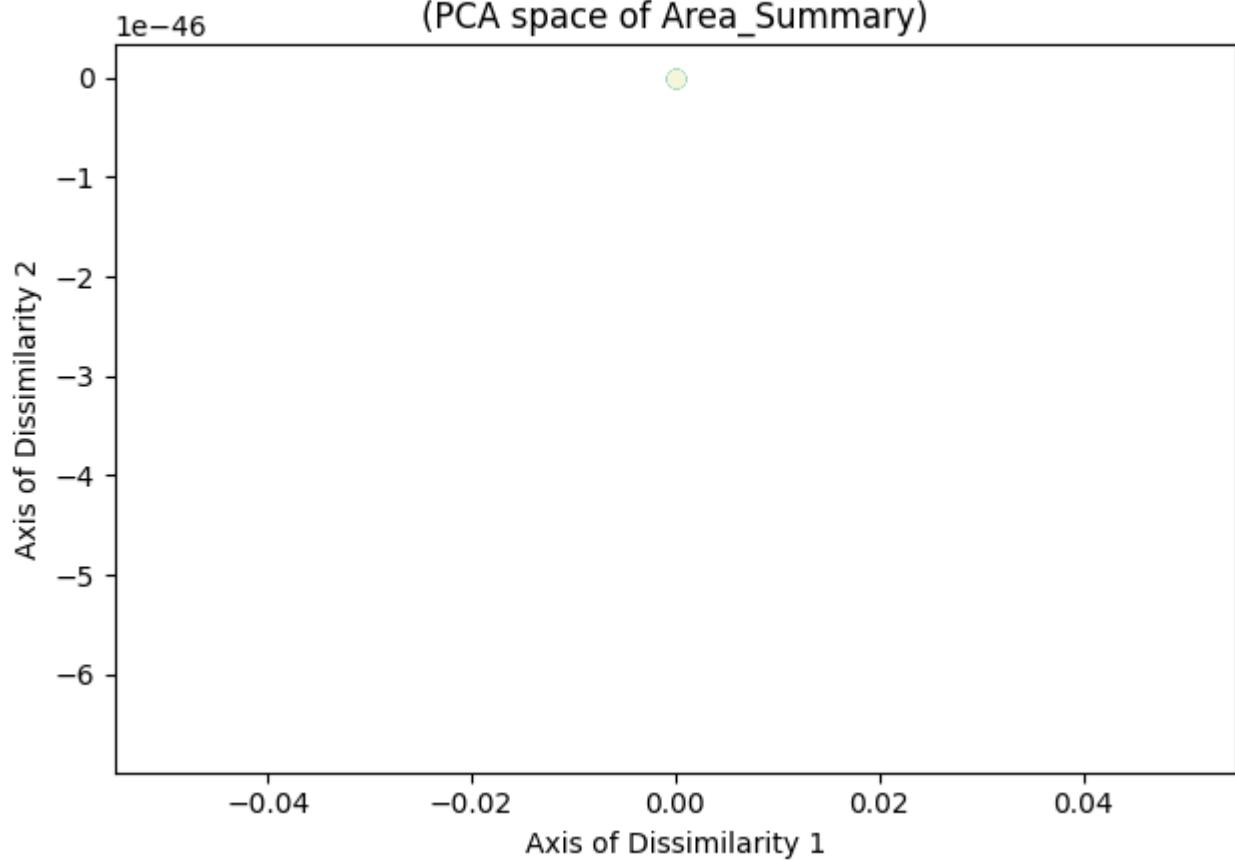


Features: ['max_vertex_degree', 'min_vertex_degree', 'mean_vertex_degree', 'std_dev_vertex_degree', 'max_weight', 'min_weight', 'mean_weight', 'std_dev_weight', 'max_edge_order', 'mean_edge_order', 'std_dev_edge_order', 'one_norm', 'log_fci_dim', 'n_elec', 'n_orbs', 'df_gap']

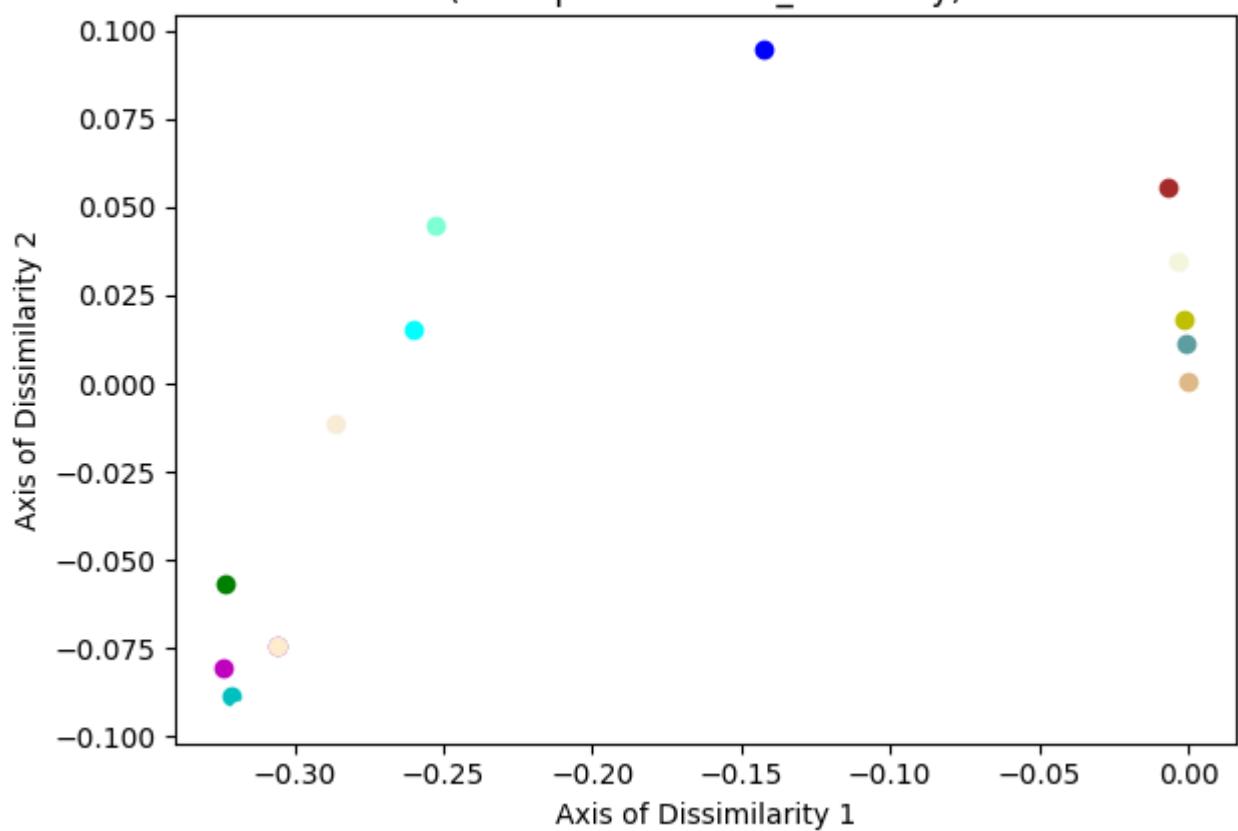
PCA Component 1: [-0.19606441 -0.19210755 -0.19466848 -0.19785564
 -0.16044022 0.36889367 0.19151328 0.14329659 -0.33728001 -0.35642778
 -0.32990174 -0.24968252 -0.24098618 -0.08184379 -0.3368266
 -0.19589773]

PCA Component 2: [0.19190723 0.13407095 0.18973626 0.19607885
 0.00984172 0.68373267 0.35862773 0.22441087 0.13916663 0.0865819
 0.15316911 0.2317319 -0.07481991 -0.29008347 0.15152307 0.08636324]

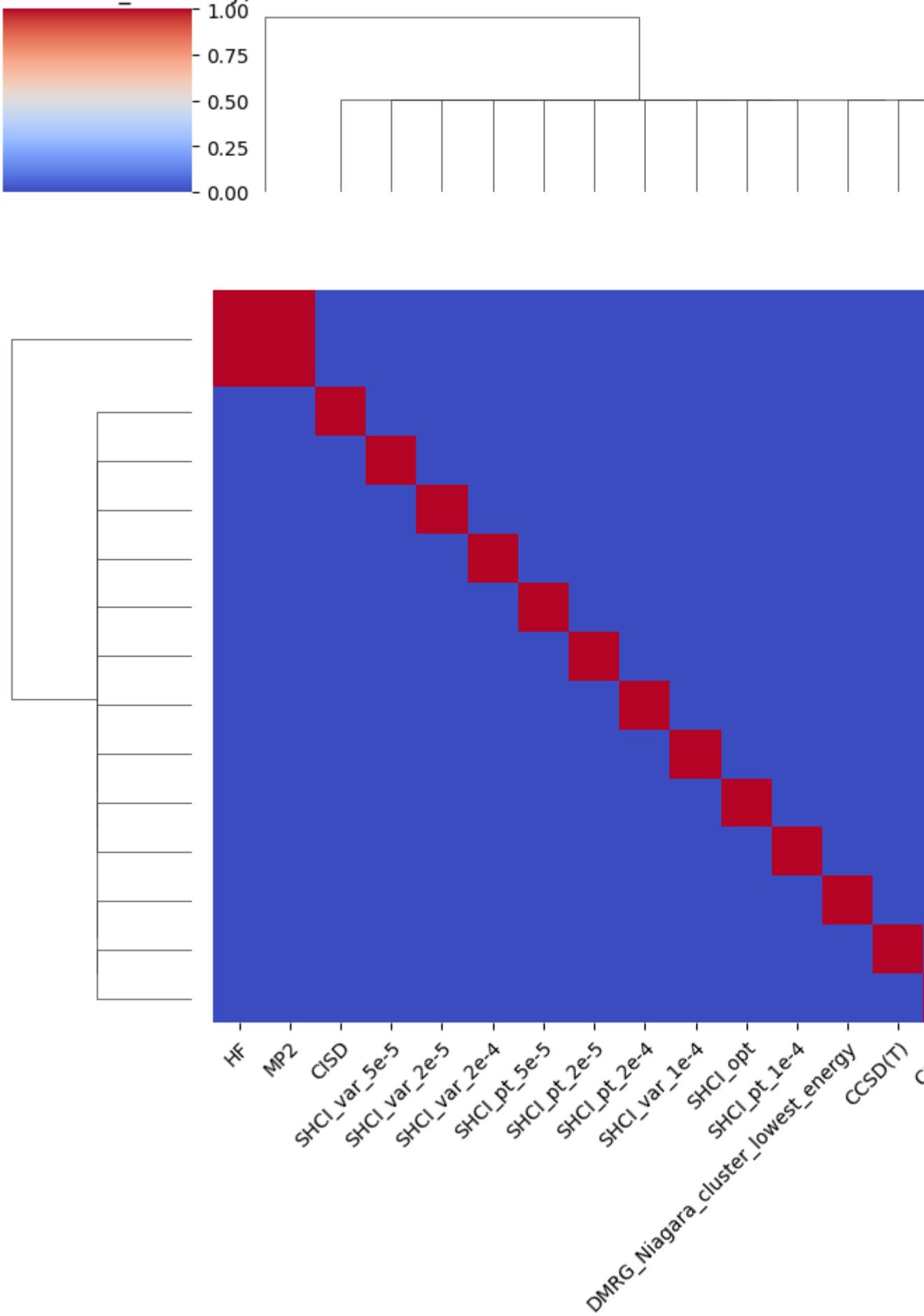
Solver points in PCA space
(PCA space of Area_Summary)



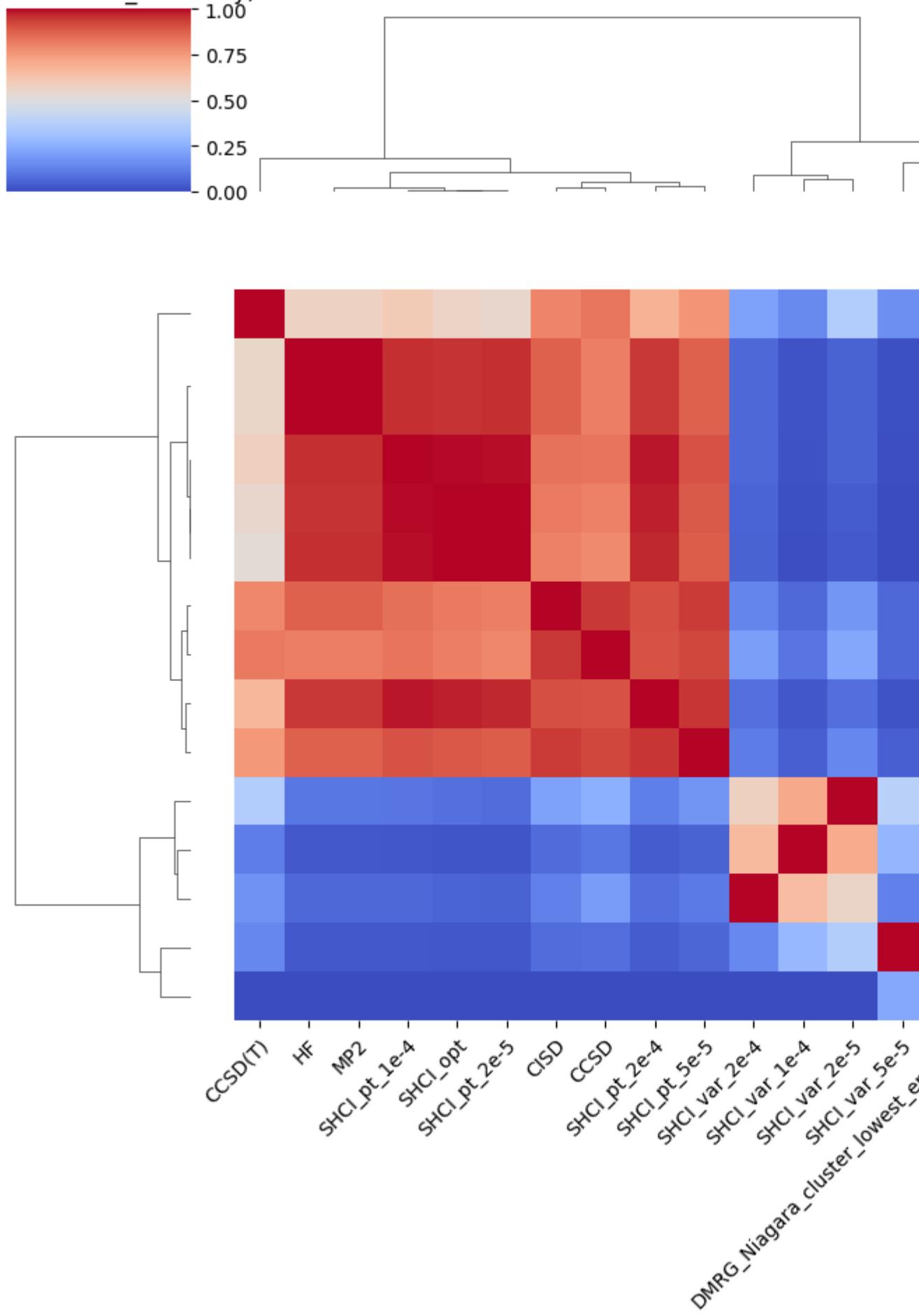
Solver points in PCA space
(PCA space of SHAP_summary)

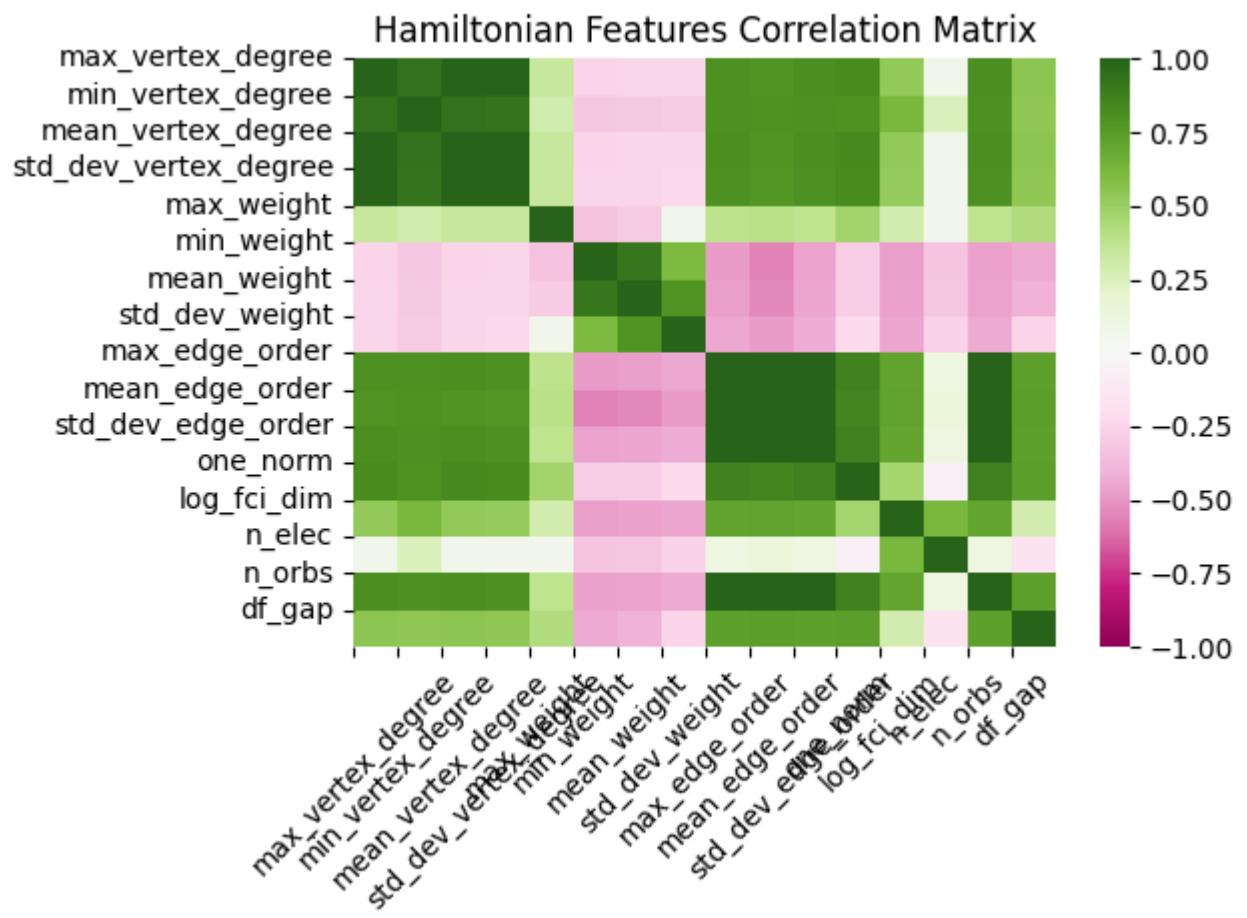


Solver similarity matrix (based on Area_Summary)

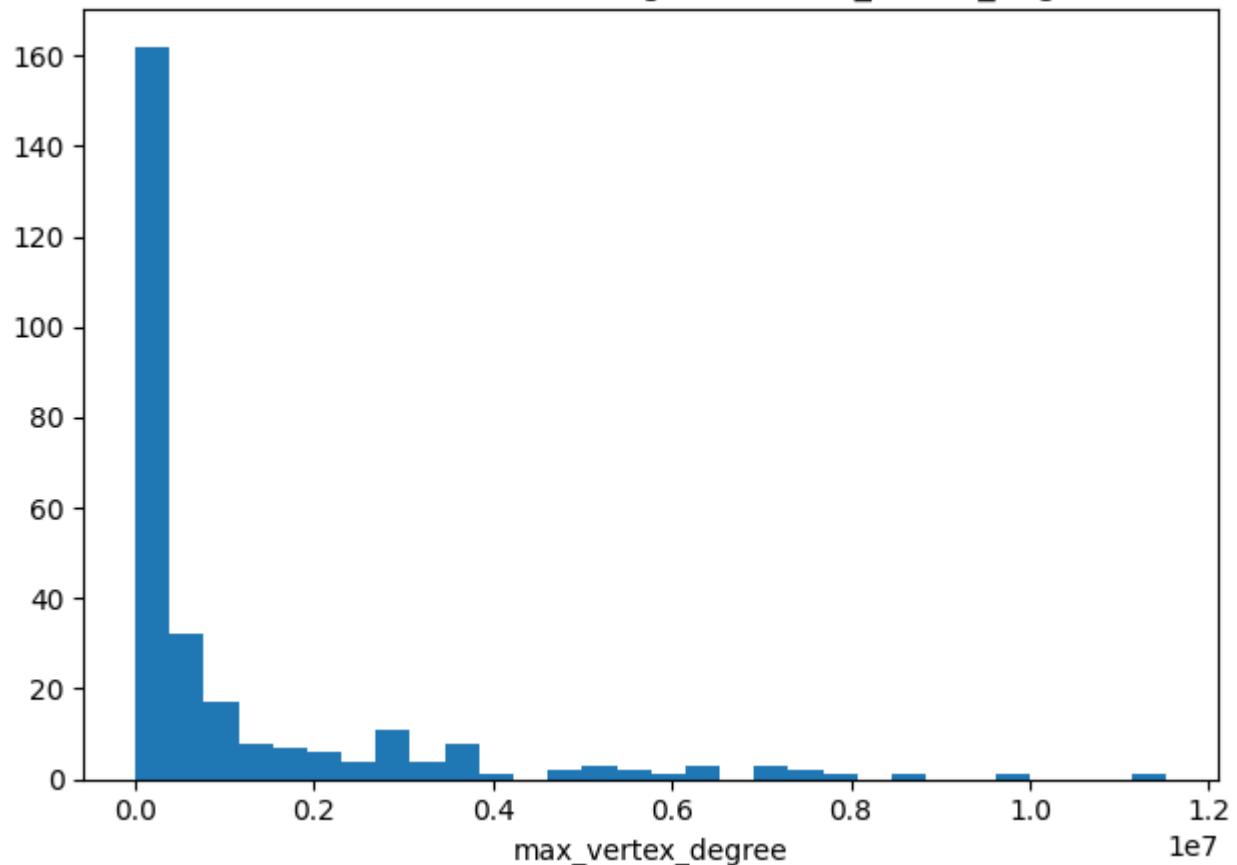


Solver similarity matrix
(based on SHAP_summary)

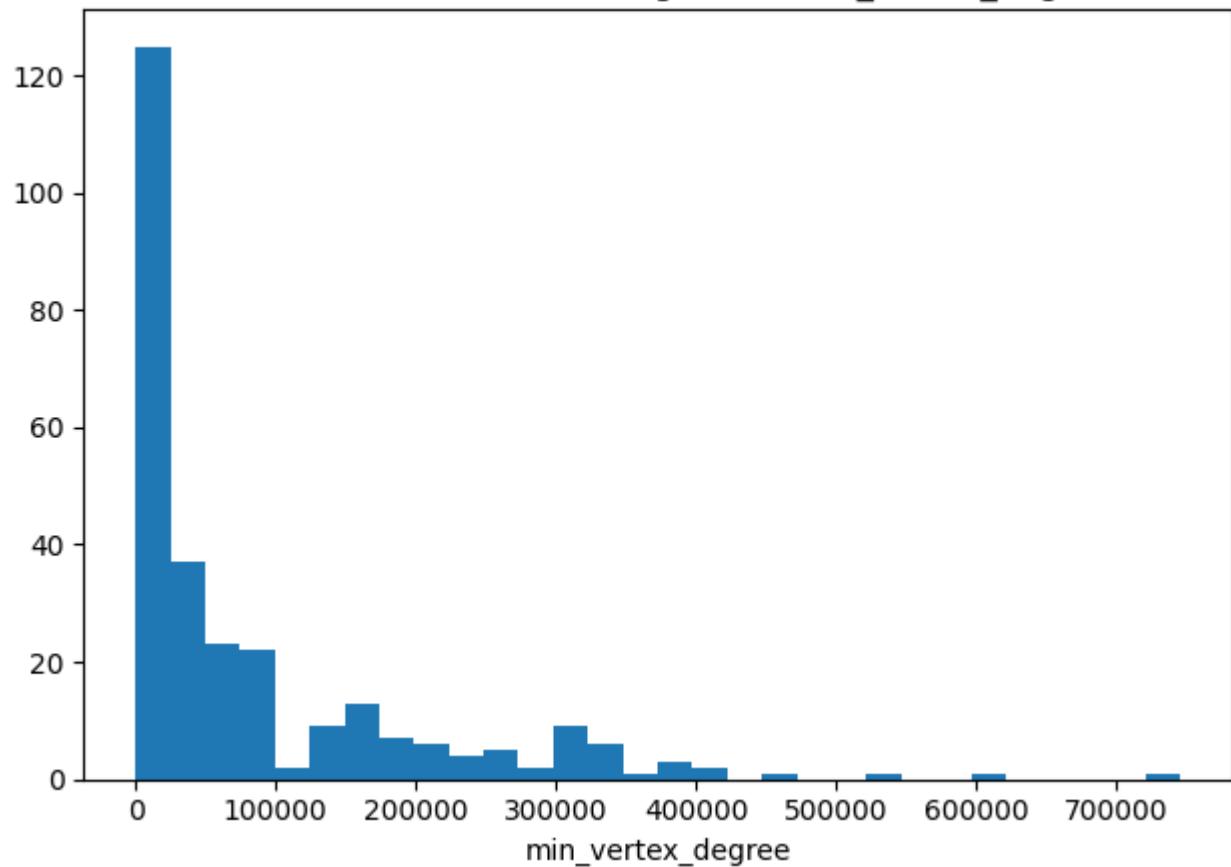




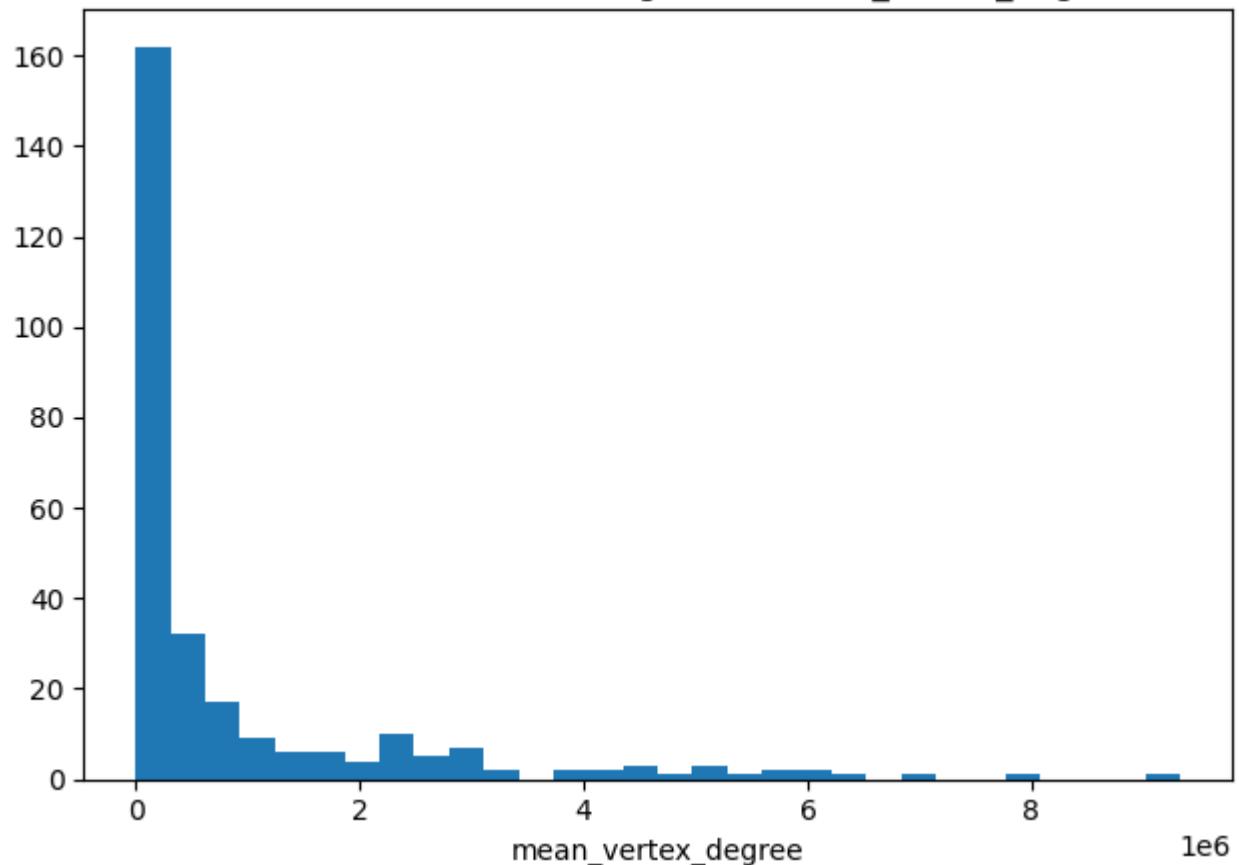
Hamiltonian features: histogram of max_vertex_degree



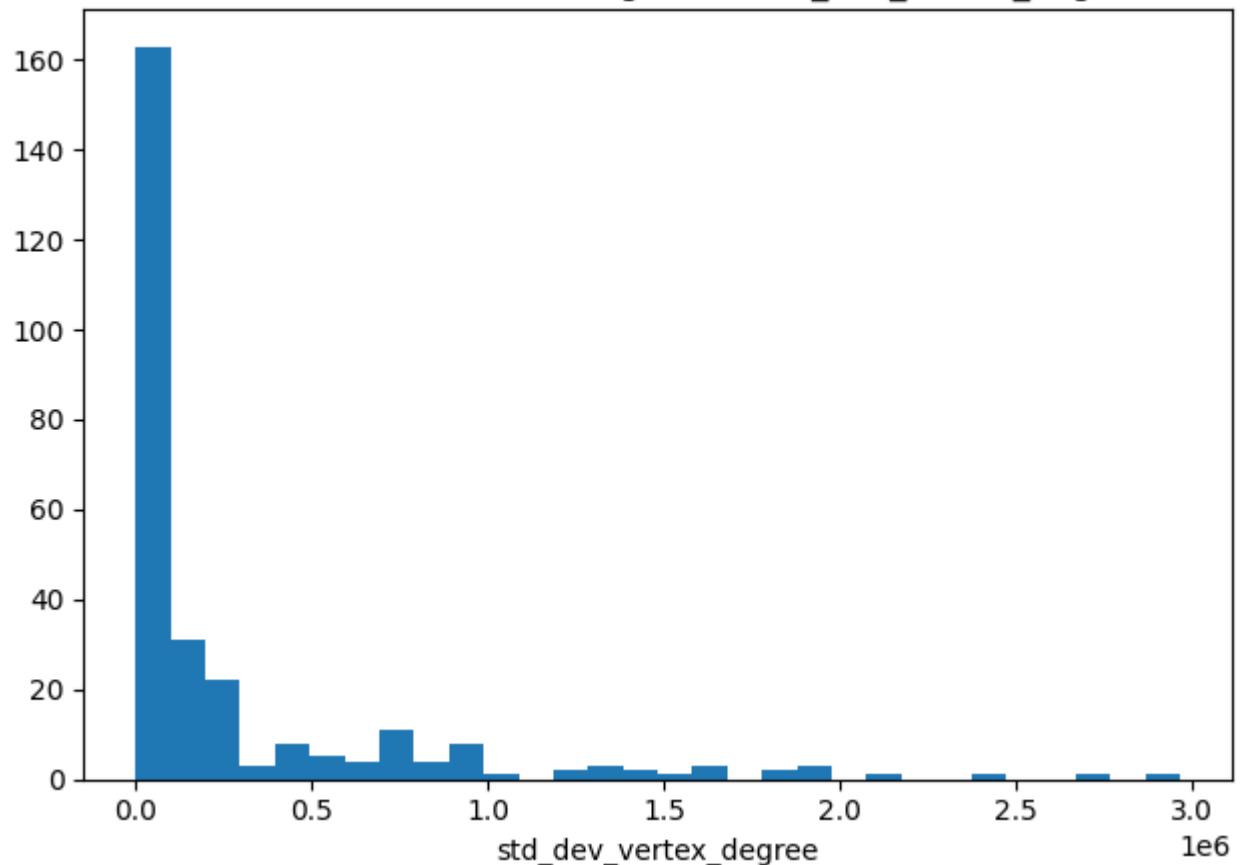
Hamiltonian features: histogram of min_vertex_degree



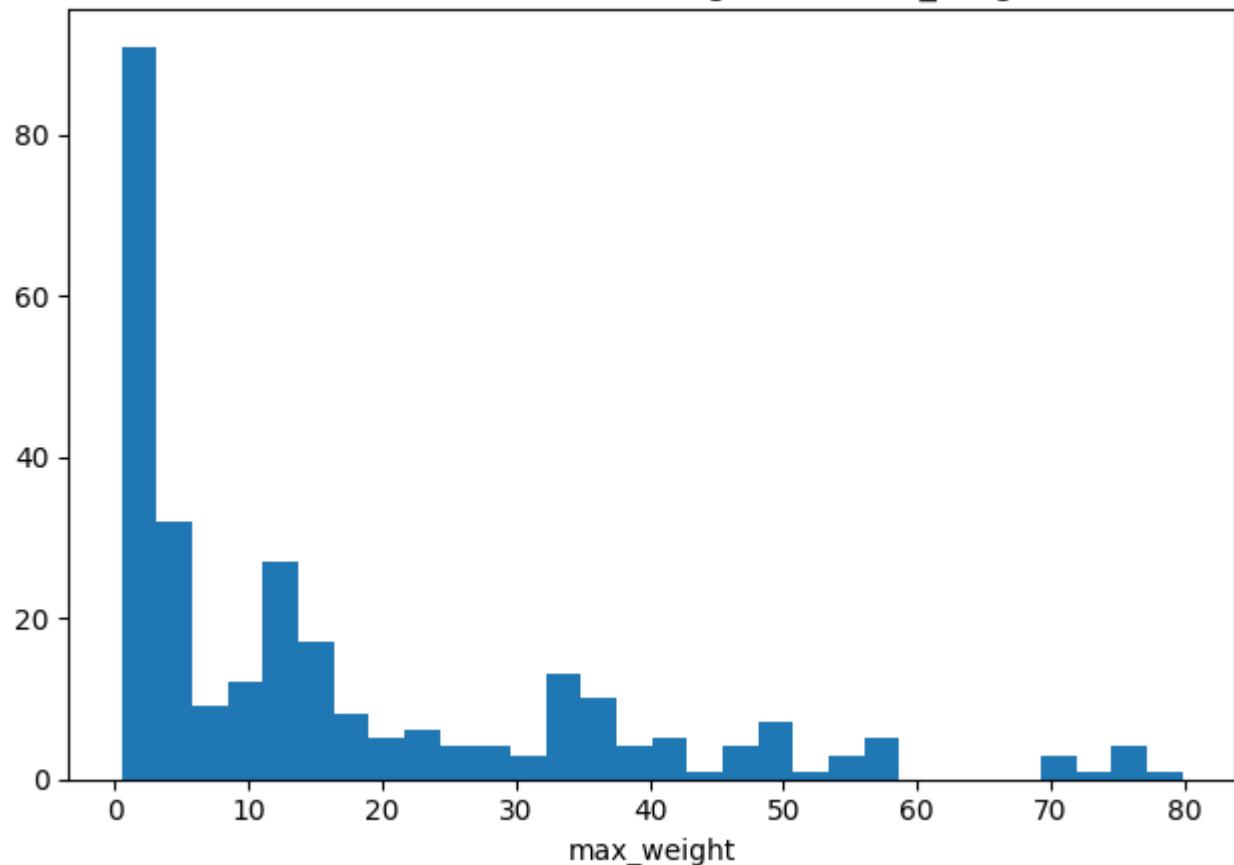
Hamiltonian features: histogram of mean_vertex_degree



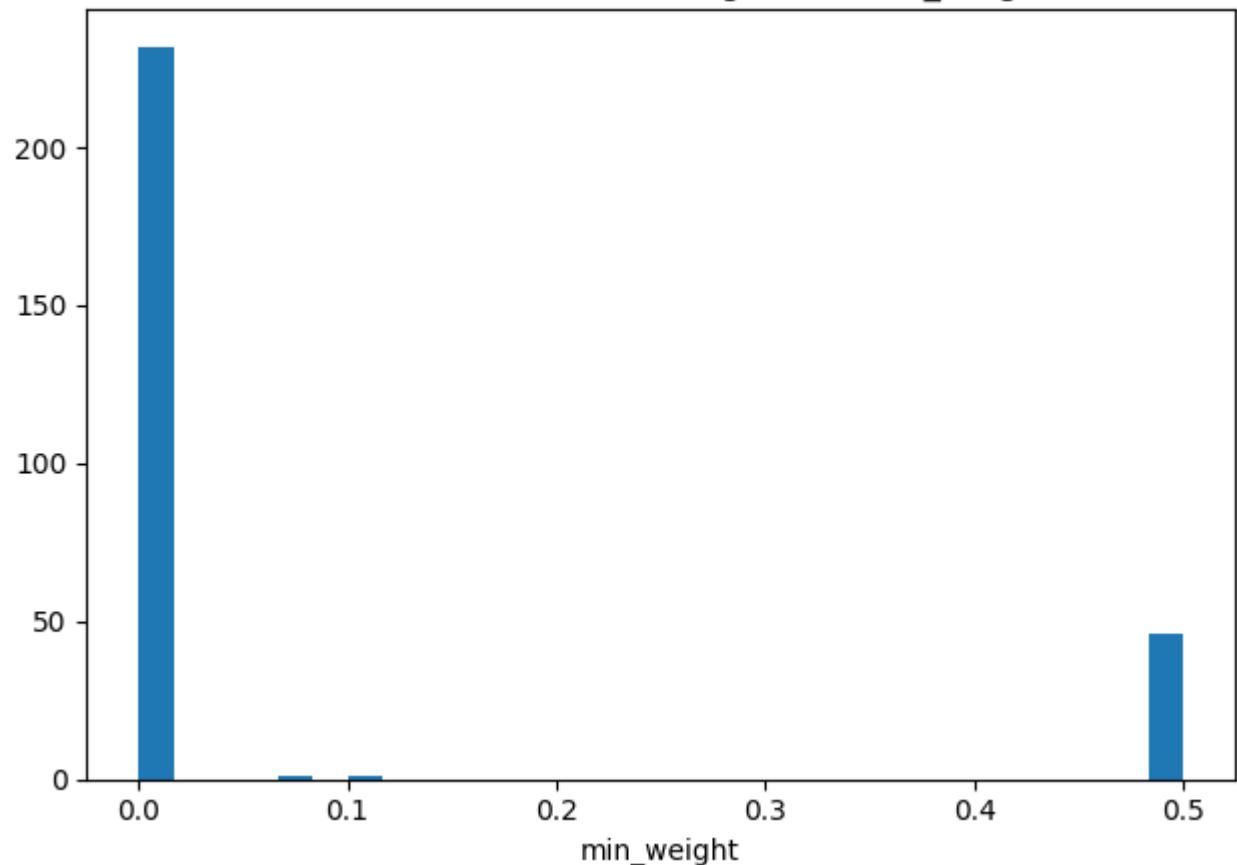
Hamiltonian features: histogram of std_dev_vertex_degree



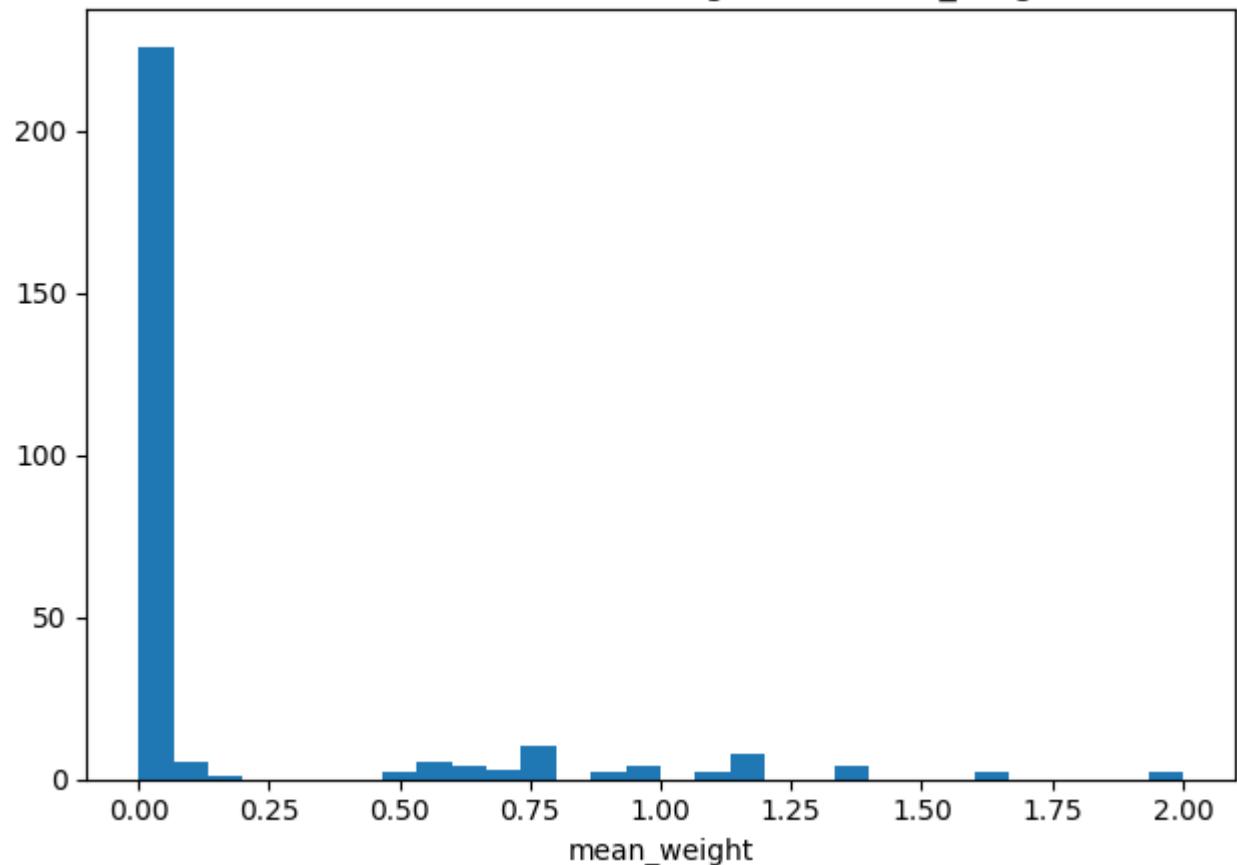
Hamiltonian features: histogram of max_weight



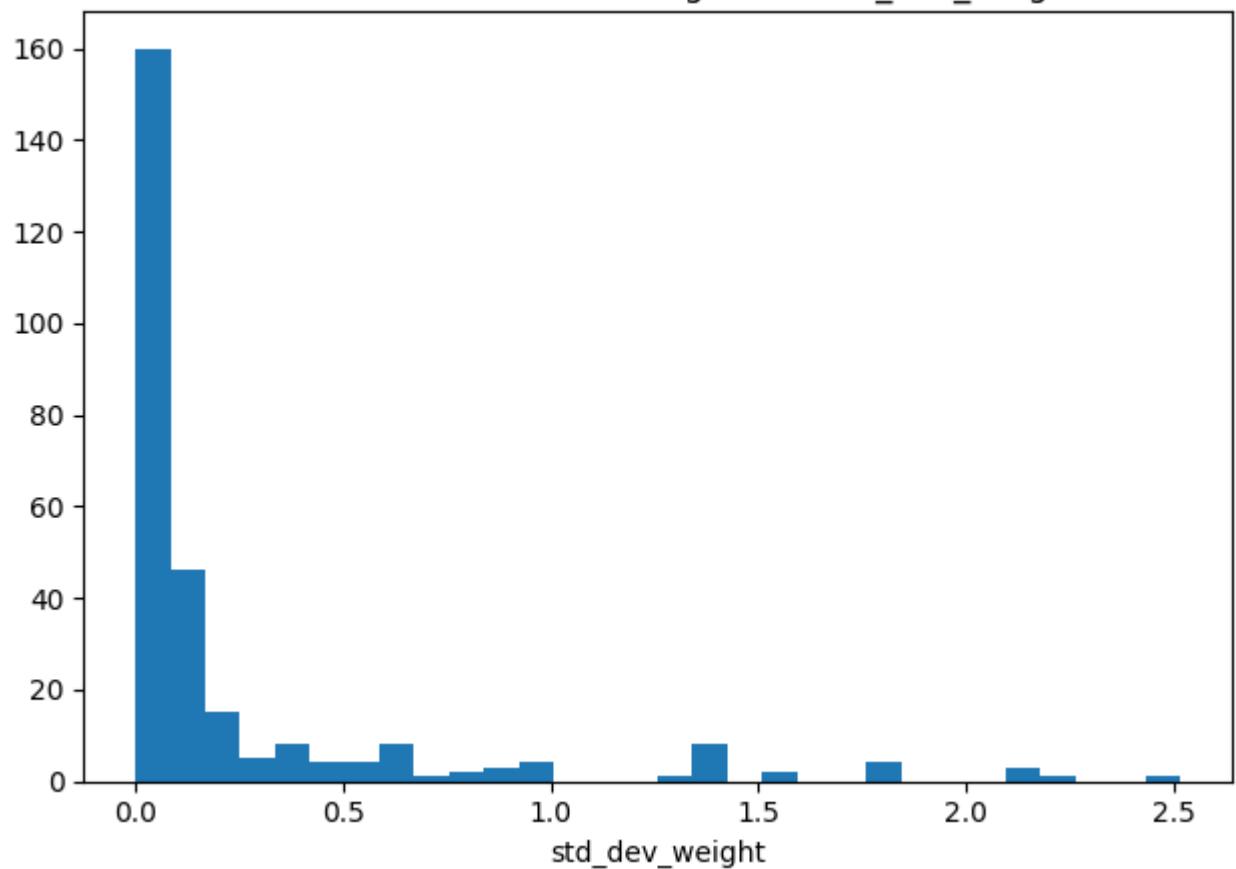
Hamiltonian features: histogram of min_weight



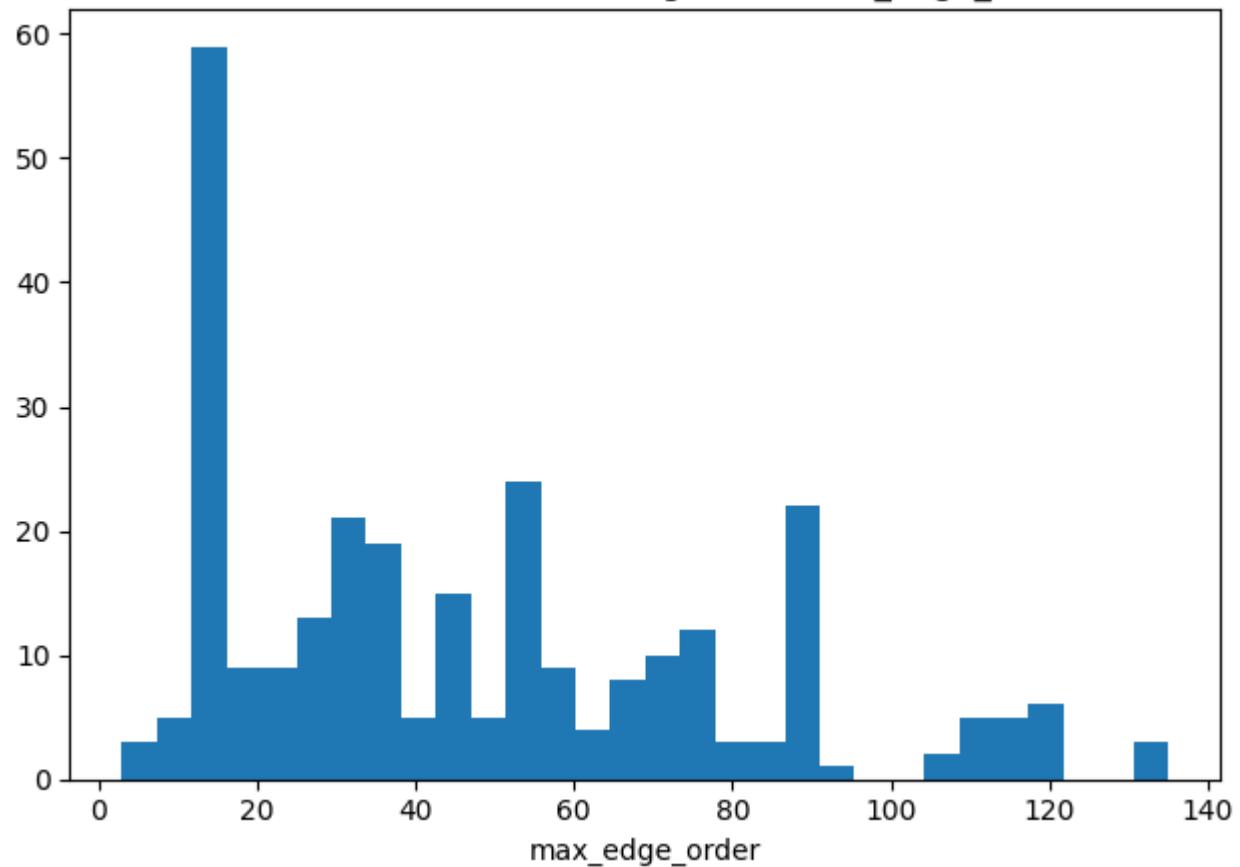
Hamiltonian features: histogram of mean_weight



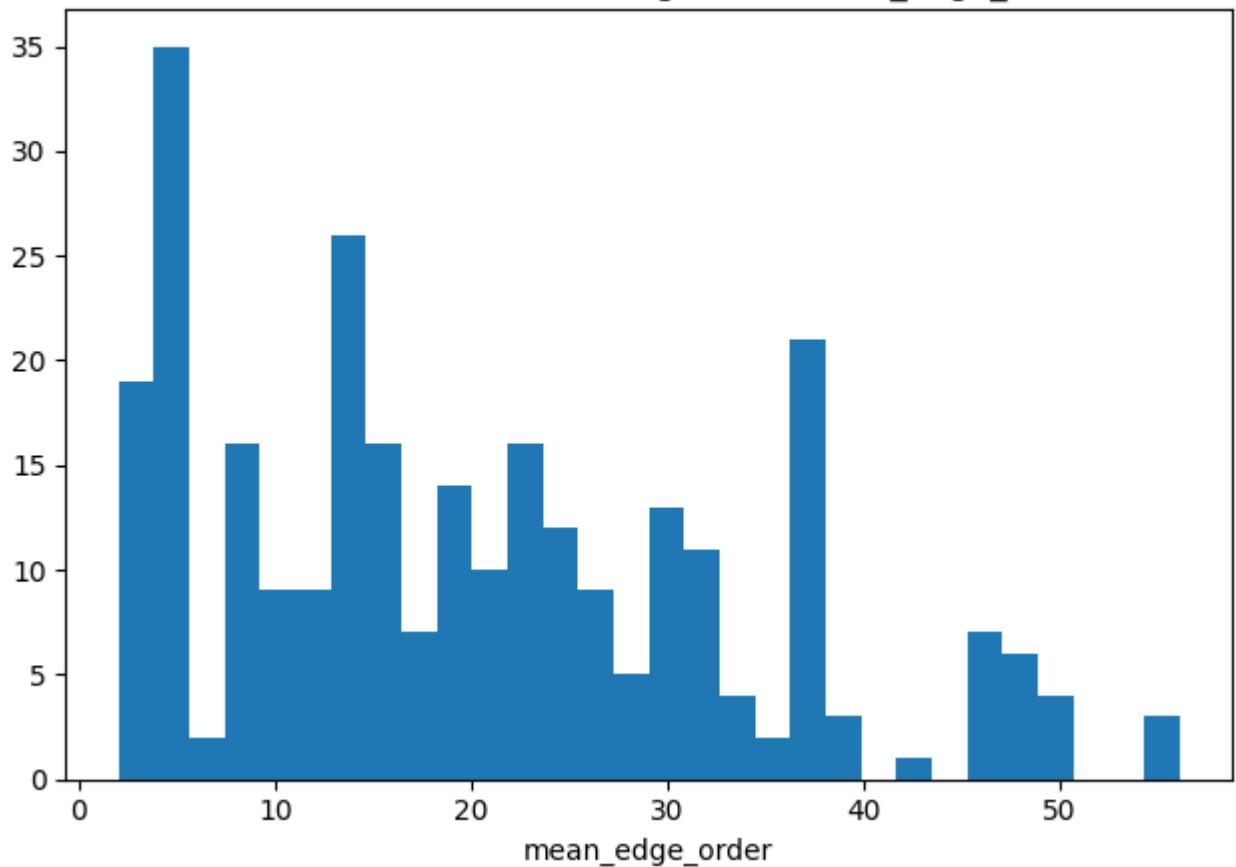
Hamiltonian features: histogram of std_dev_weight



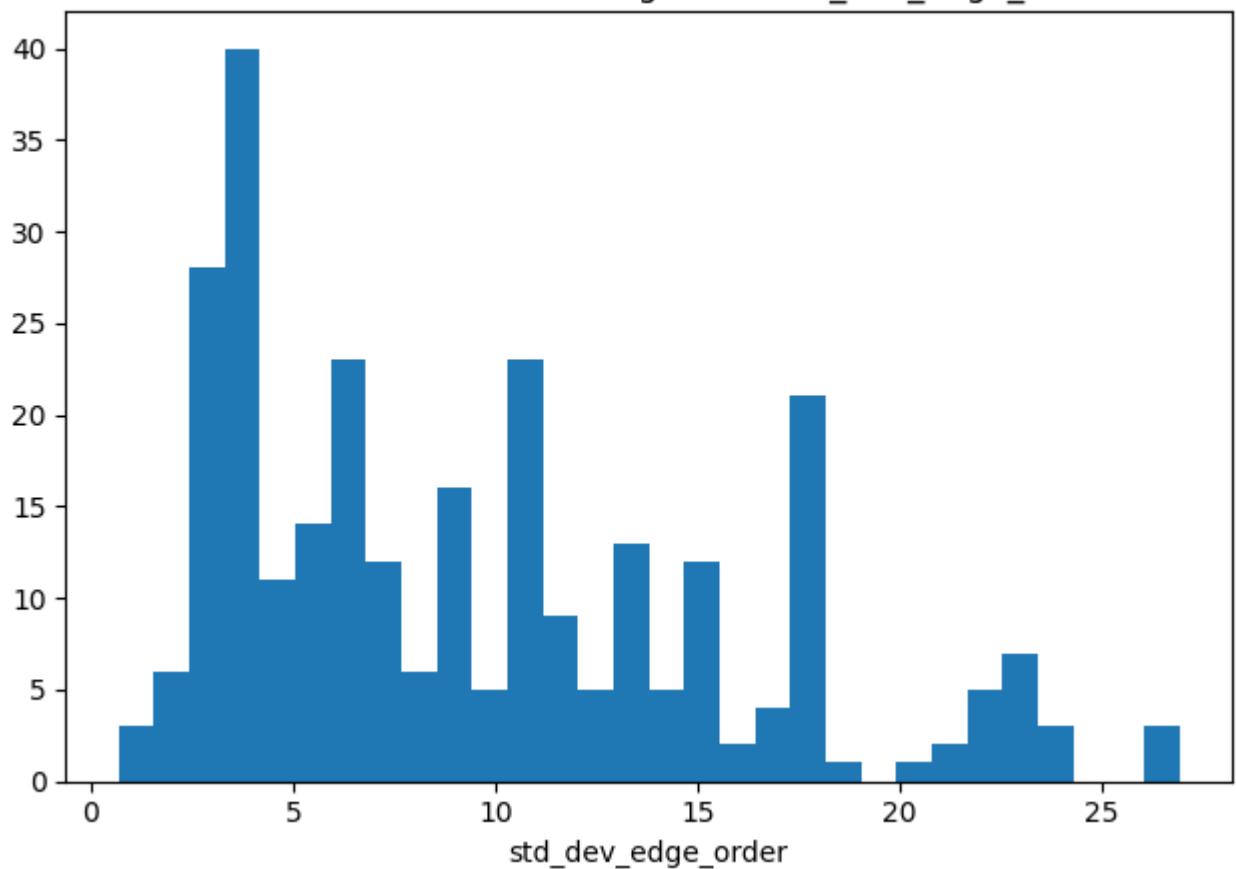
Hamiltonian features: histogram of max_edge_order



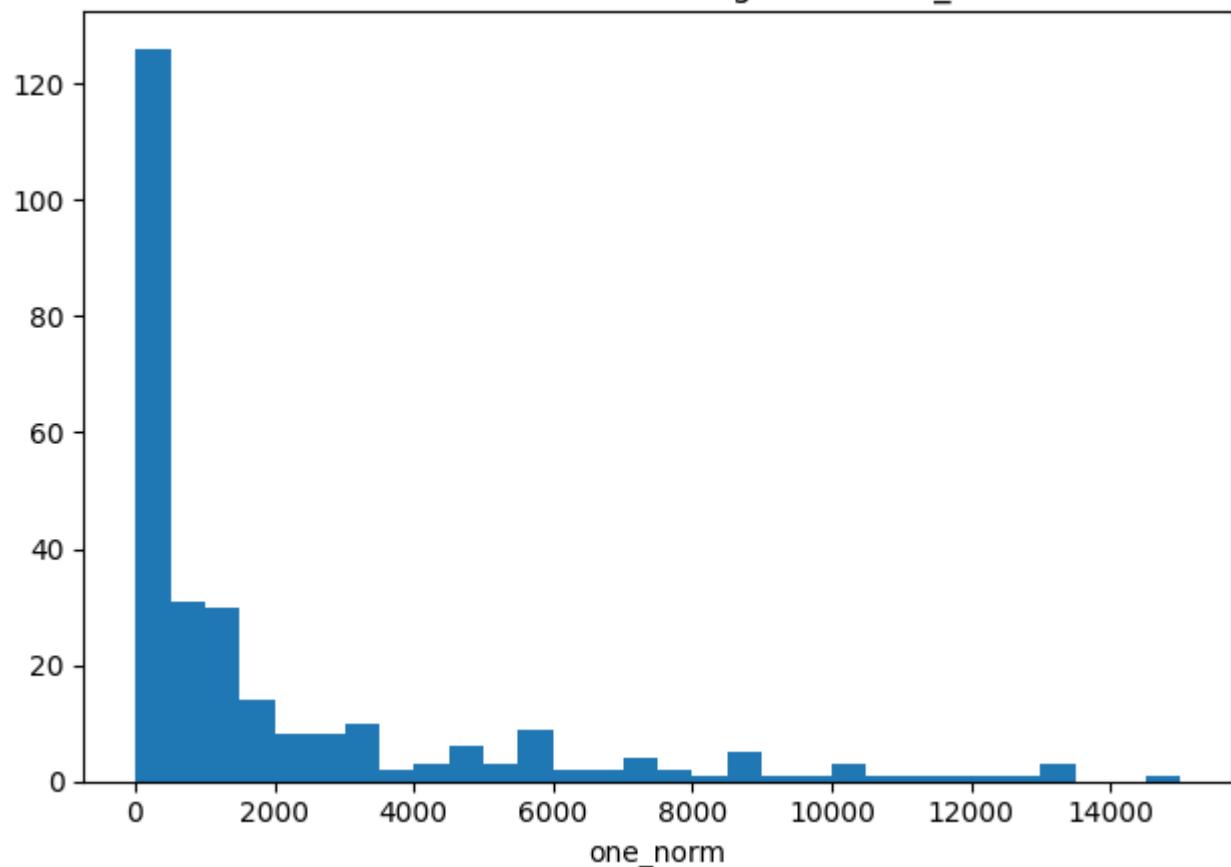
Hamiltonian features: histogram of mean_edge_order



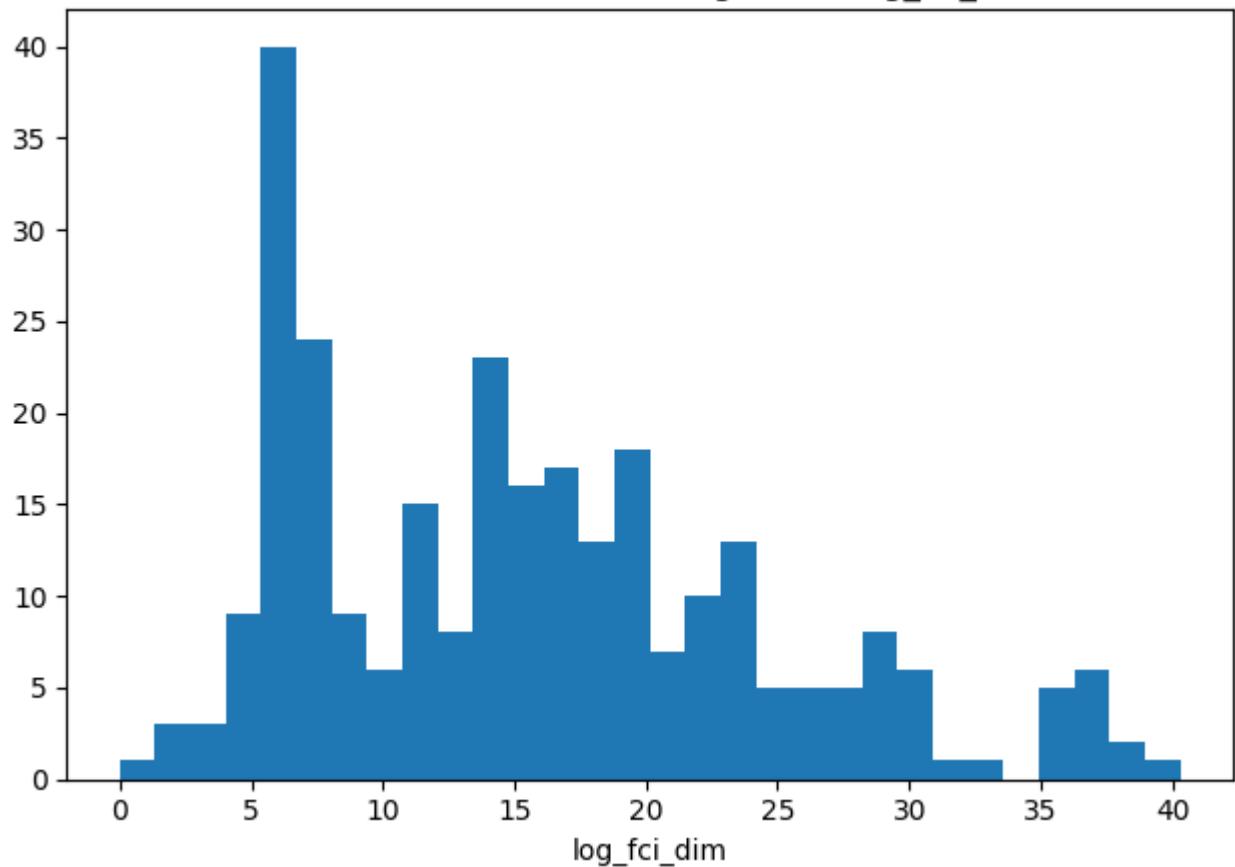
Hamiltonian features: histogram of std_dev_edge_order



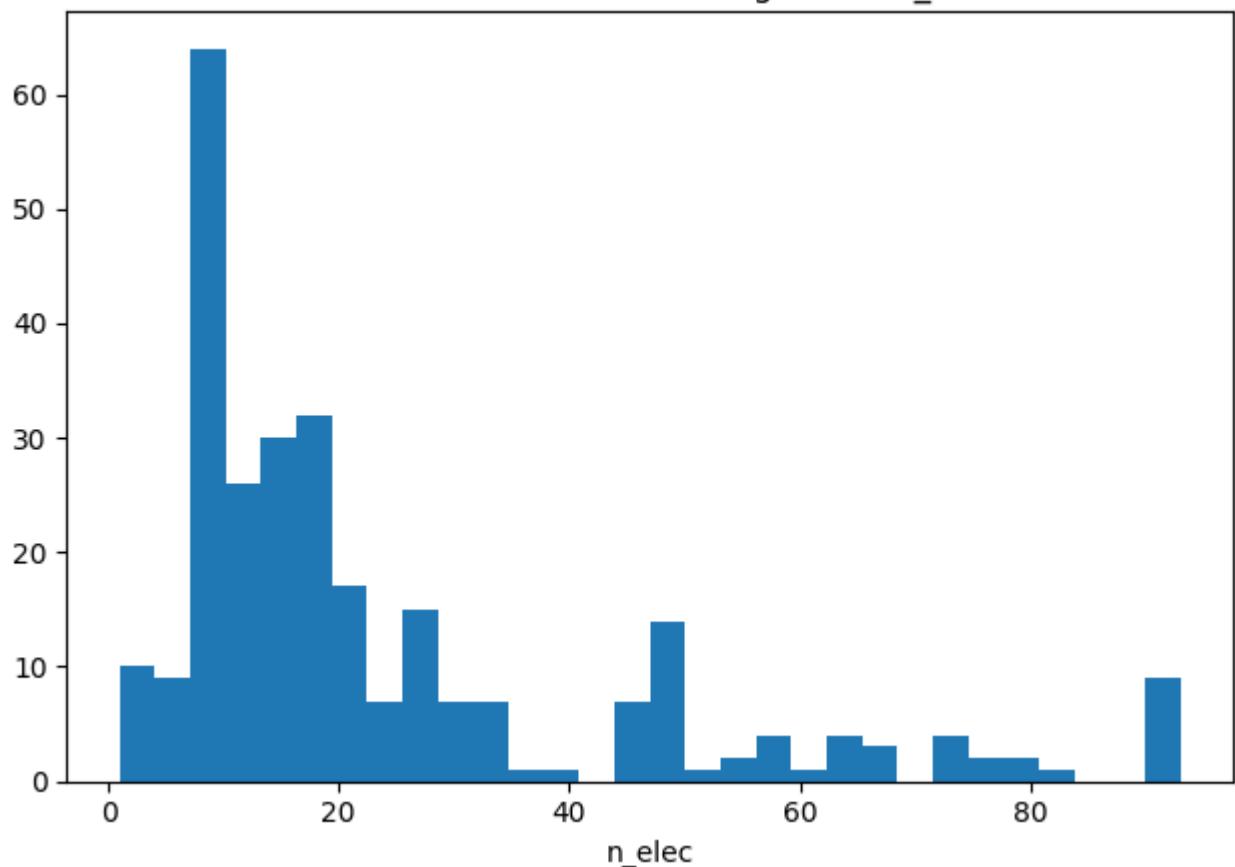
Hamiltonian features: histogram of one_norm



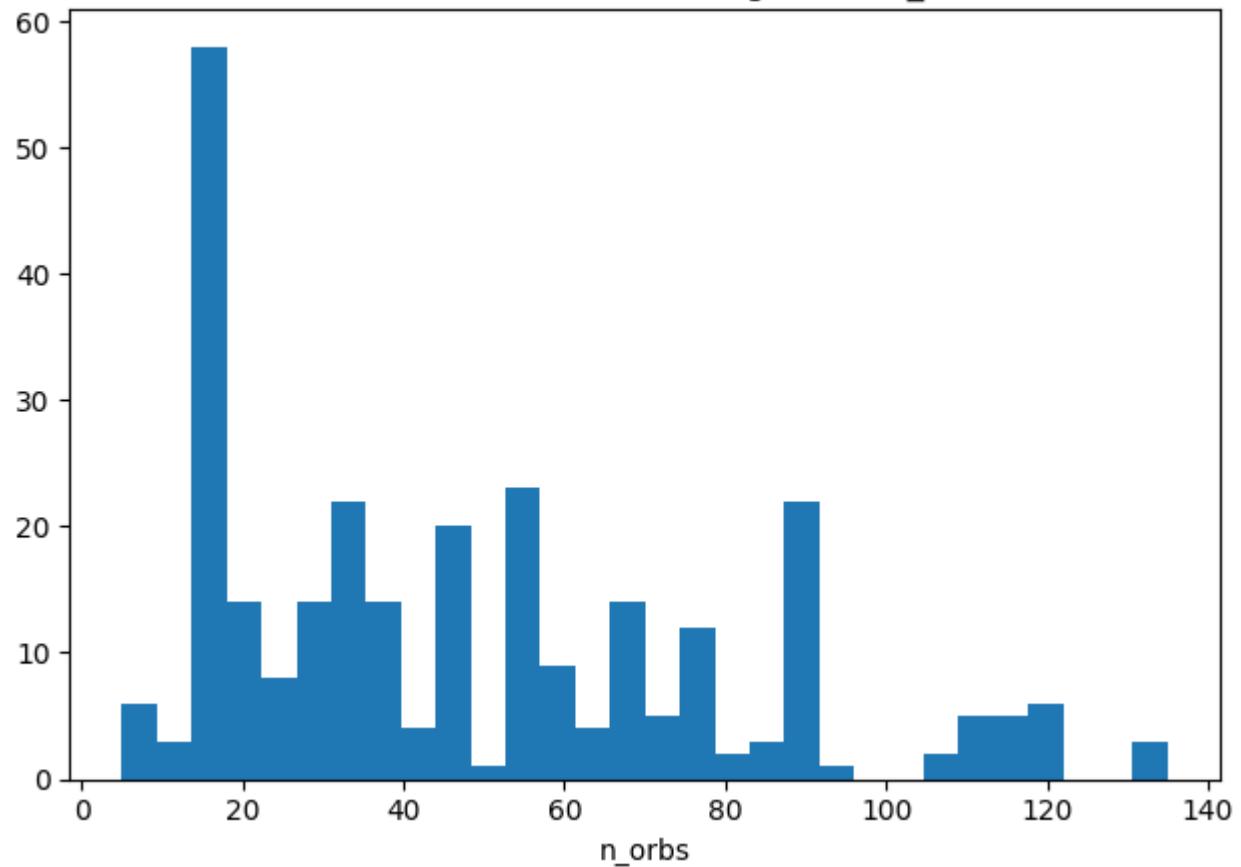
Hamiltonian features: histogram of log_fci_dim



Hamiltonian features: histogram of n_elec



Hamiltonian features: histogram of n_orbs



Hamiltonian features: histogram of df_gap

