

GSEE Benchmark Standard Report

Report based on data from 2025-01-30T17:45:00.466432+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Wed Jan 29 10:24:10 2025

Input data: GSEE -
`HC_utility_estimates_all_instances_task_uuids_v2.csv`, last modified
Thu Jan 9 12:11:19 2025

Latest creation time for a `problem_instance.json` file: Mon Jan 27 11:42:37 2025

Latest creation time for a `solution.json` file: Thu Jan 30 12:27:04 2025

Problem Instance Summary Statistics

number of `problem_instances`: 84.

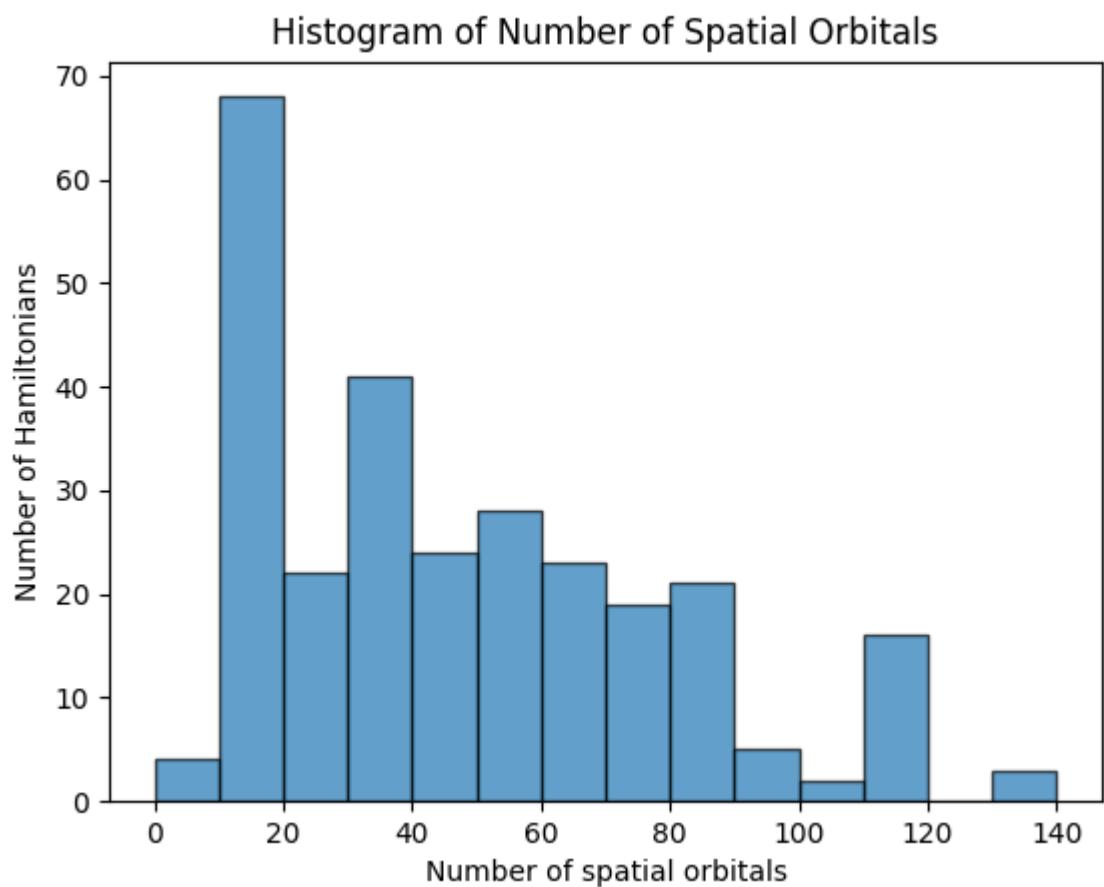
`problem_instance.json` with the most tasks: 30 (`hubbard_square/614c4444-a31a-4348-b24d-01040208651c`)

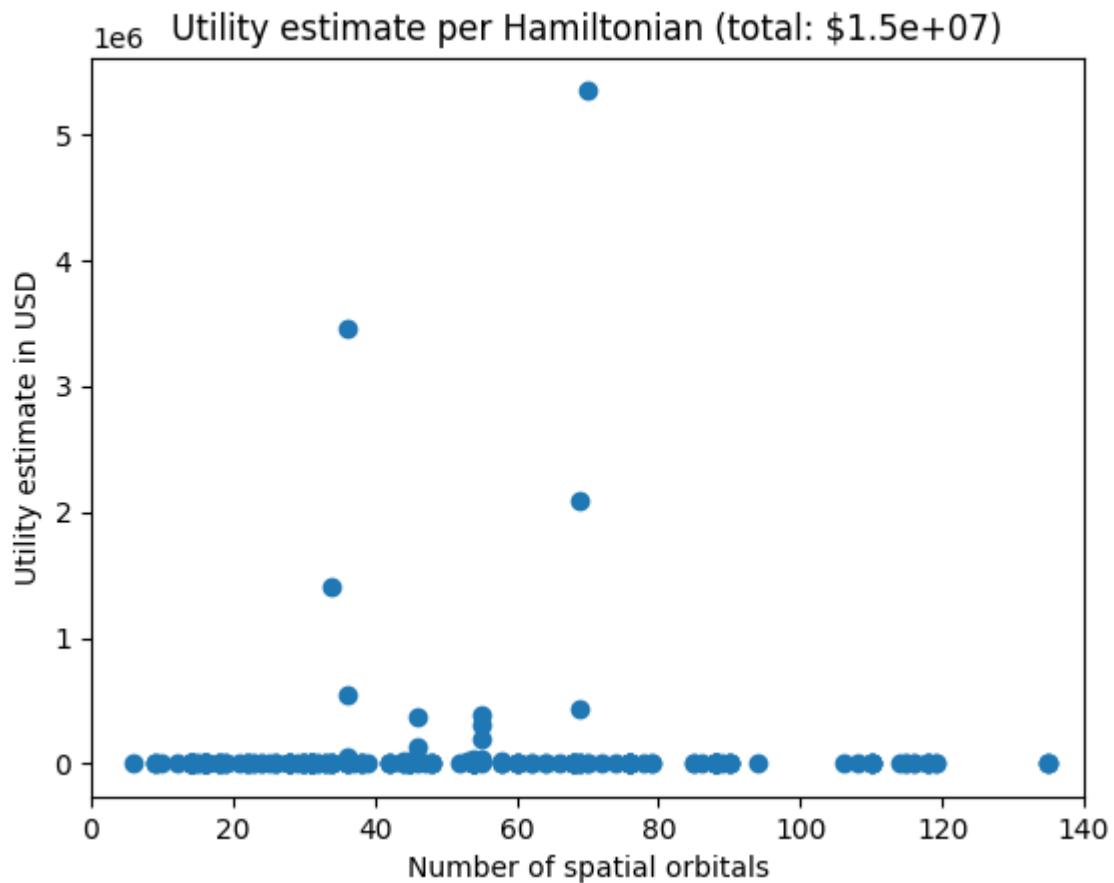
number of Hamiltonians (i.e., tasks) we have features calculated for: 276

minimum number of orbitals: 6

median number of orbitals: 42.0

maximum number of orbitals: 135





Solver Summary Statistics

number of unique participating solvers: 17

Solver: SHCI_opt/2dde727e-a881-44fa-aabf-bba6248e4baf, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.83333333 0.99342105]

Solver: SHCI_pt_1e-4/4ed500f1-0650-41e3-af00-e4d0359394b4, ML Solvability Ratio: {'PCA': 0.9707, 'NNMF': 0.9859}, F1 Score: [0.71428571 0.97222222]

Solver: SHCI_var_1e-4/7e730dfb-57ee-480b-a8a1-4b73f5f07c54, ML Solvability Ratio: {'PCA': 0.8691, 'NNMF': 0.8794}, F1 Score: [0.99212598 0.99470899]

Solver: SHCI_pt_2e-4/ad964781-302e-4728-a26d-39918e0a6cdb, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.64516129 0.96140351]

Solver: SHCI_pt_2e-5/c71b90bd-3250-4c0c-b4e7-fc9878f141f6, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.375 0.96666667]

Solver: SHCI_pt_5e-5/d626506c-7aae-4ad6-802a-b29af5f2bb93, ML Solvability Ratio: {'PCA': 1.0, 'NNMF': 1.0}, F1 Score: [0.9375 0.99295775]

Solver: SHCI_var_2e-4/0db183e3-a86d-491b-9125-599556e37c7a, ML
Solvability Ratio: {'PCA': 0.3499, 'NNMF': 0.0833}, F1 Score: [0.95364238
0.95757576]

Solver: SHCI_var_2e-5/86bfe50c-9342-4d54-bb68-abc8abd95688, ML
Solvability Ratio: {'PCA': 0.5812, 'NNMF': 0.3942}, F1 Score: [0.8627451
0.97358491]

Solver: SHCI_var_5e-5/01949b95-c427-4693-9134-01f47f688c09, ML
Solvability Ratio: {'PCA': 0.6393, 'NNMF': 0.3549}, F1 Score: [0.83950617
0.94468085]

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

Solver: CISD/418f060e-496b-4024-8d2d-9b1f8791e76d, ML Solvability
Ratio: {'PCA': 0.0079, 'NNMF': 0.003}, F1 Score: [0.97826087 0.85]

Solver: CCSD(T)/c09217e6-d0f7-4b0f-81c4-79210b7ac878, ML Solvability
Ratio: {'PCA': 0.6011, 'NNMF': 0.8102}, F1 Score: [0.86956522
0.86451613]

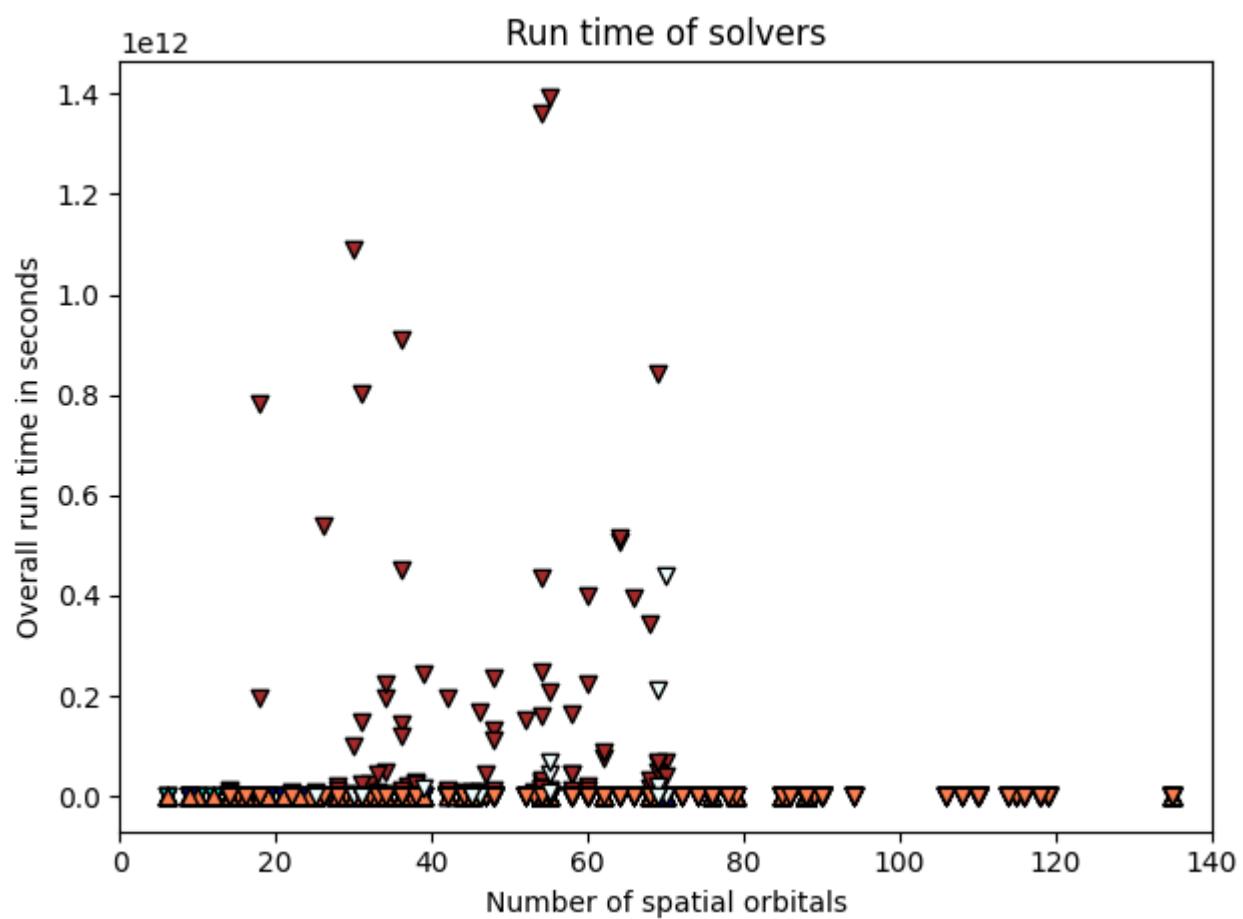
Solver: HF/5f5e617a-19c2-4d82-bebc-b2d6b3dc012, ML Solvability Ratio:
{'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98675497 0.71428571]

Solver: MP2/b420358b-5def-41e6-8c5d-b9d93b6aec02, ML Solvability Ratio:
{'PCA': 0.0, 'NNMF': 0.0}, F1 Score: [0.98675497 0.71428571]

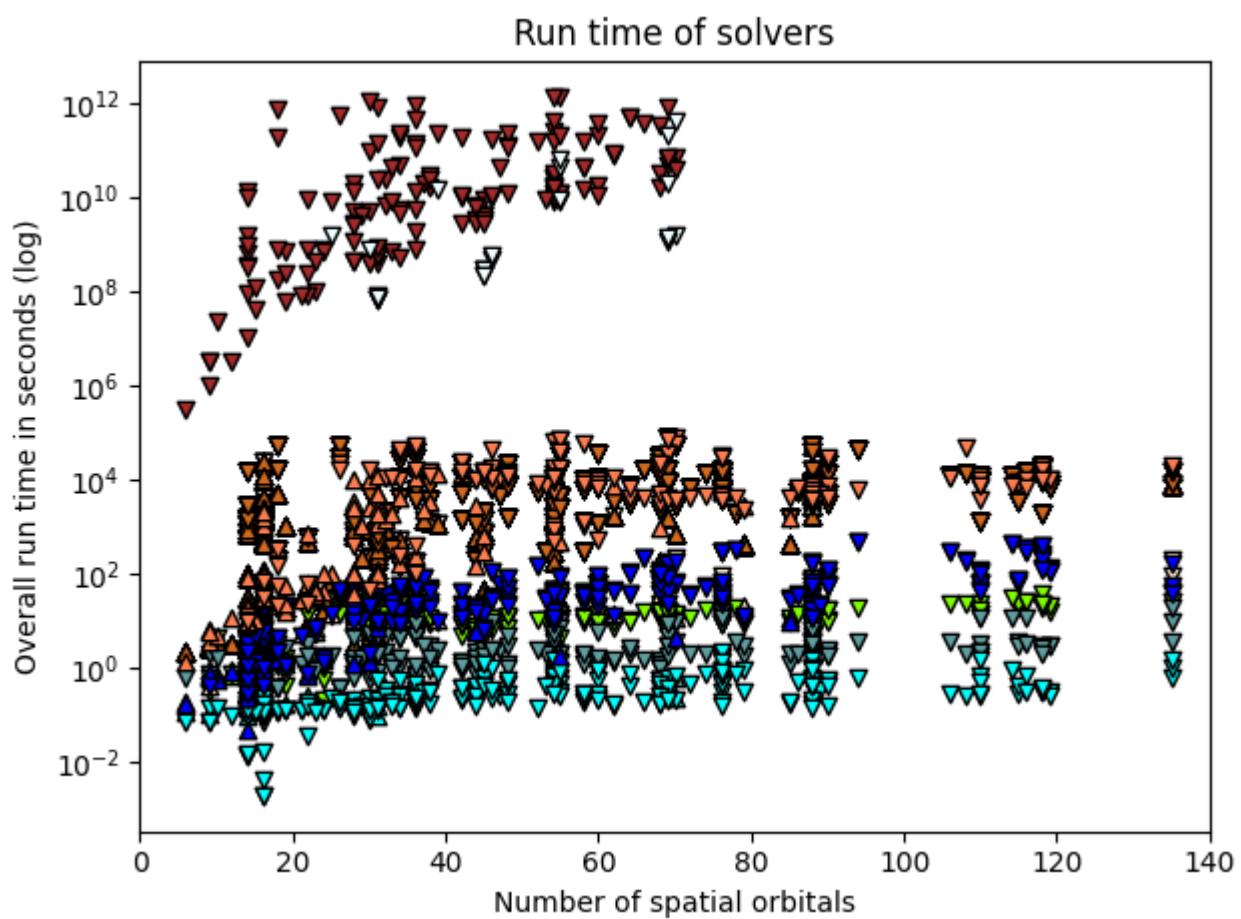
Solver: CCSD/0a29e54f-bef9-4d19-bafa-d94b1c4b37aa, ML Solvability Ratio:
{'PCA': 0.0, 'NNMF': 0.0197}, F1 Score: [0.98867925 0.94117647]

Solver: DMRG_Niagara_cluster_lowest_energy/16537433-9f4c-4eae-
a65d-787dc3b35b59, ML Solvability Ratio: {'PCA': 0.5461, 'NNMF':
0.6106}, F1 Score: [0.96629213 0.98678414]

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

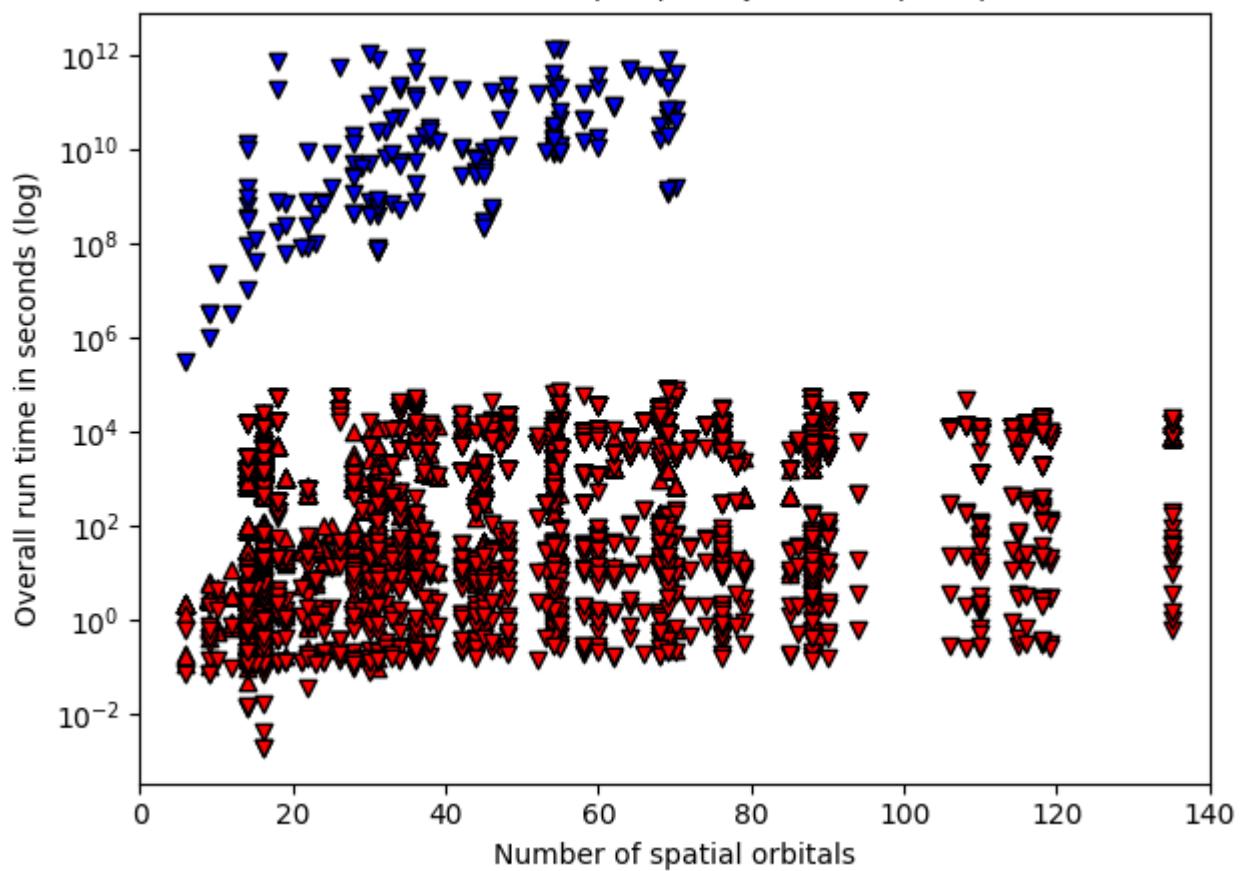


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

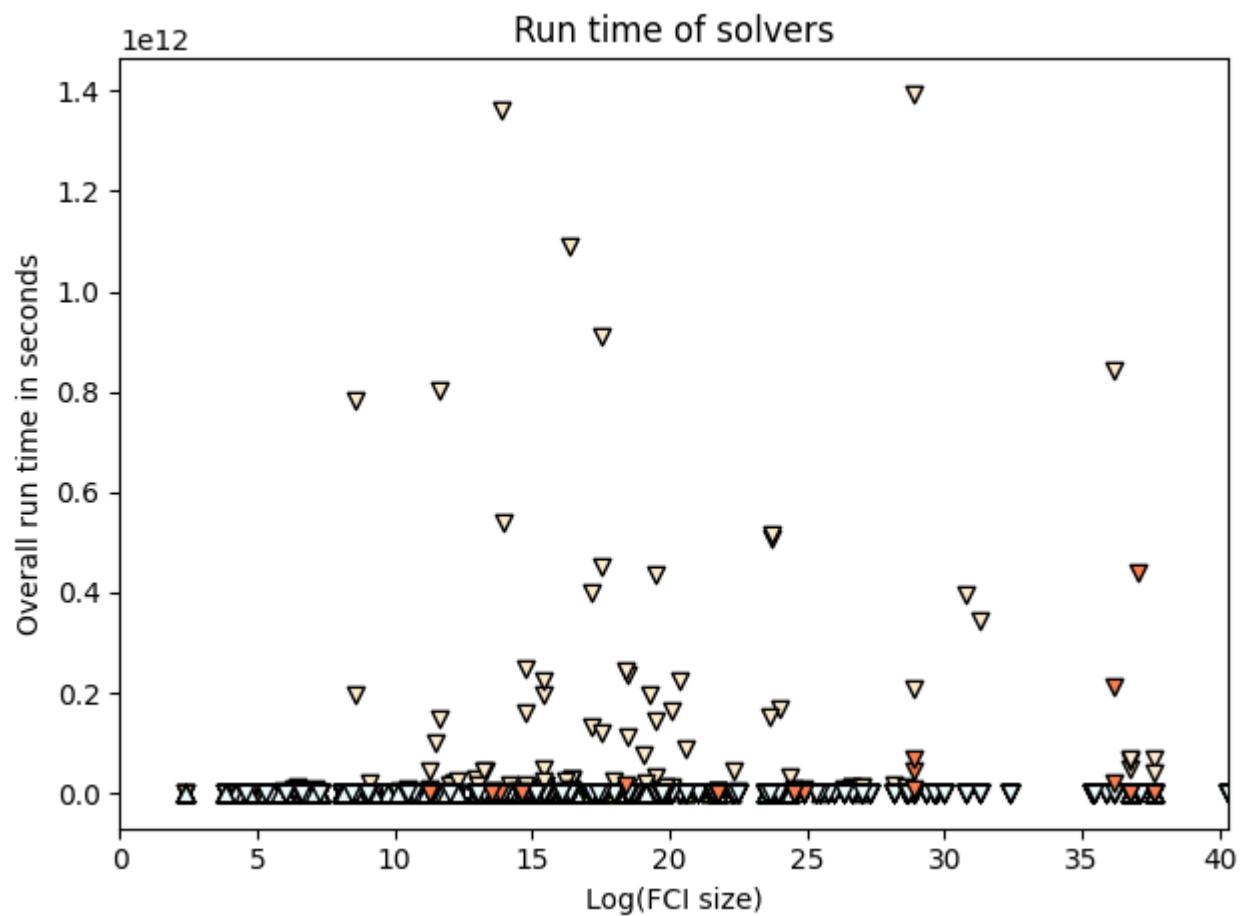


NOTE: only attempted tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.

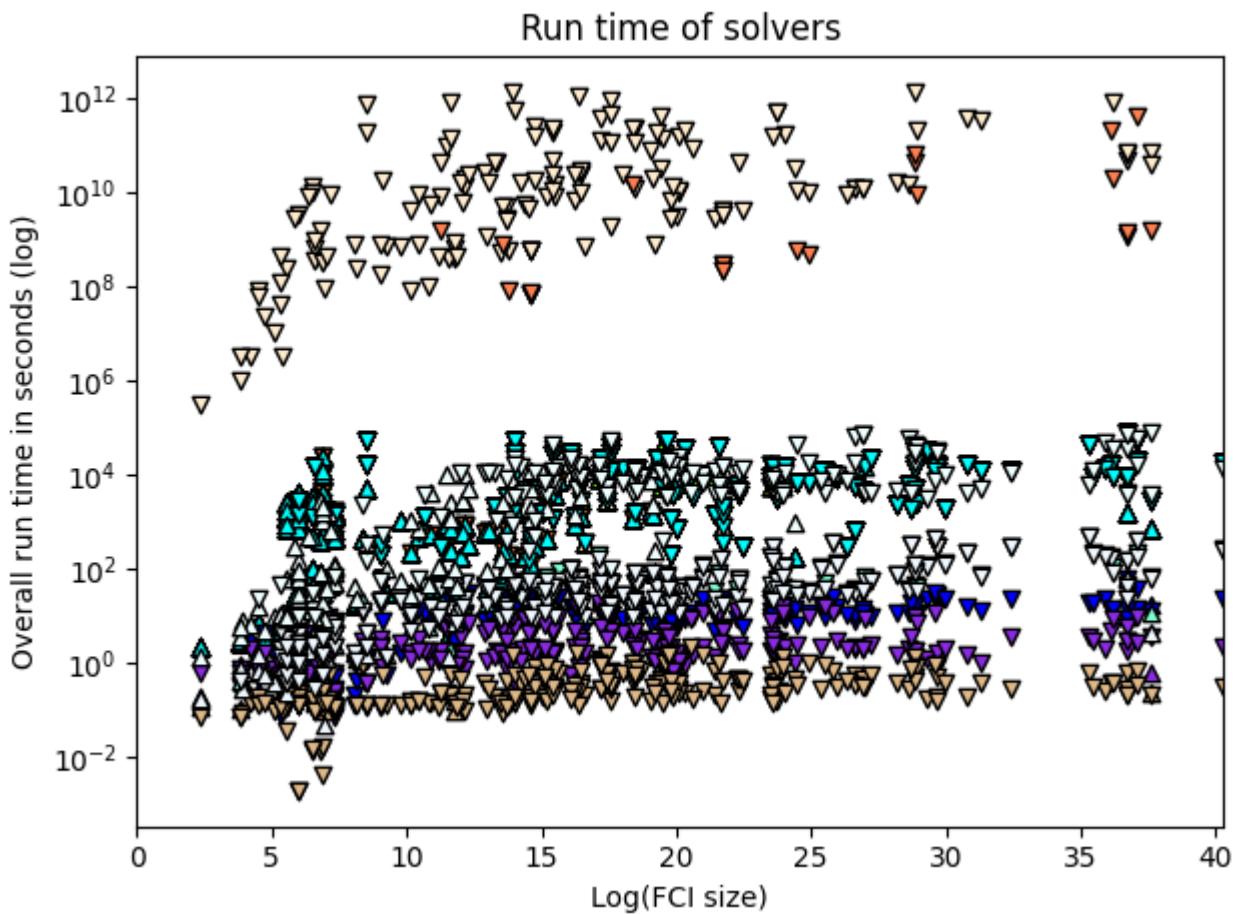
Run time of Classical (red) vs Quantum (blue) solvers



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



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

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

solver_short_name:SHCI_opt

compute.hardware_type:classical_computer

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

algorithm_details:SHCI with optimized orbitals followed by SHCI+PT

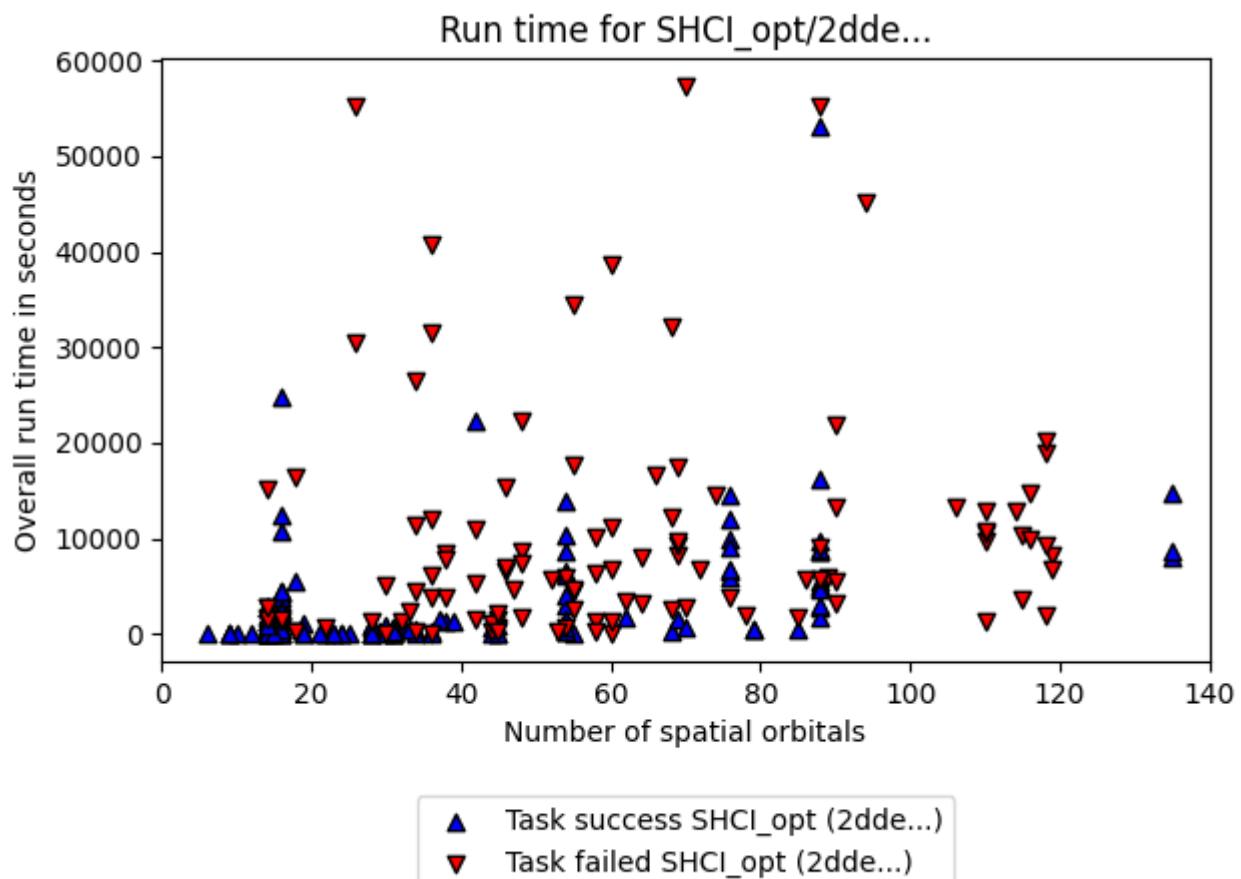
software_details:SHCI Arrow Code (<https://github.com/QMC-Cornell/shci>).

performance_metrics_uuid: 8dbde2d7-1d3f-4c17-9c77-2edf63490d19

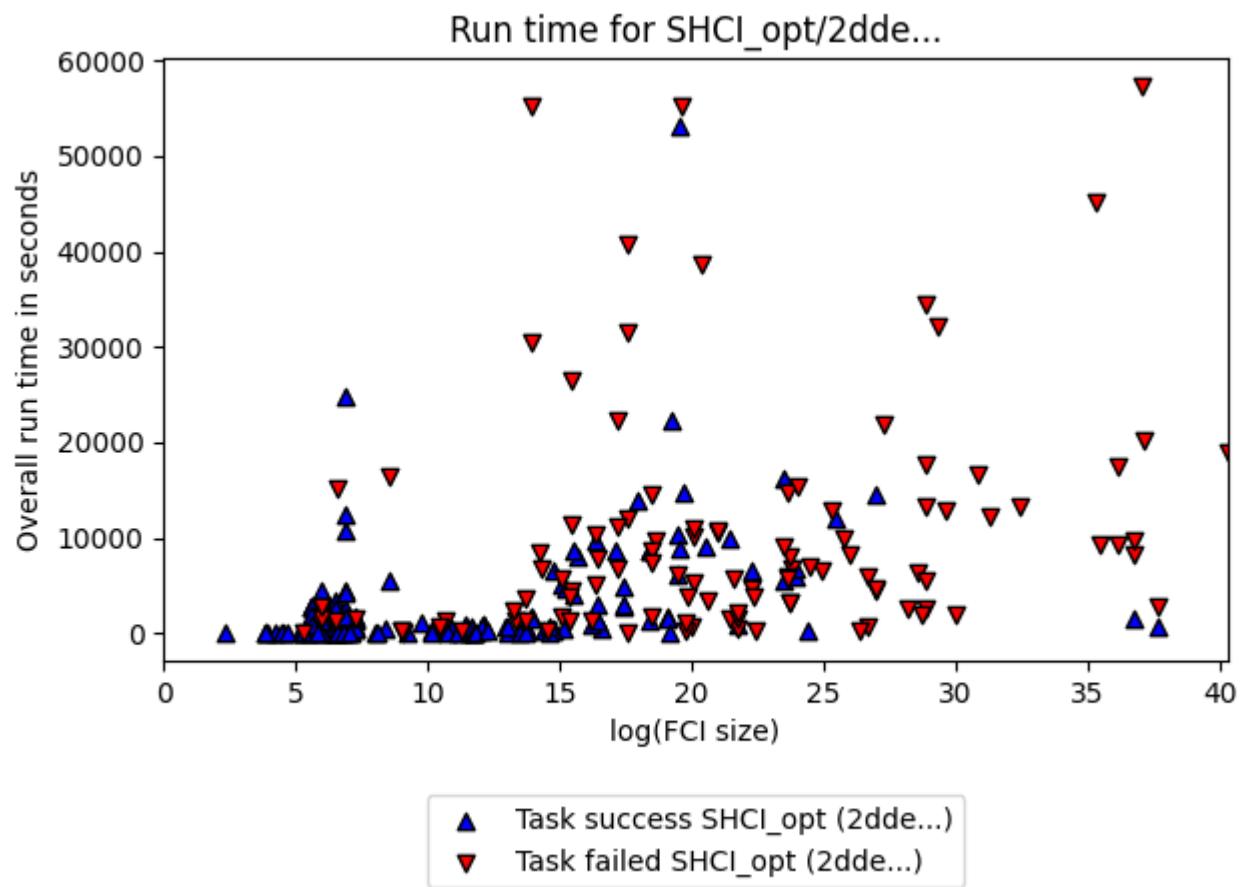
creation_timestamp: 2025-01-30T17:45:00.466432+00:00

number_of_problem_instances: 84

```
number_of_problem_instances_attempted: 80
number_of_problem_instances_solved: 33
number_of_tasks: 276
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: [0.8333333333333334, 0.993421052631579]
ml_metrics_calculator_version: 1
```



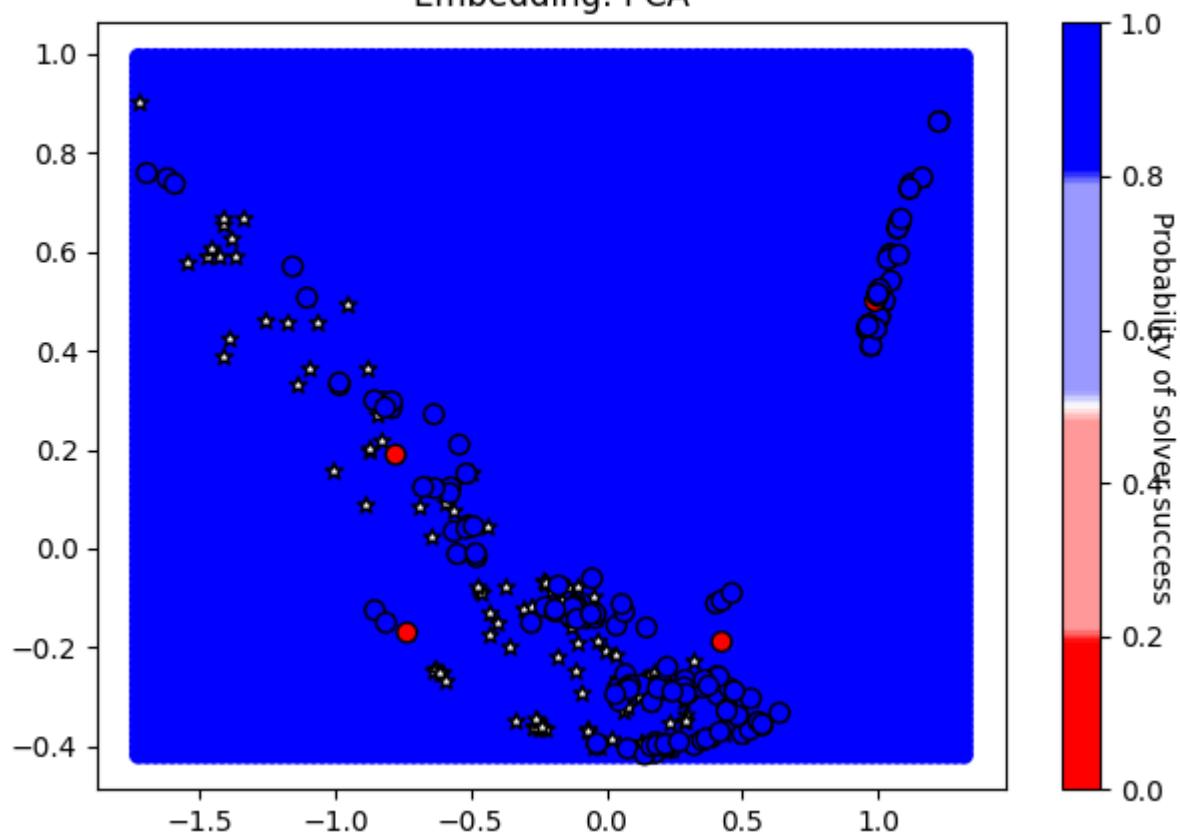
Note: plot only contains attempted tasks.



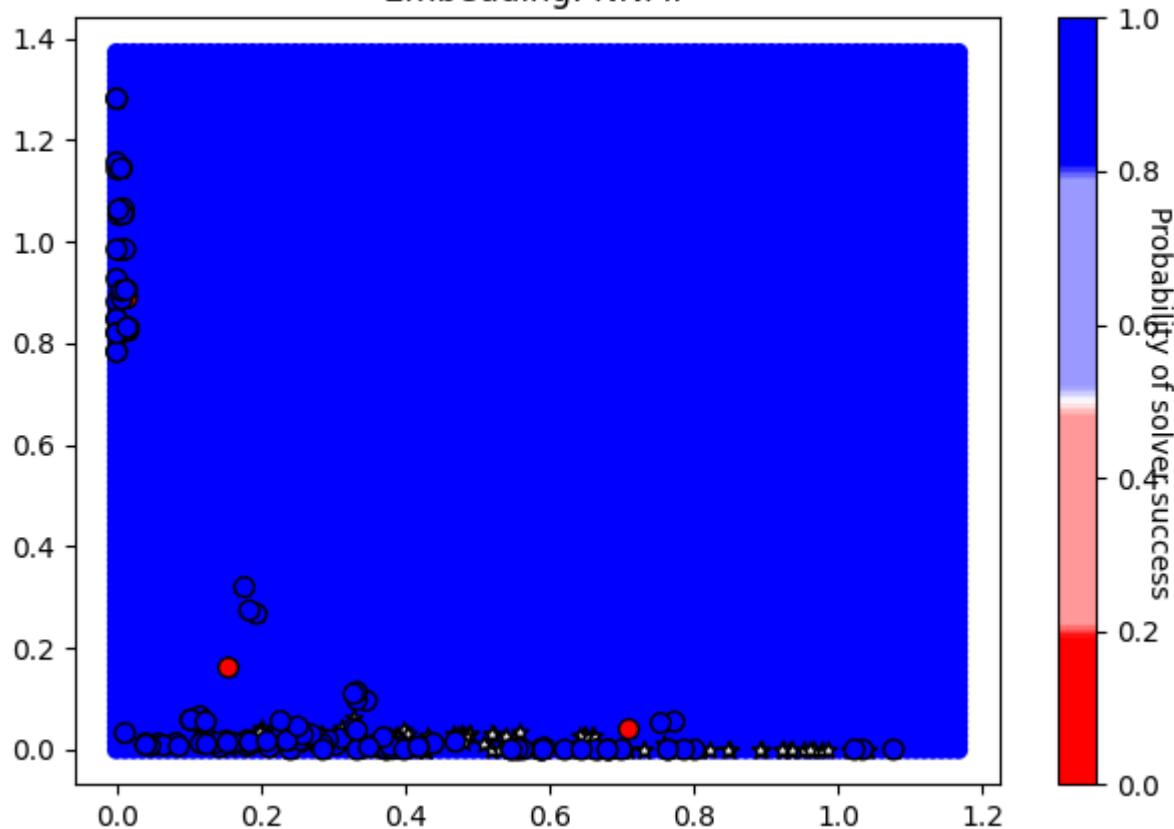
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_2dde727e-a881-44fa-aabf-bba6248e4baf_utility_capture_plot.png)

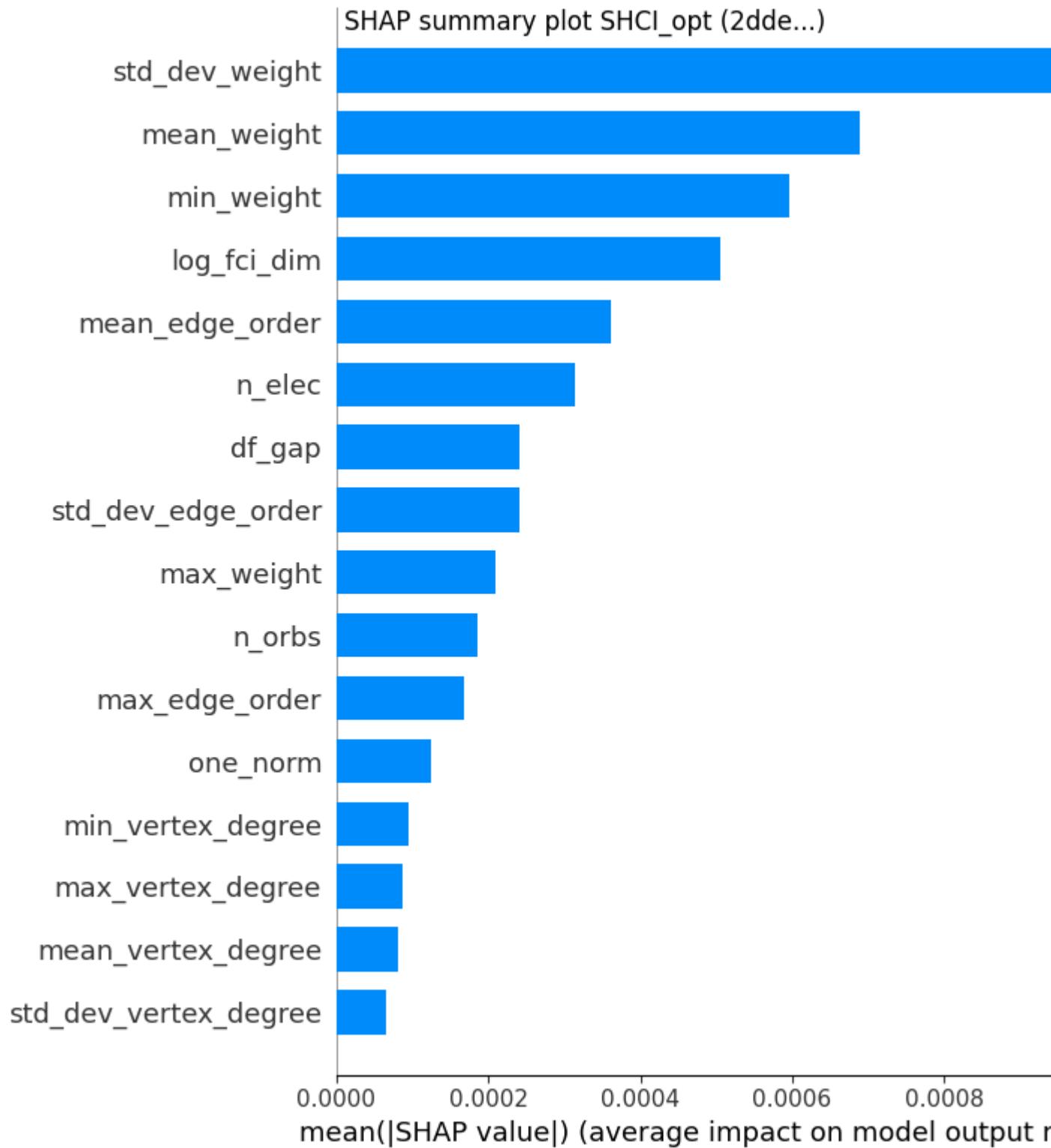
Solver SHCI_opt (2dde...)
Embedding: PCA



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.

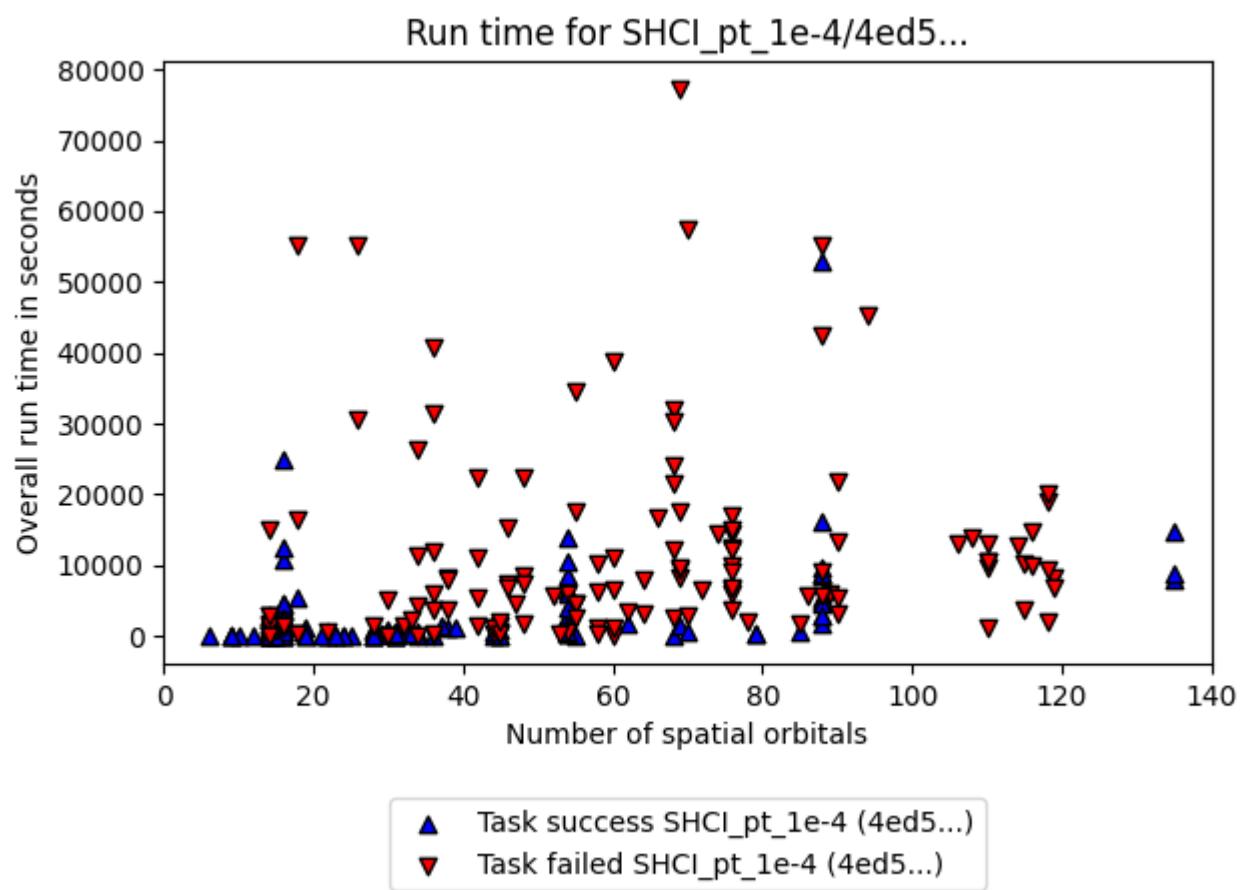


Solver SHCI_pt_1e-4, 4ed500f1-0650-41e3-af00-e4d0359394b4

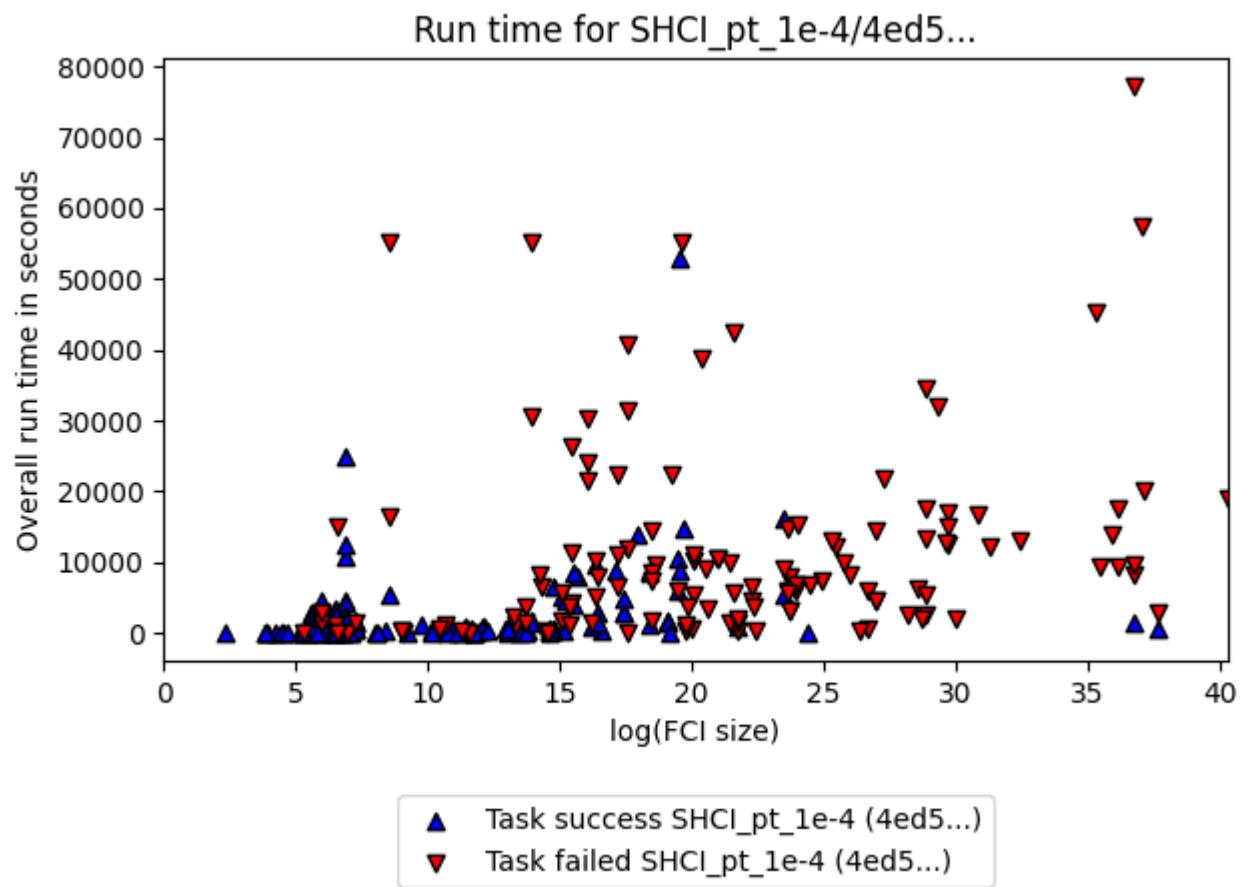
solver_uuid:4ed500f1-0650-41e3-af00-e4d0359394b4

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: ffb46f81-e8eb-46c3-8204-6a14b32b30ed
creation.timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 22
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 140
number_of_tasks_solved_within_run_time_limit: 275
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: 0.9707
comment: solvability ratio based on PCA embedding.
f1_score: [0.7142857142857143, 0.9722222222222222]
ml.metrics_calculator_version: 1



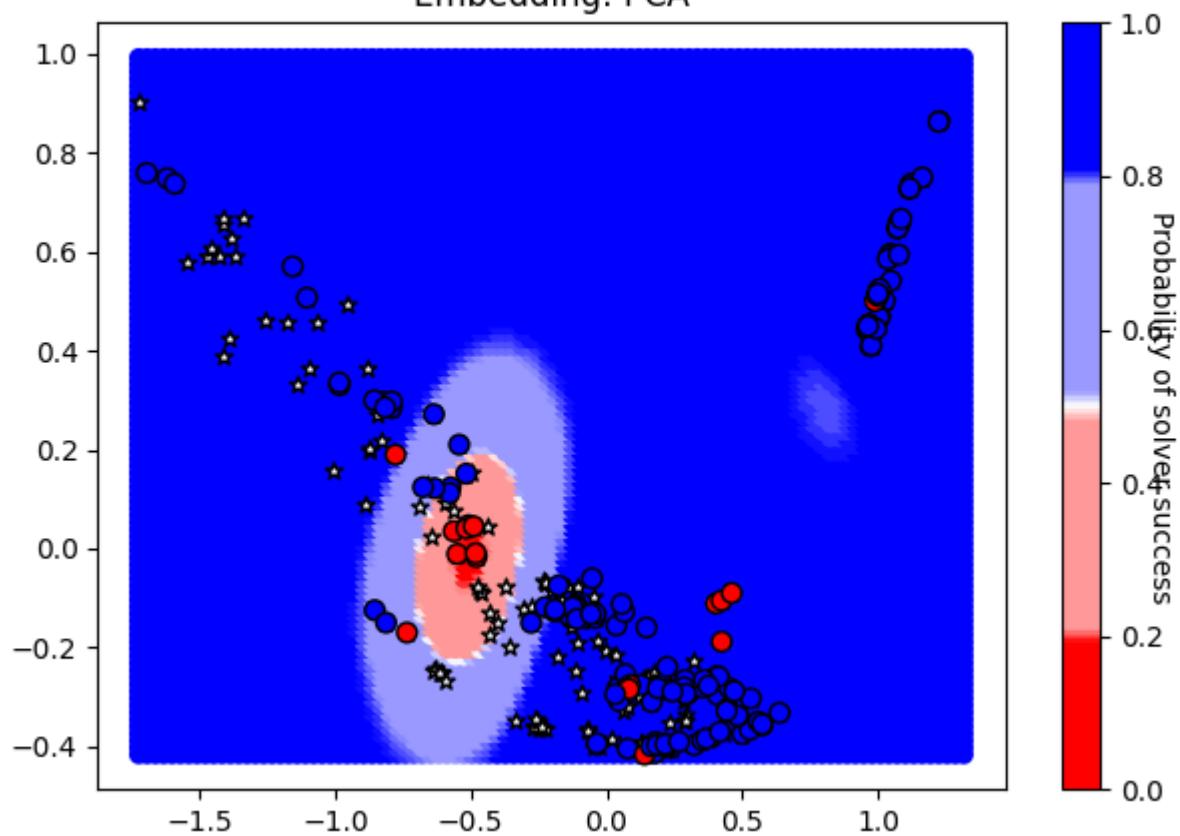
Note: plot only contains attempted tasks.



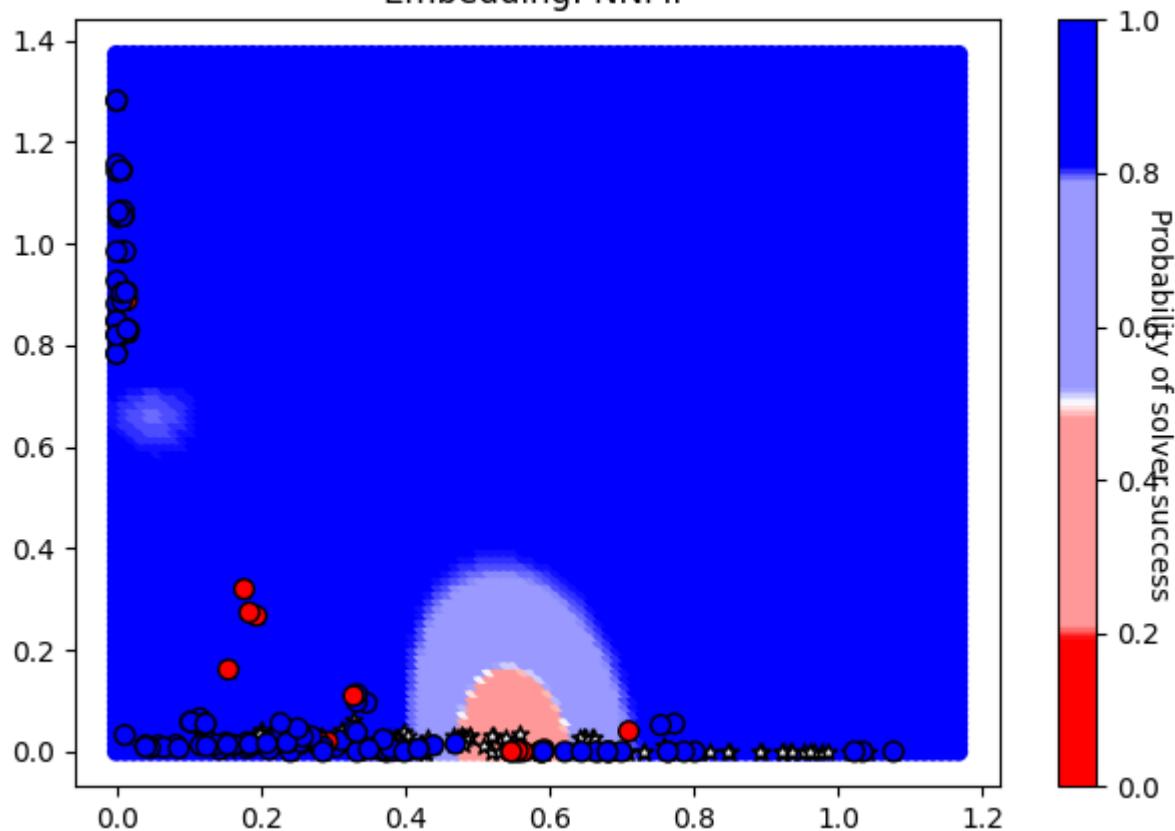
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_4ed500f1-0650-41e3-af00-e4d0359394b4_utility_capture_plot.png)

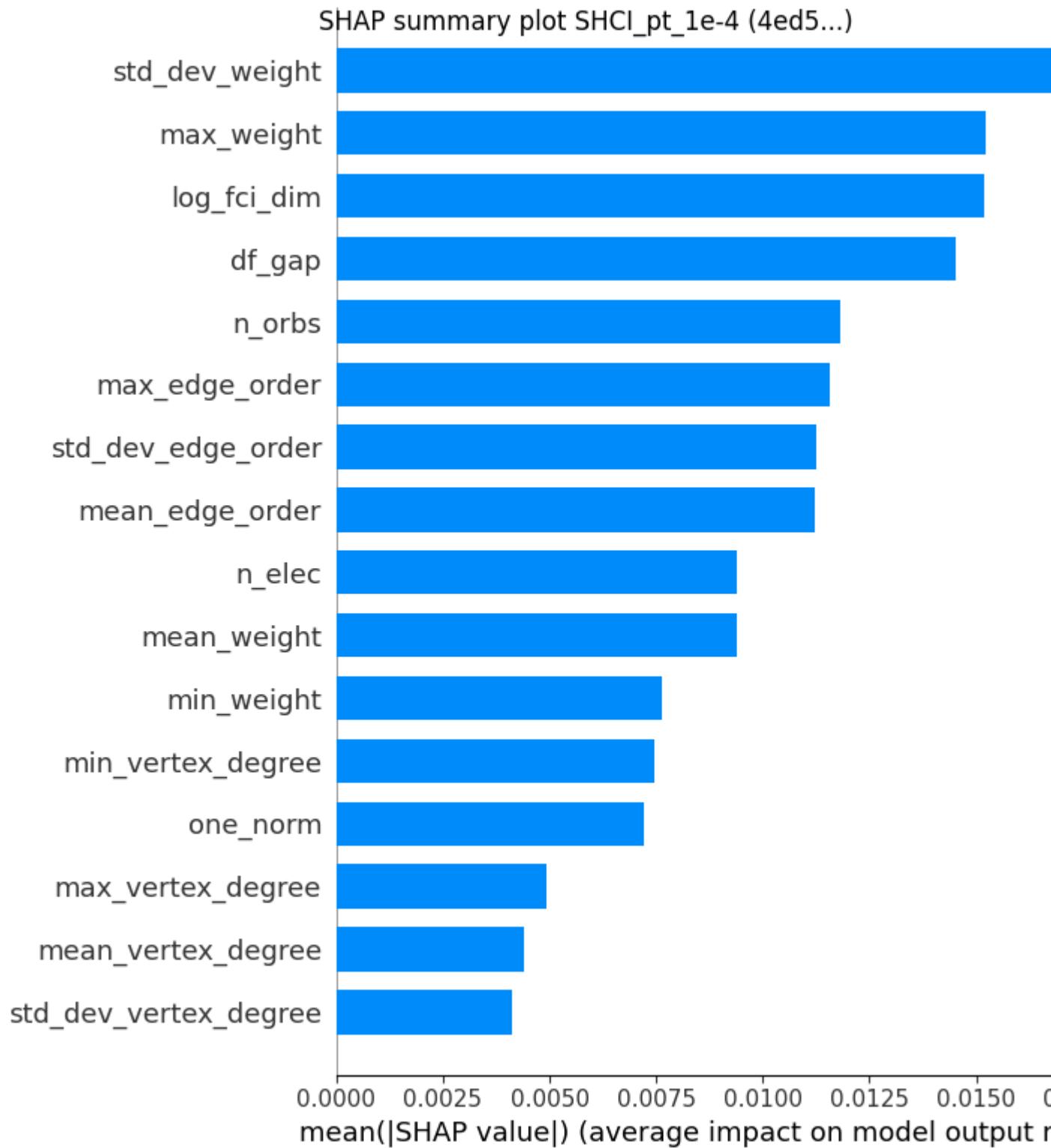
Solver SHCI_pt_1e-4 (4ed5...)
Embedding: PCA



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.

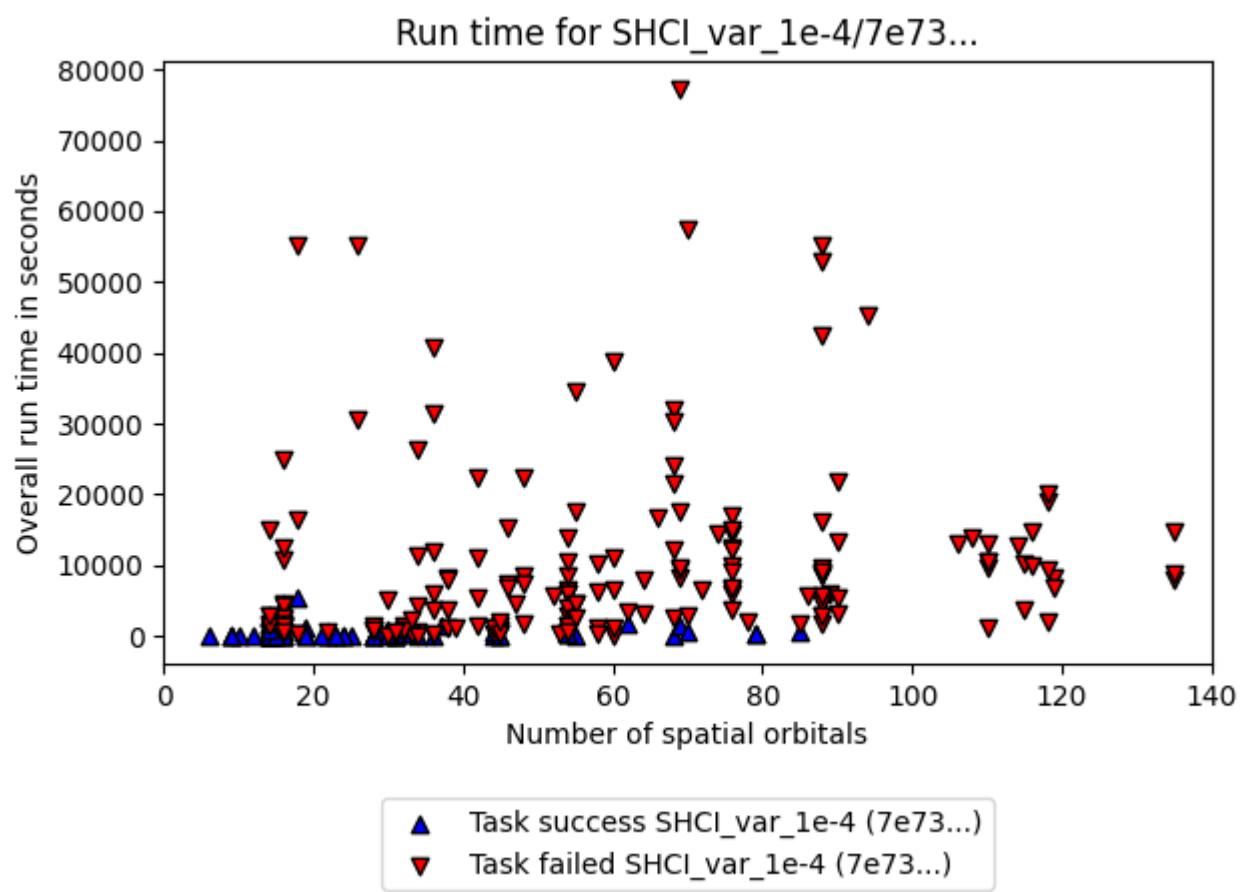


Solver SHCI_var_1e-4, 7e730dfb-57ee-480b-a8a1-4b73f5f07c54

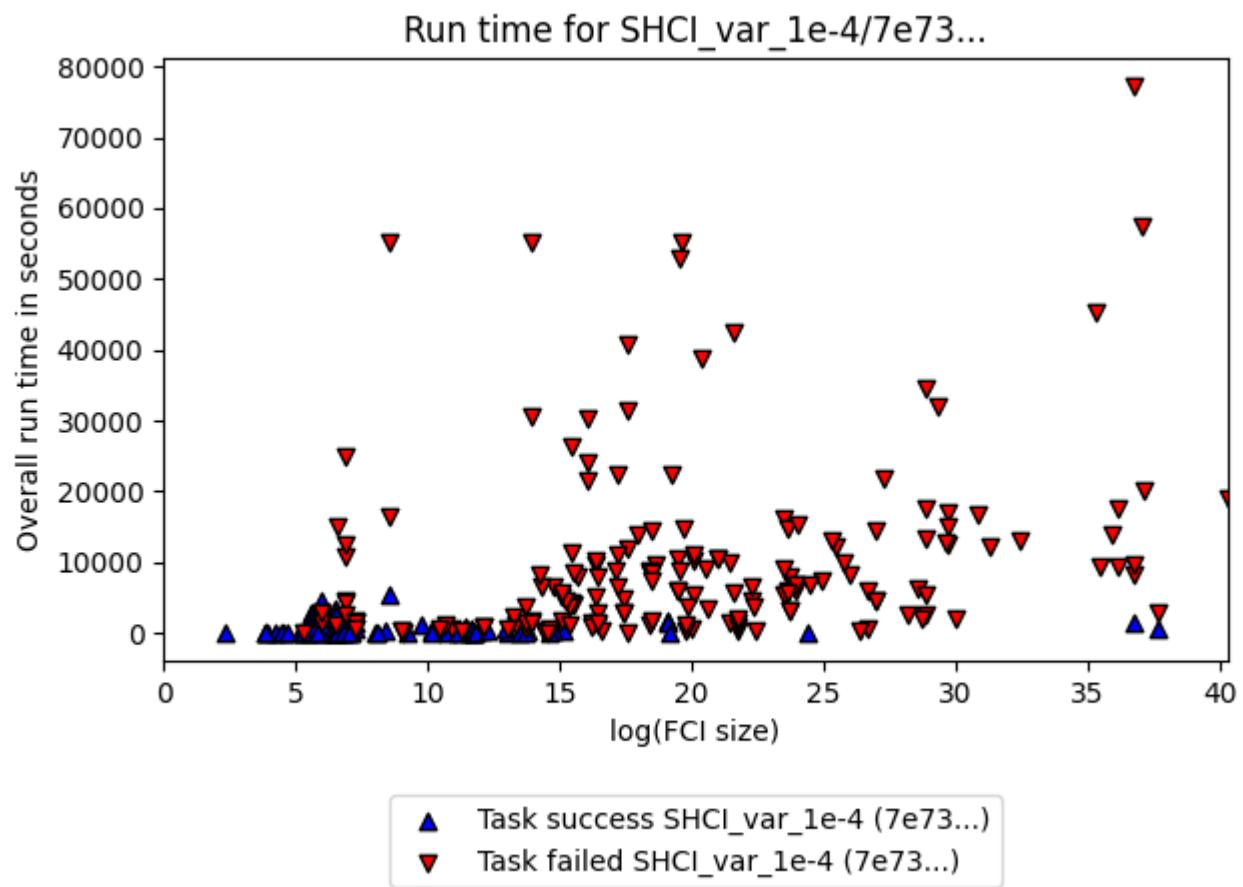
solver_uuid:7e730dfb-57ee-480b-a8a1-4b73f5f07c54

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: d8eada75-7c35-411f-8de3-0829015df276
creation.timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 13
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 95
number_of_tasks_solved_within_run_time_limit: 275
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: 0.8691
comment: solvability ratio based on PCA embedding.
f1_score: [0.9921259842519685, 0.9947089947089947]
ml.metrics_calculator_version: 1



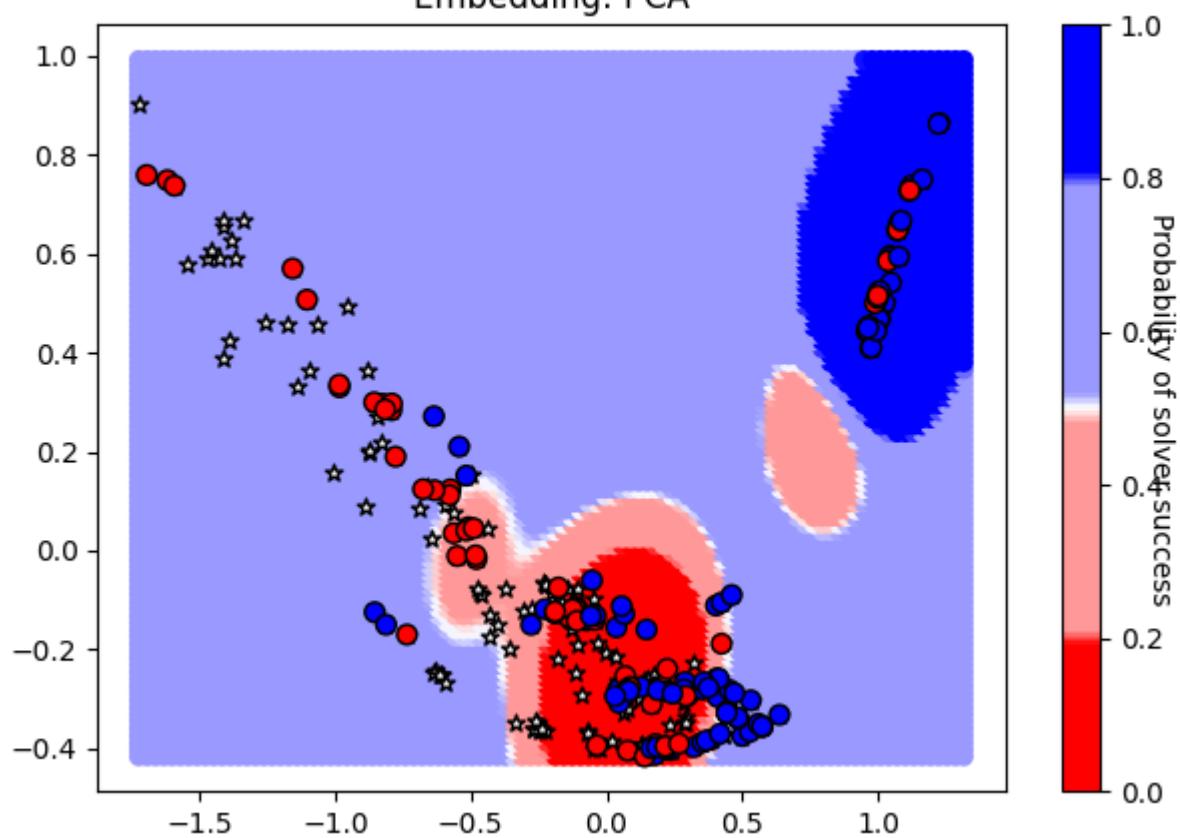
Note: plot only contains attempted tasks.



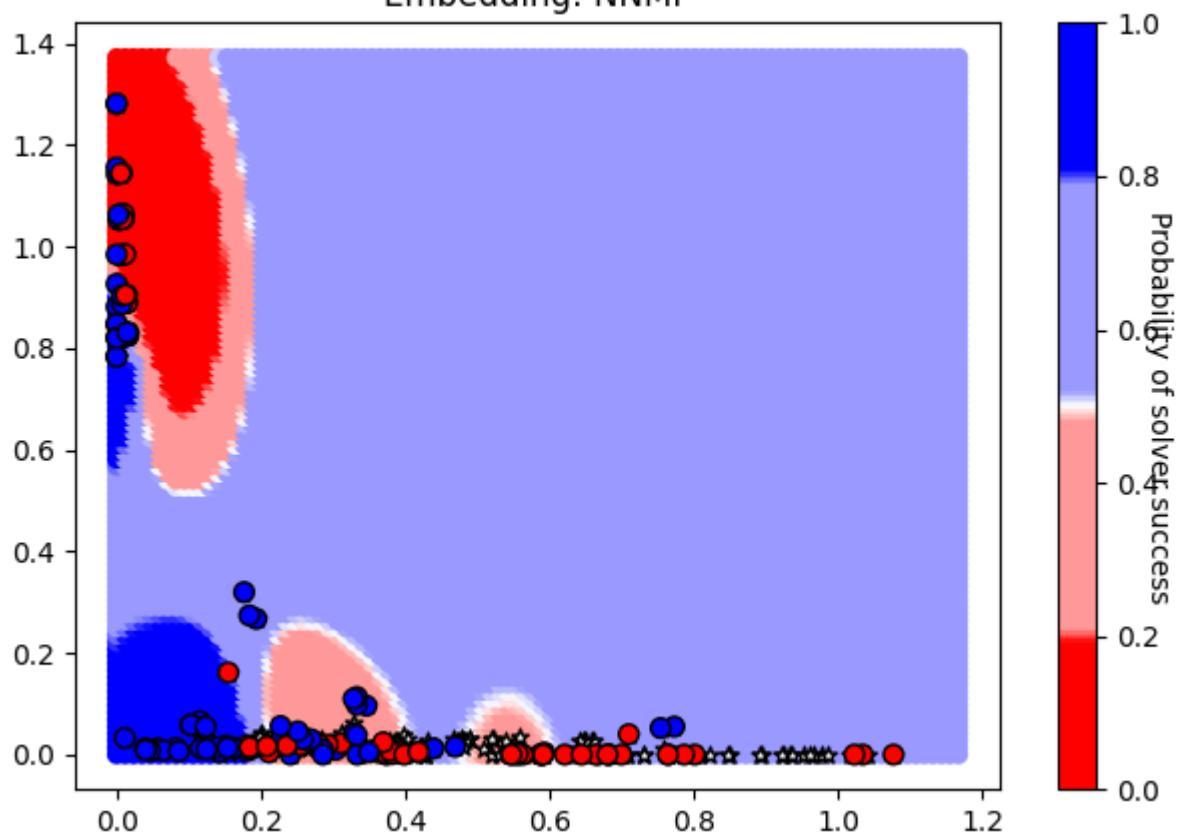
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_7e730dfb-57ee-480b-a8a1-4b73f5f07c54_utility_capture_plot.png)

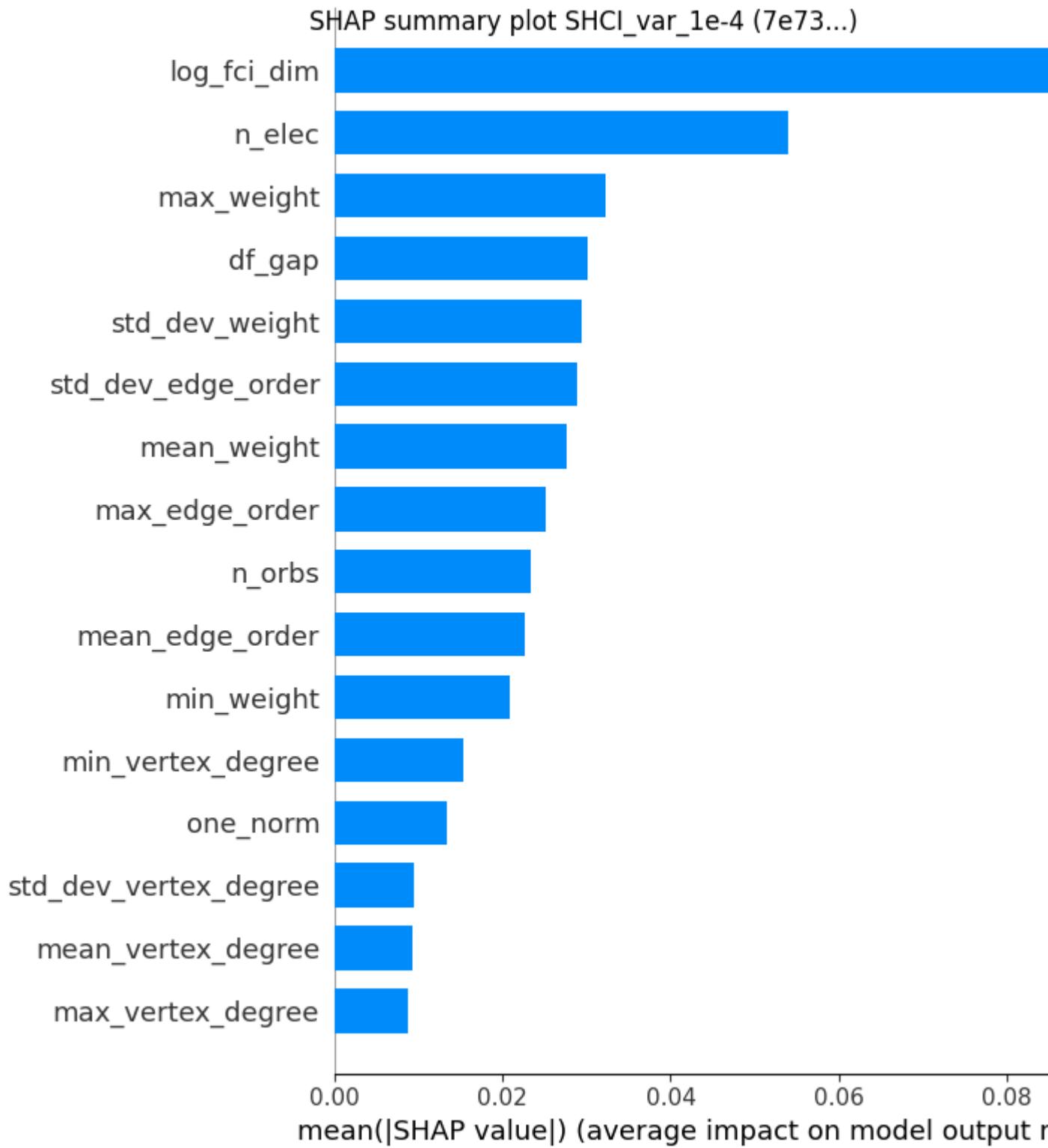
Solver SHCI_var_1e-4 (7e73...)
Embedding: PCA



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.

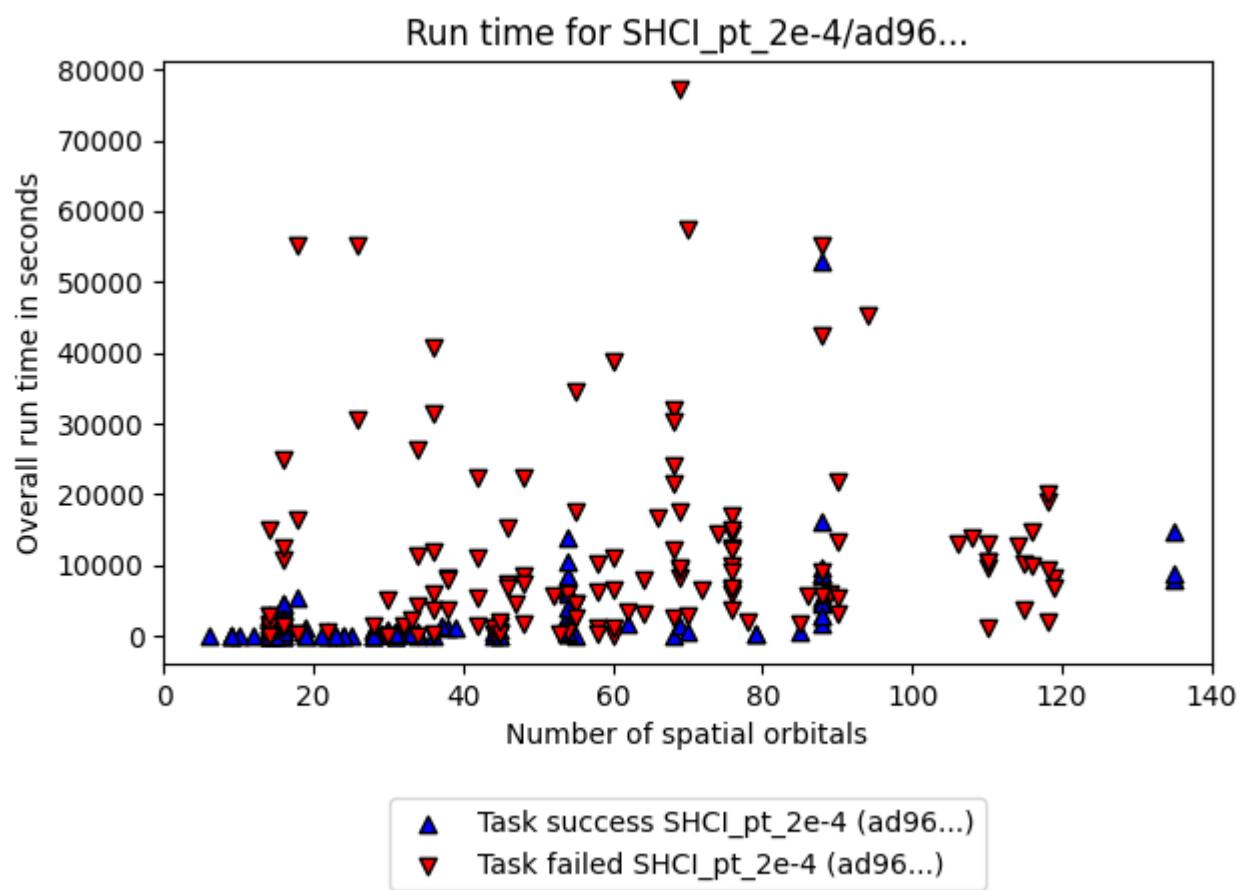


Solver SHCI_pt_2e-4, ad964781-302e-4728-a26d-39918e0a6cdb

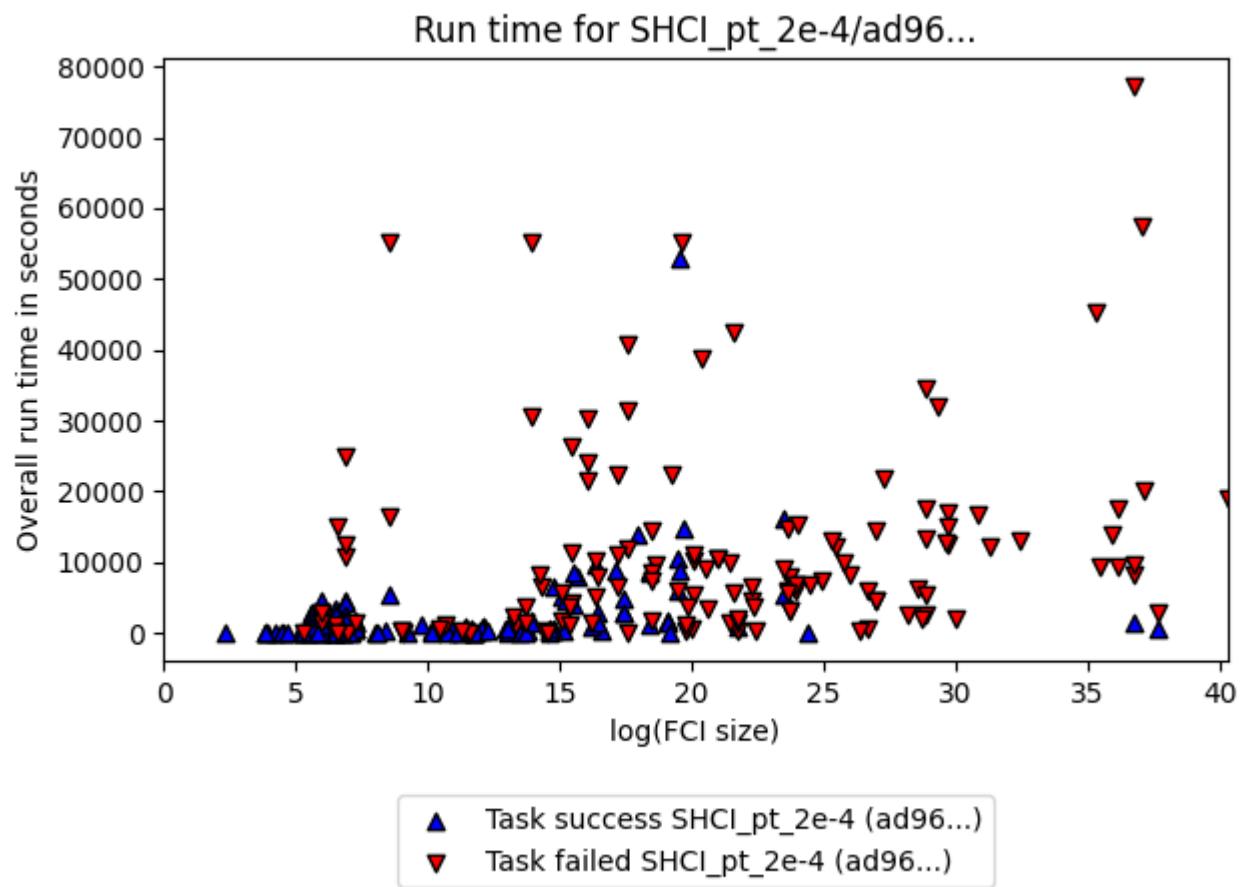
solver_uuid:ad964781-302e-4728-a26d-39918e0a6cdb

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: 9ff7cdc4-75a1-4f59-add9-1b73e9362e32
creation.timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 22
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 137
number_of_tasks_solved_within_run_time_limit: 275
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: [0.6451612903225806, 0.9614035087719298]
ml.metrics_calculator_version: 1



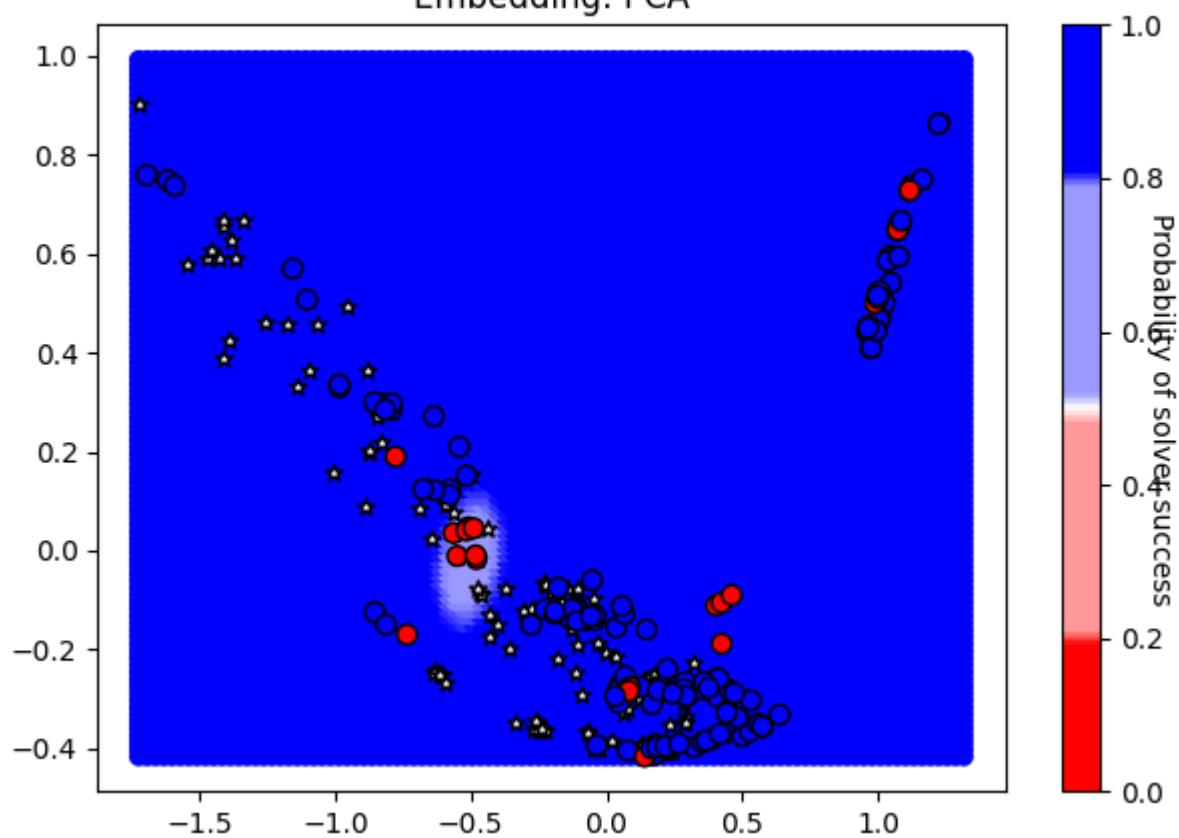
Note: plot only contains attempted tasks.



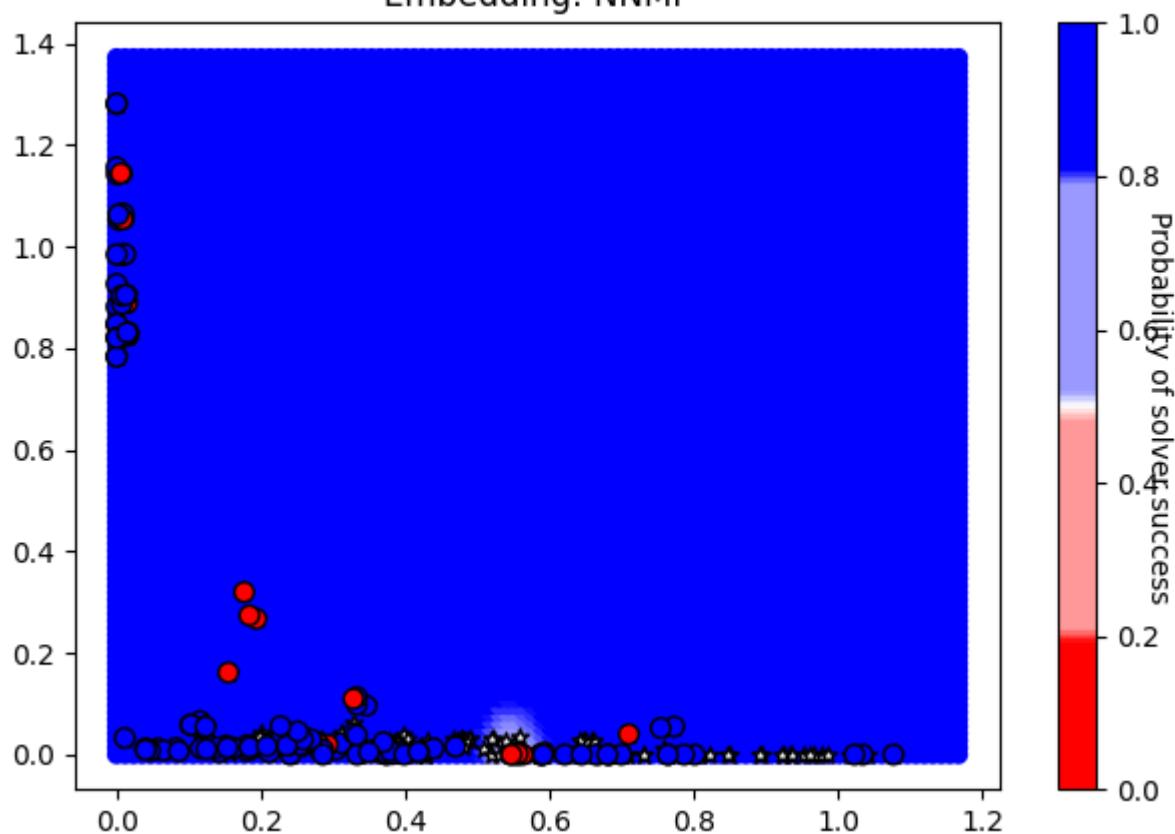
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_ad964781-302e-4728-a26d-39918e0a6cdb_utility_capture_plot.png)

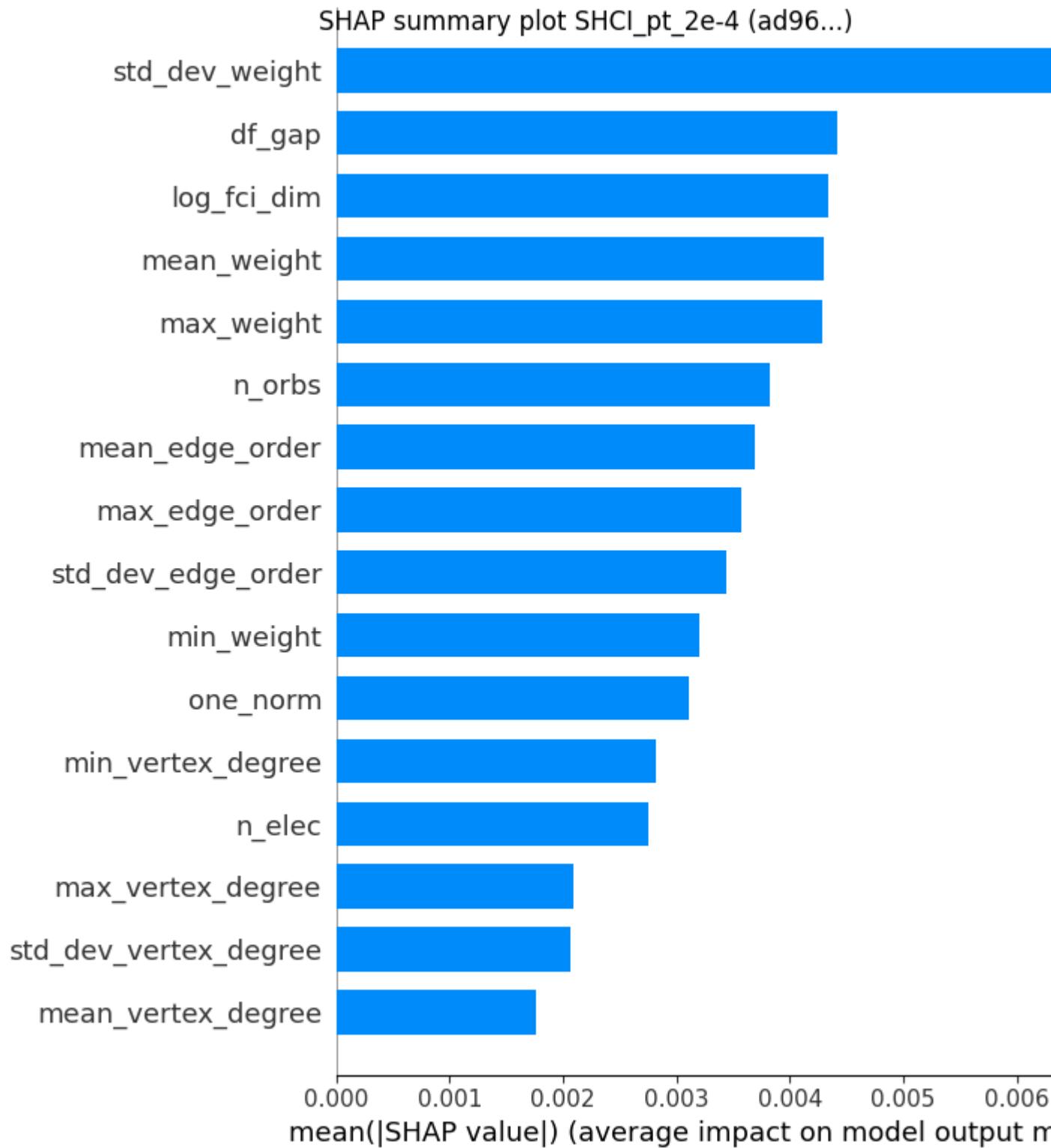
Solver SHCI_pt_2e-4 (ad96...)
Embedding: PCA



Solver SHCI_pt_2e-4 (ad96...)
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.



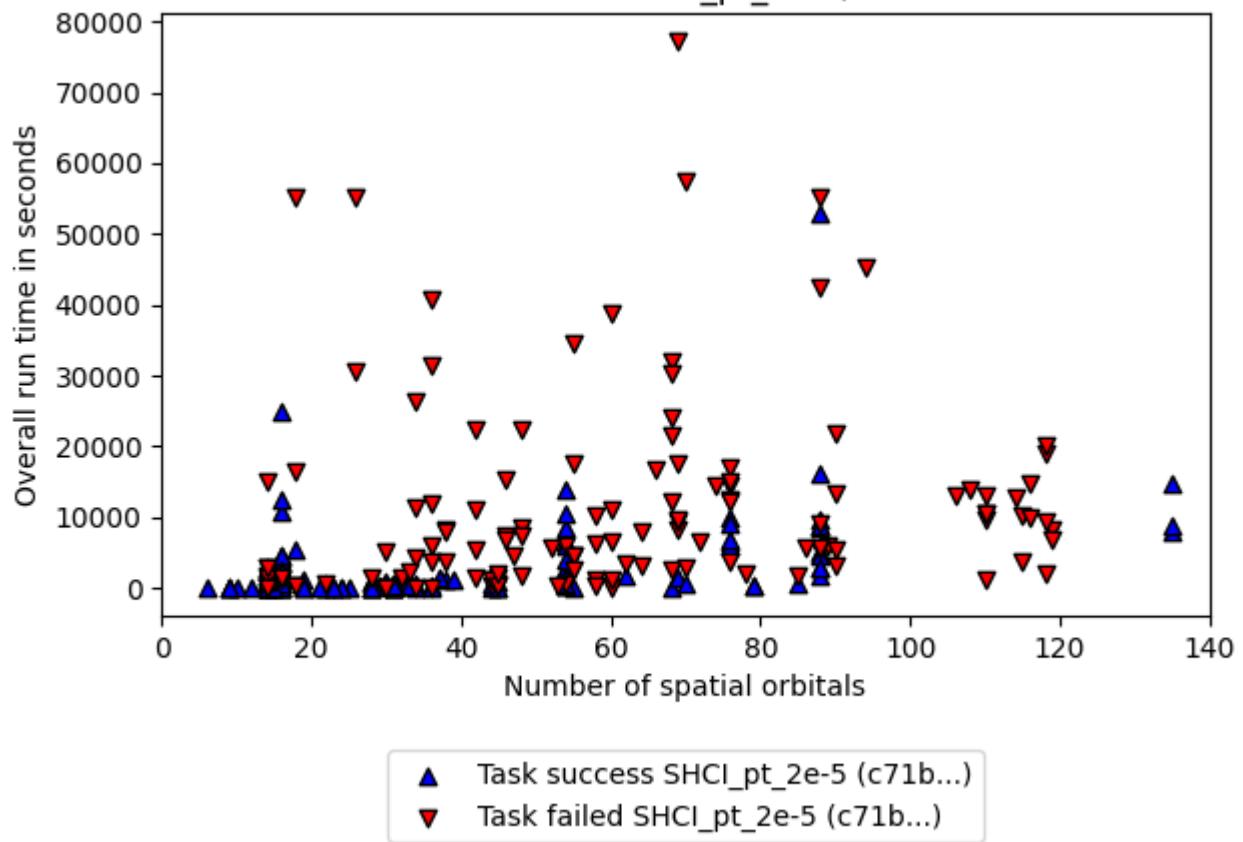
Solver SHCI_pt_2e-5, c71b90bd-3250-4c0c-b4e7-fc9878f141f6

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

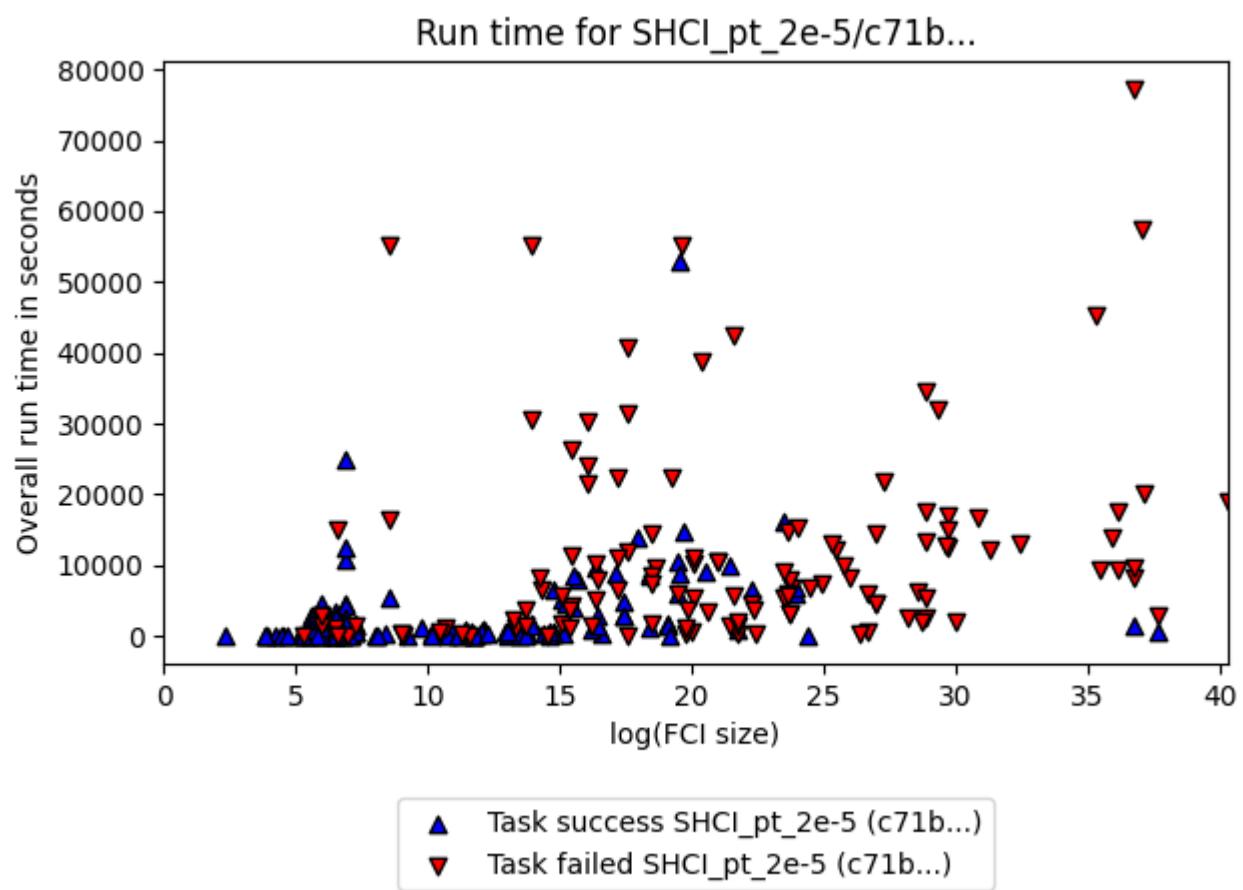
solver_short_name:SHCI_pt_2e-5

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: c8b06cd5-765a-4d01-8394-58cbe98b3be7
creation.timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 26
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 145
number_of_tasks_solved_within_run_time_limit: 275
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: [0.375, 0.9666666666666667]
ml.metrics_calculator_version: 1

Run time for SHCI_pt_2e-5/c71b...



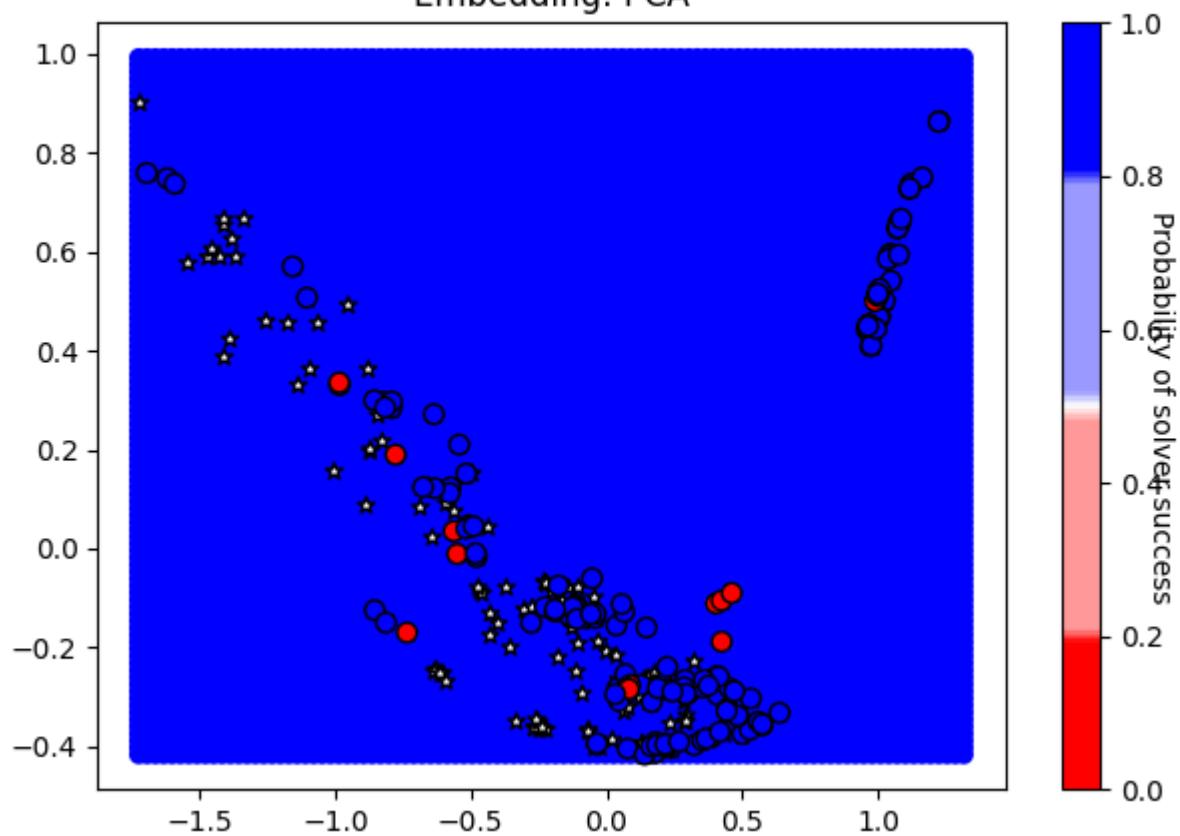
Note: plot only contains attempted tasks.



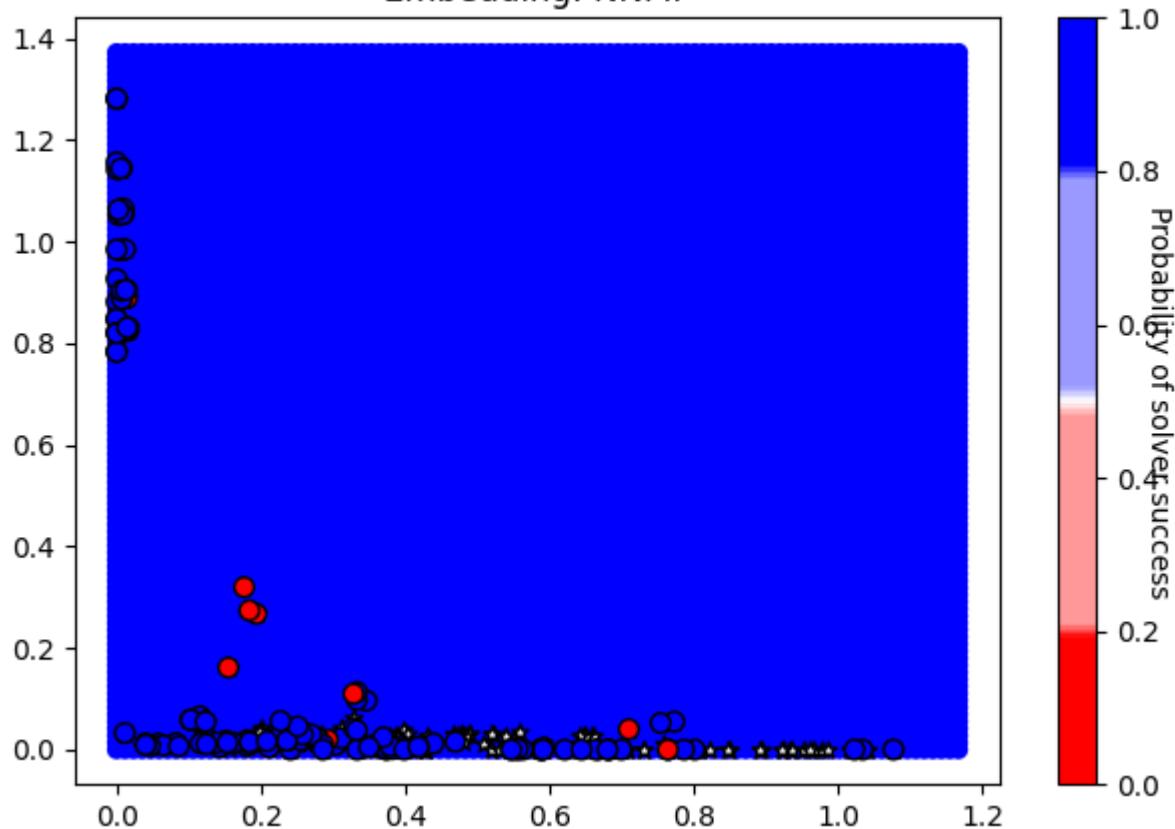
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_c71b90bd-3250-4c0c-b4e7-fc9878f141f6_utility_capture_plot.png)

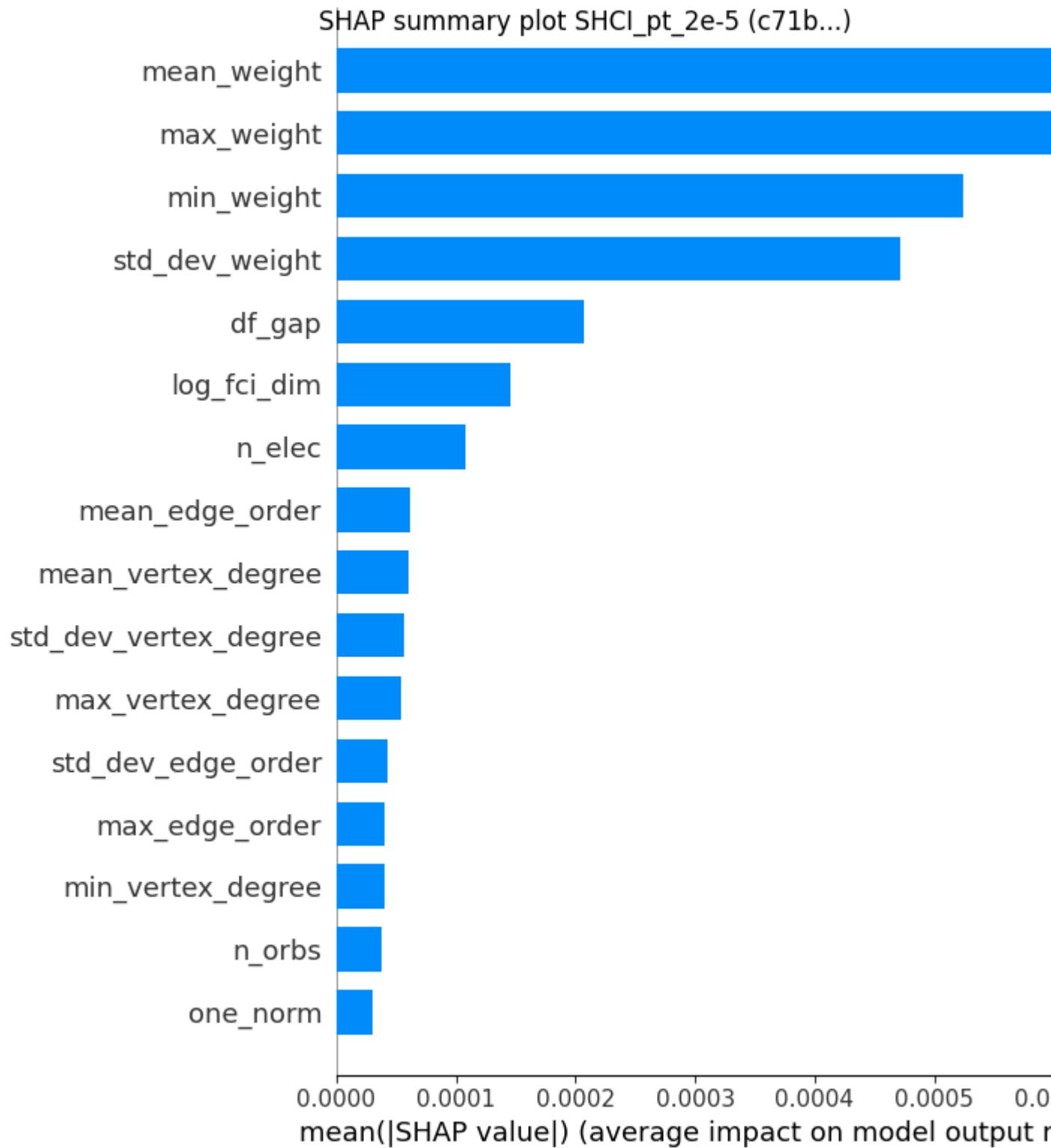
Solver SHCI_pt_2e-5 (c71b...)
Embedding: PCA



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.

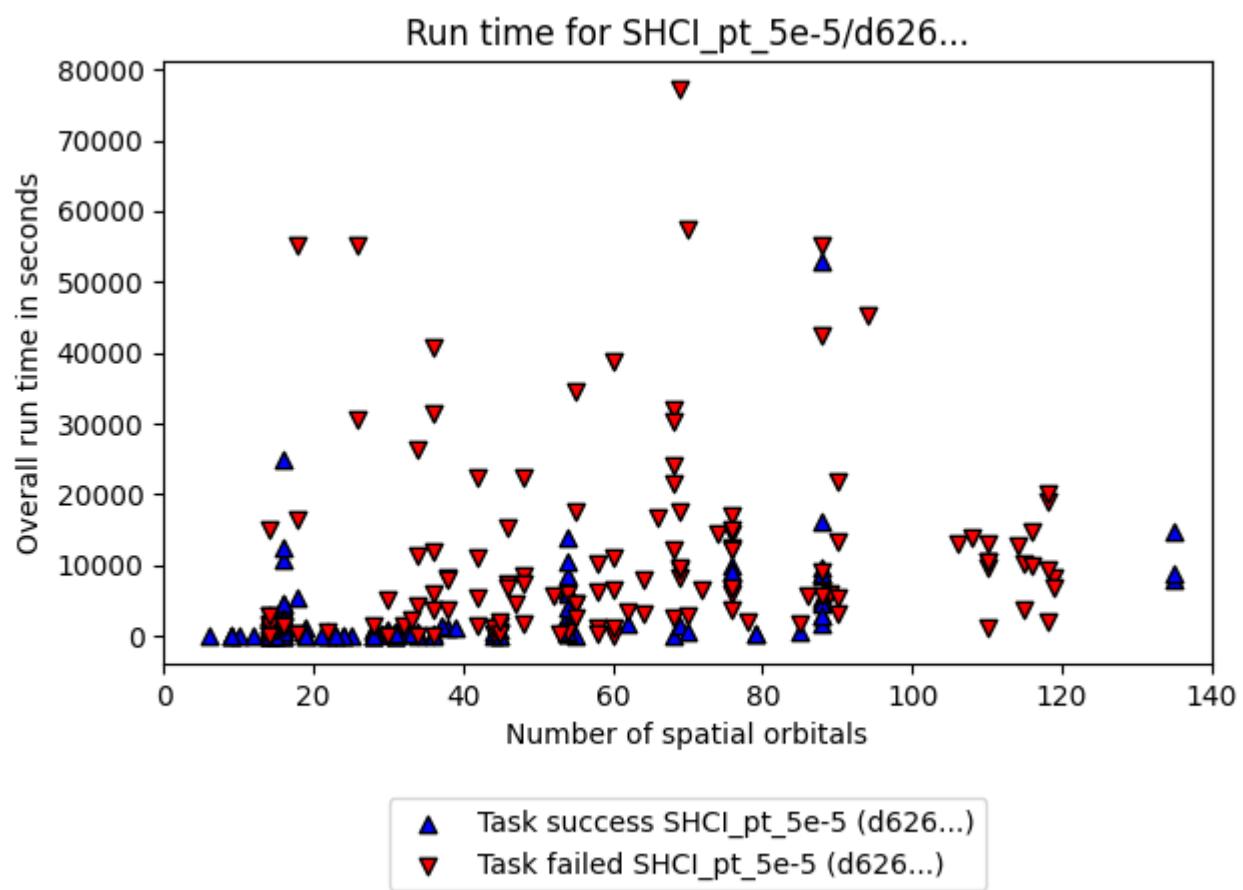


Solver SHCI_pt_5e-5, d626506c-7aae-4ad6-802a-b29af5f2bb93

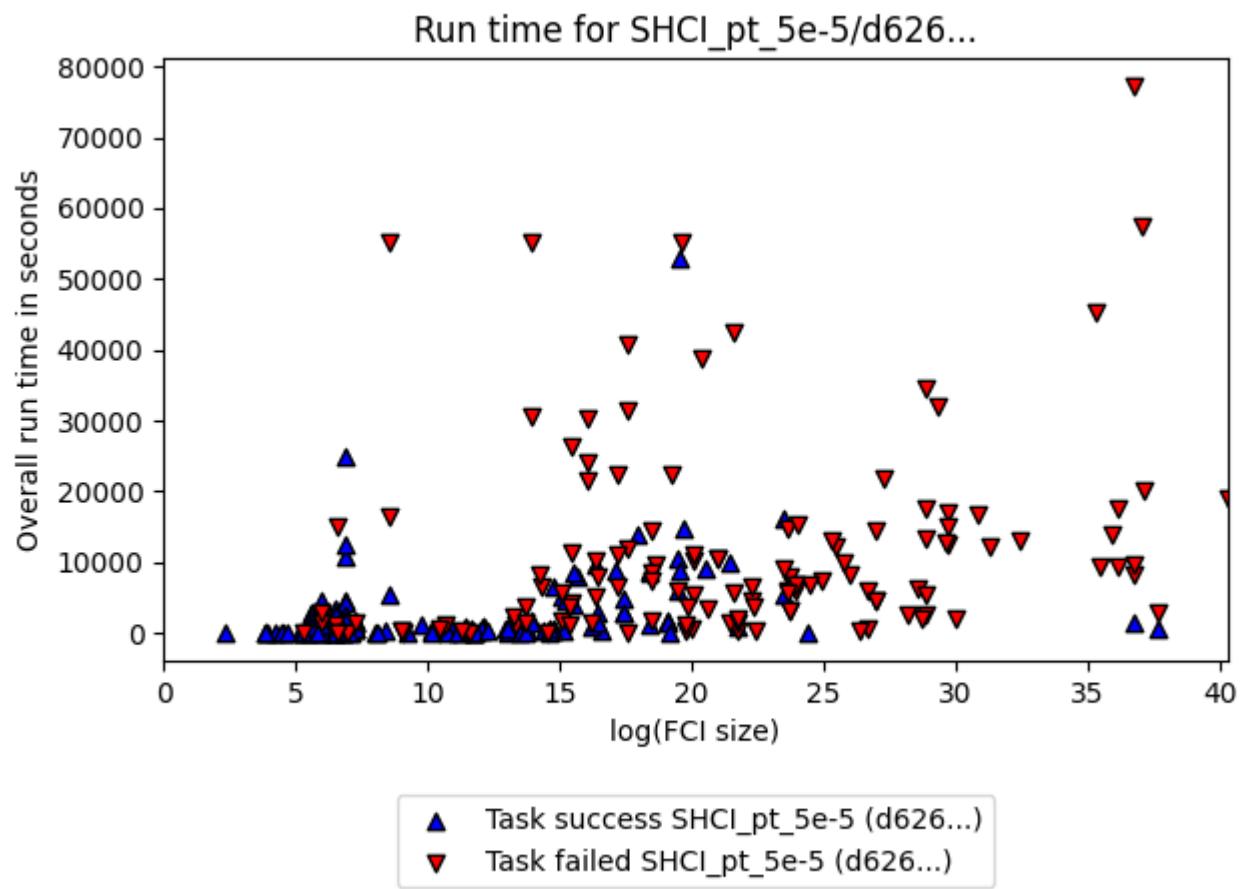
solver_uuid:d626506c-7aae-4ad6-802a-b29af5f2bb93

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: dca2c01a-ca56-45c7-a2c6-7eafcc6e63eb
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 24
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 143
number_of_tasks_solved_within_run_time_limit: 275
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: 1.0
comment: solvability ratio based on PCA embedding.
f1_score: [0.9375, 0.9929577464788732]
ml_metrics_calculator_version: 1



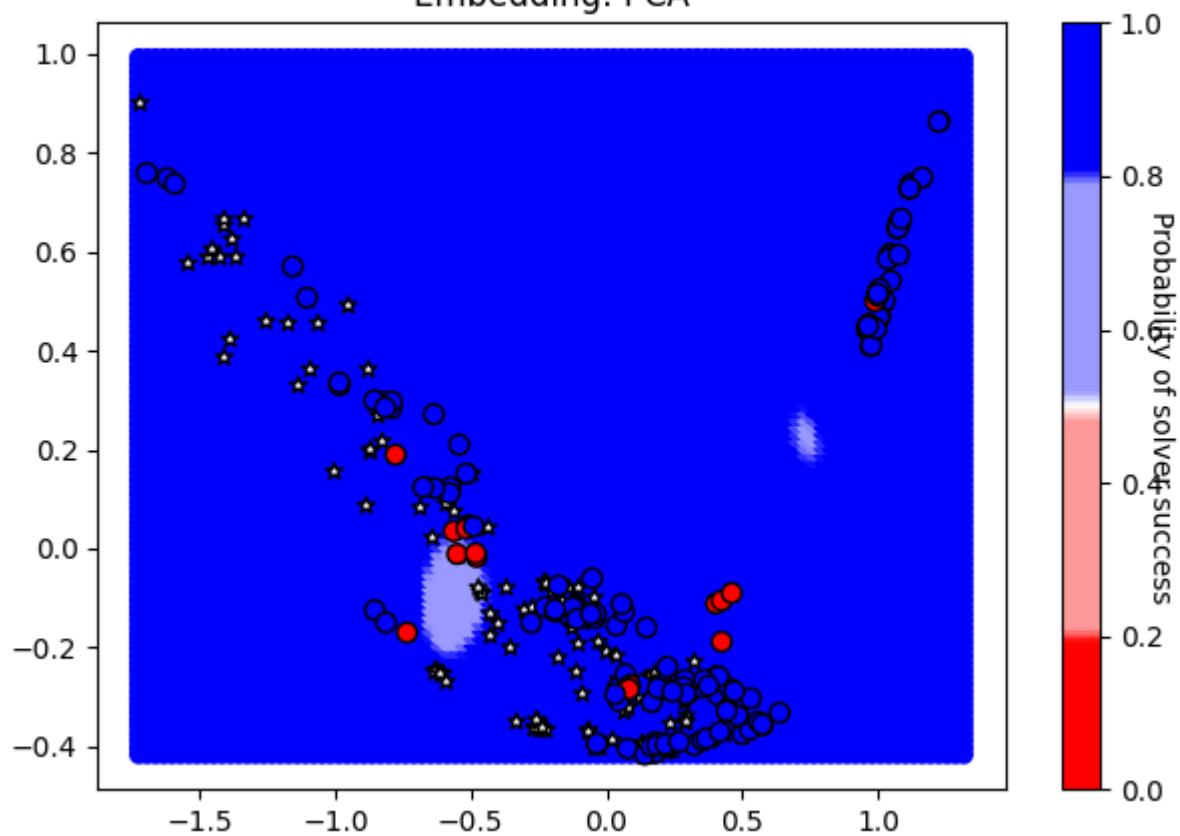
Note: plot only contains attempted tasks.



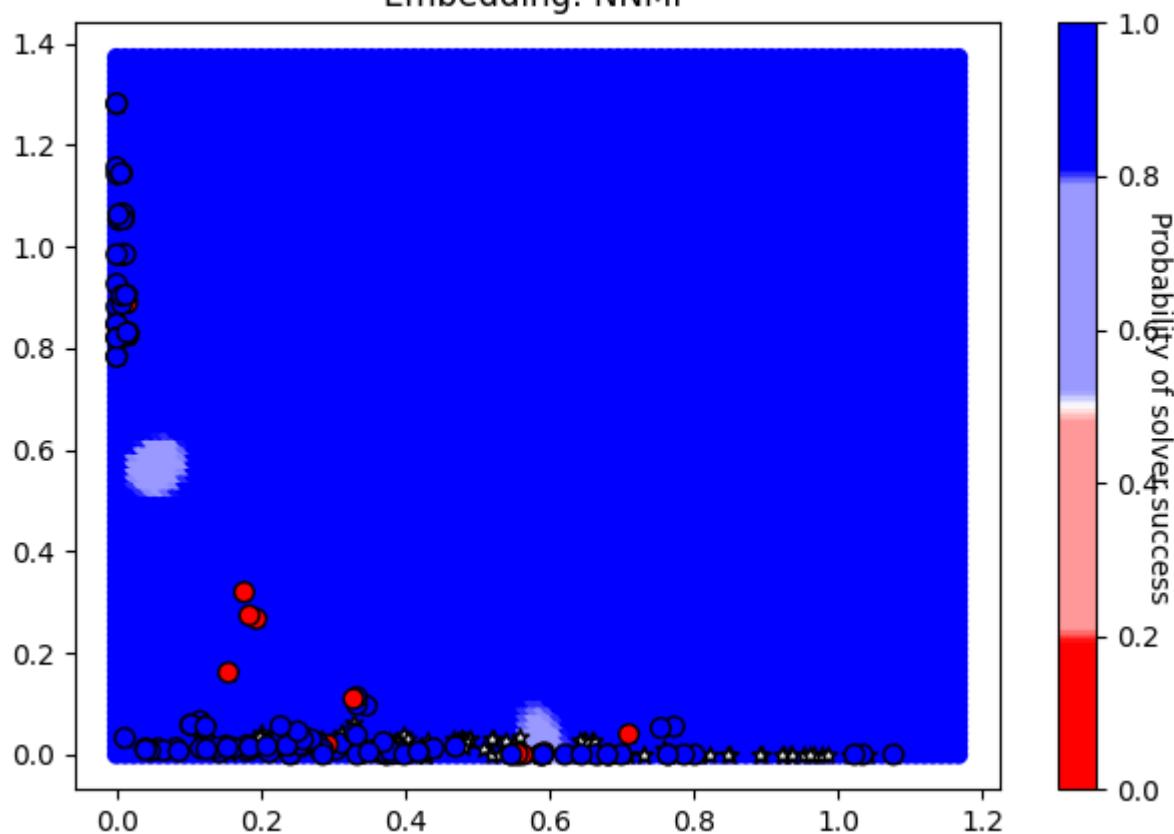
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/
(solver_d626506c-7aae-4ad6-802a-b29af5f2bb93_utility_capture_plot.png)

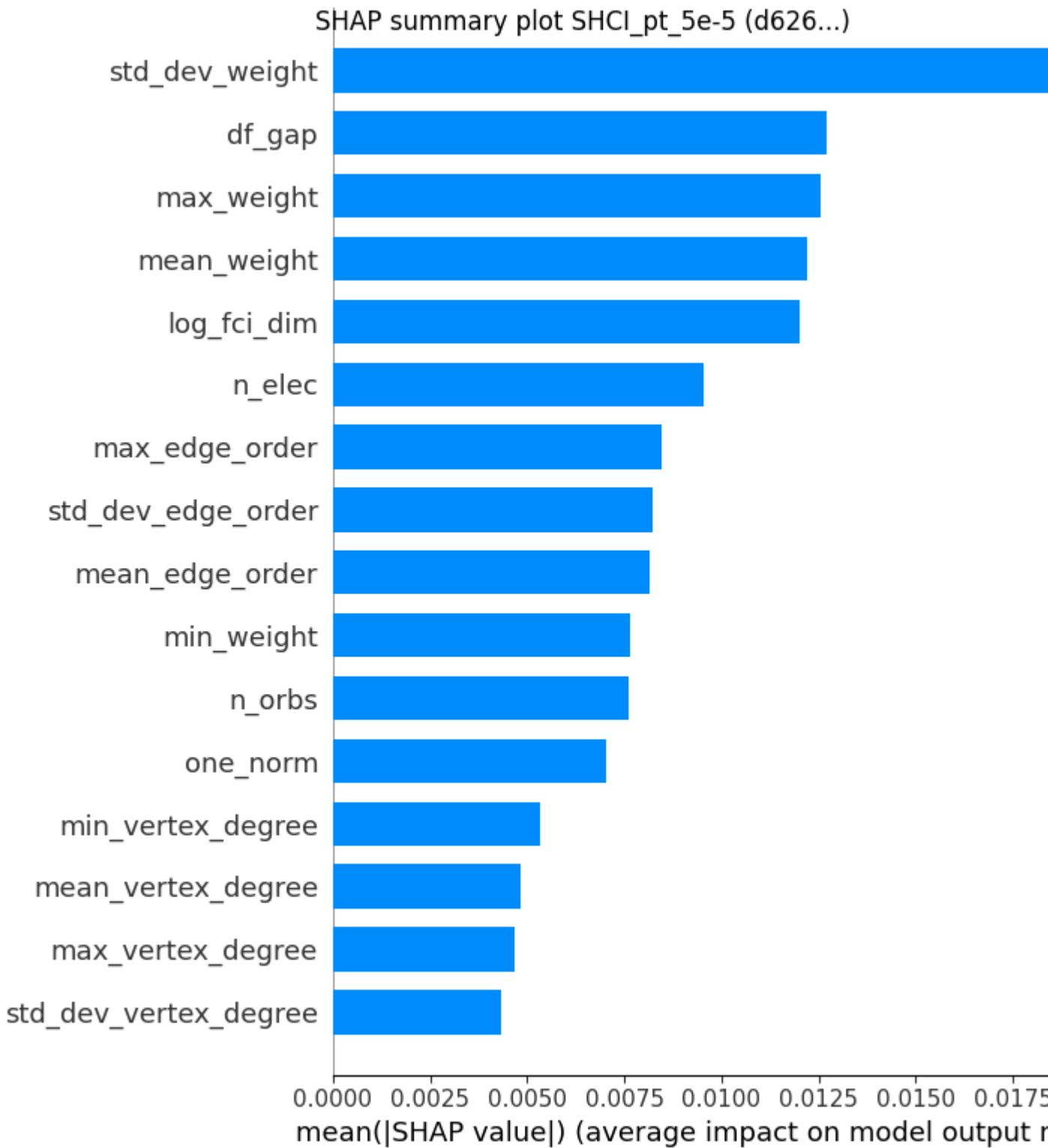
Solver SHCI_pt_5e-5 (d626...)
Embedding: PCA



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.

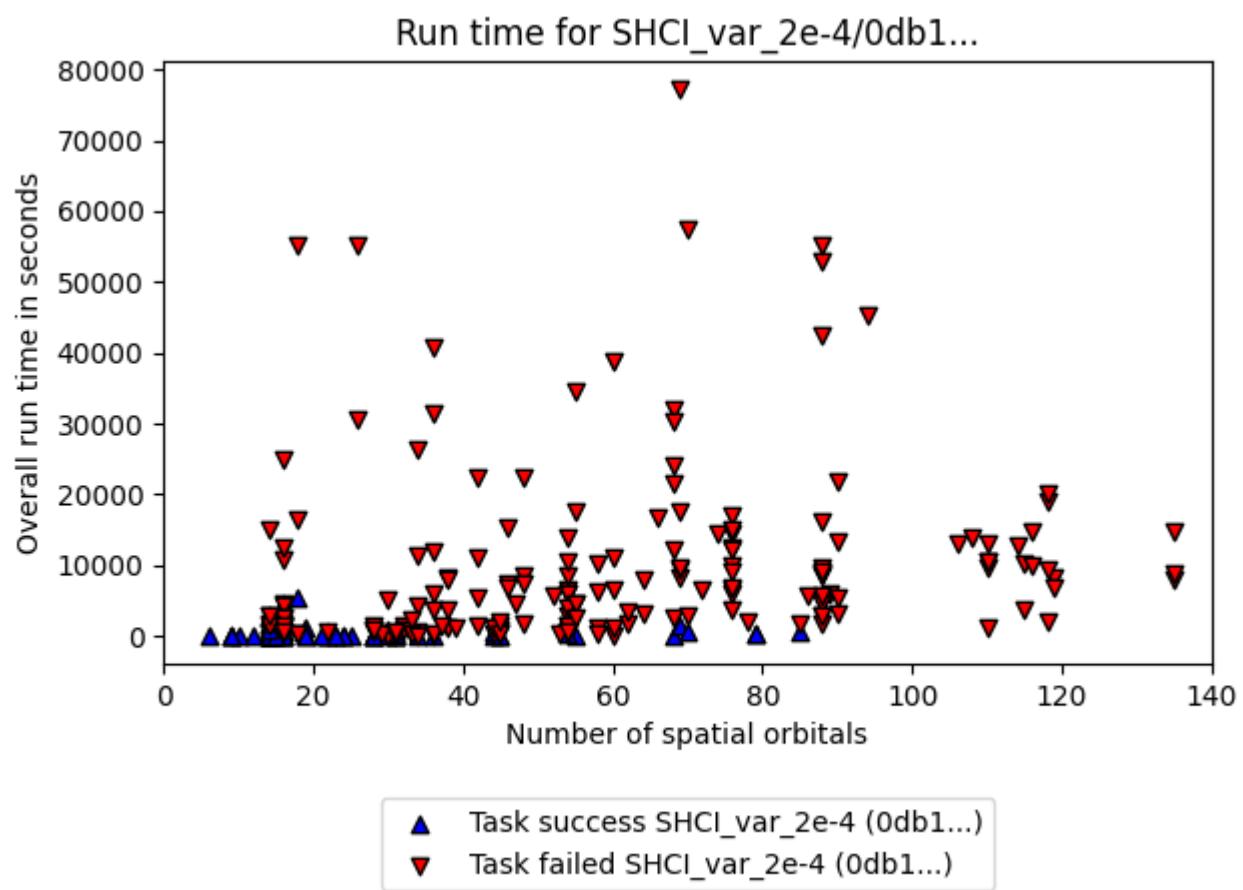


Solver SHCI_var_2e-4, 0db183e3-a86d-491b-9125-599556e37c7a

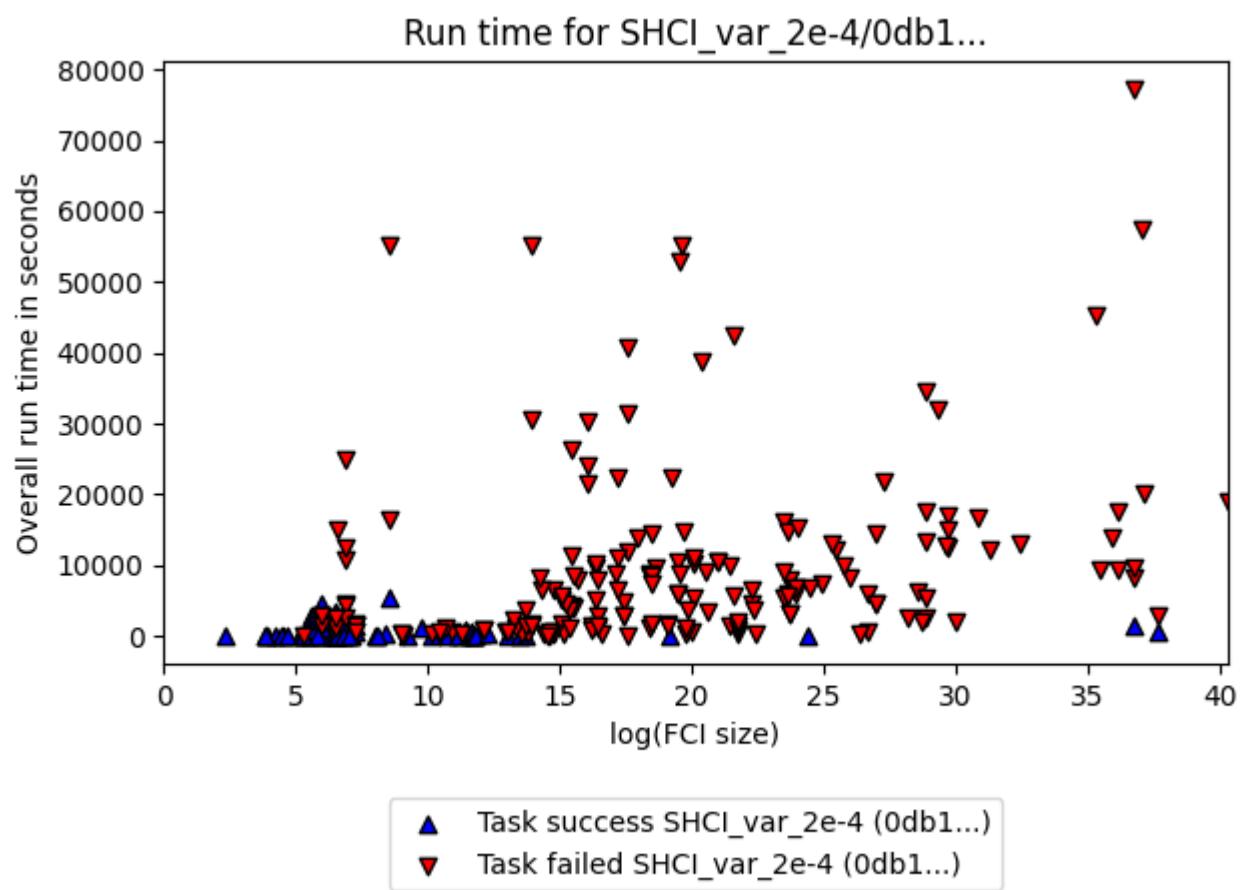
solver_uuid:0db183e3-a86d-491b-9125-599556e37c7a

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: e740bd1c-eab8-4fef-9062-b7ccd11a0334
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 13
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 84
number_of_tasks_solved_within_run_time_limit: 275
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: 0.3499
comment: solvability ratio based on PCA embedding.
f1_score: [0.9536423841059603, 0.95757575757575]
ml_metrics_calculator_version: 1



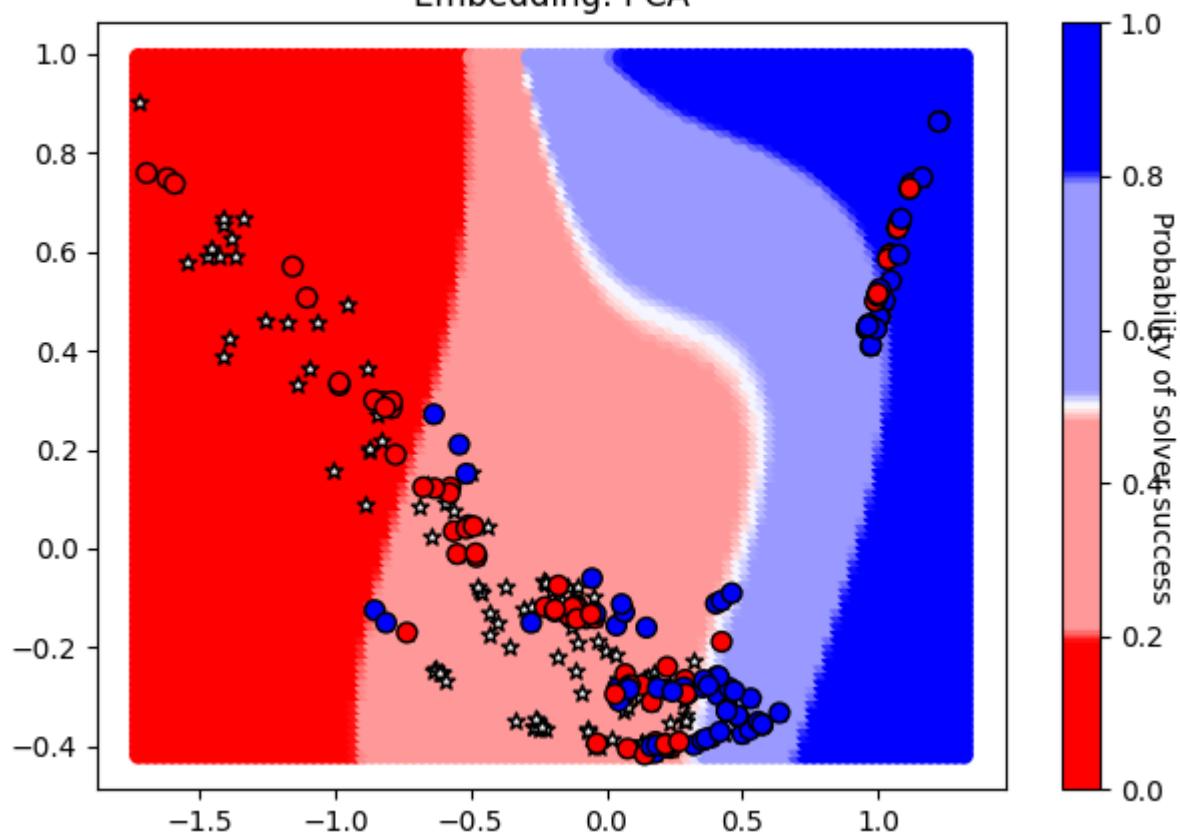
Note: plot only contains attempted tasks.



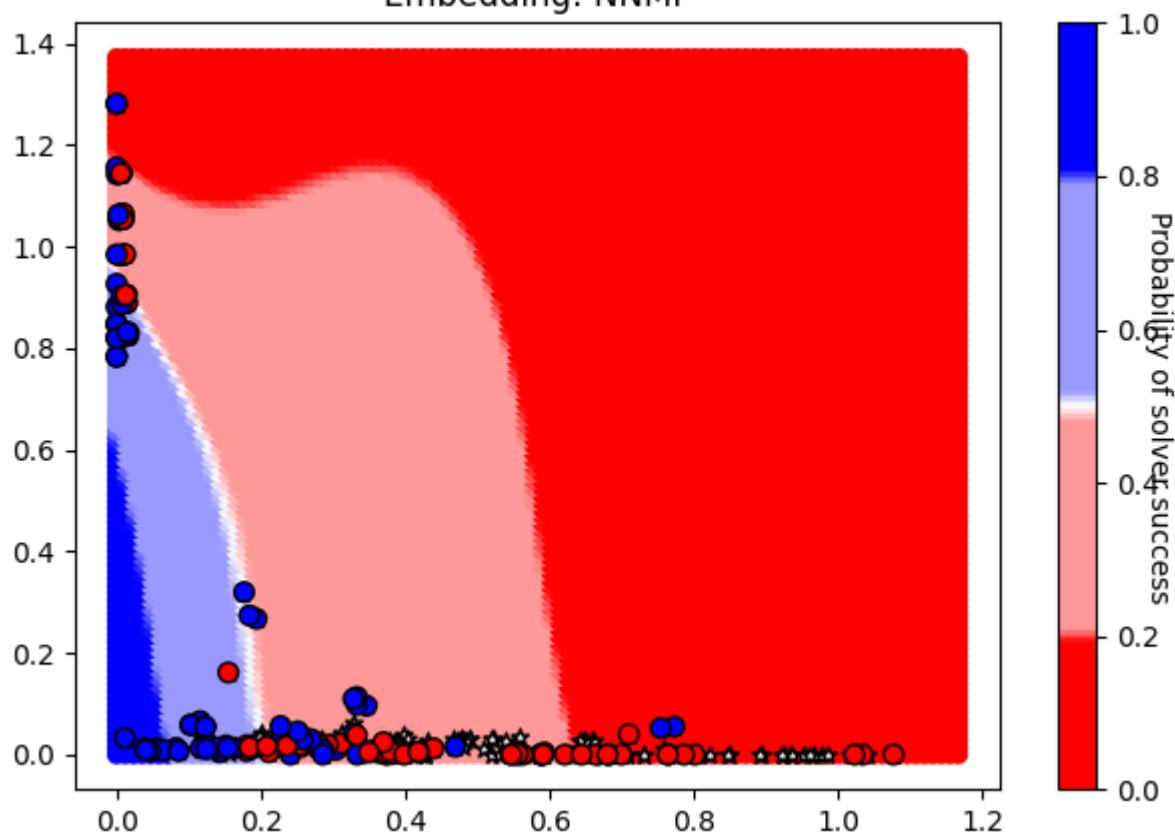
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_0db183e3-a86d-491b-9125-599556e37c7a_utility_capture_plot.png)

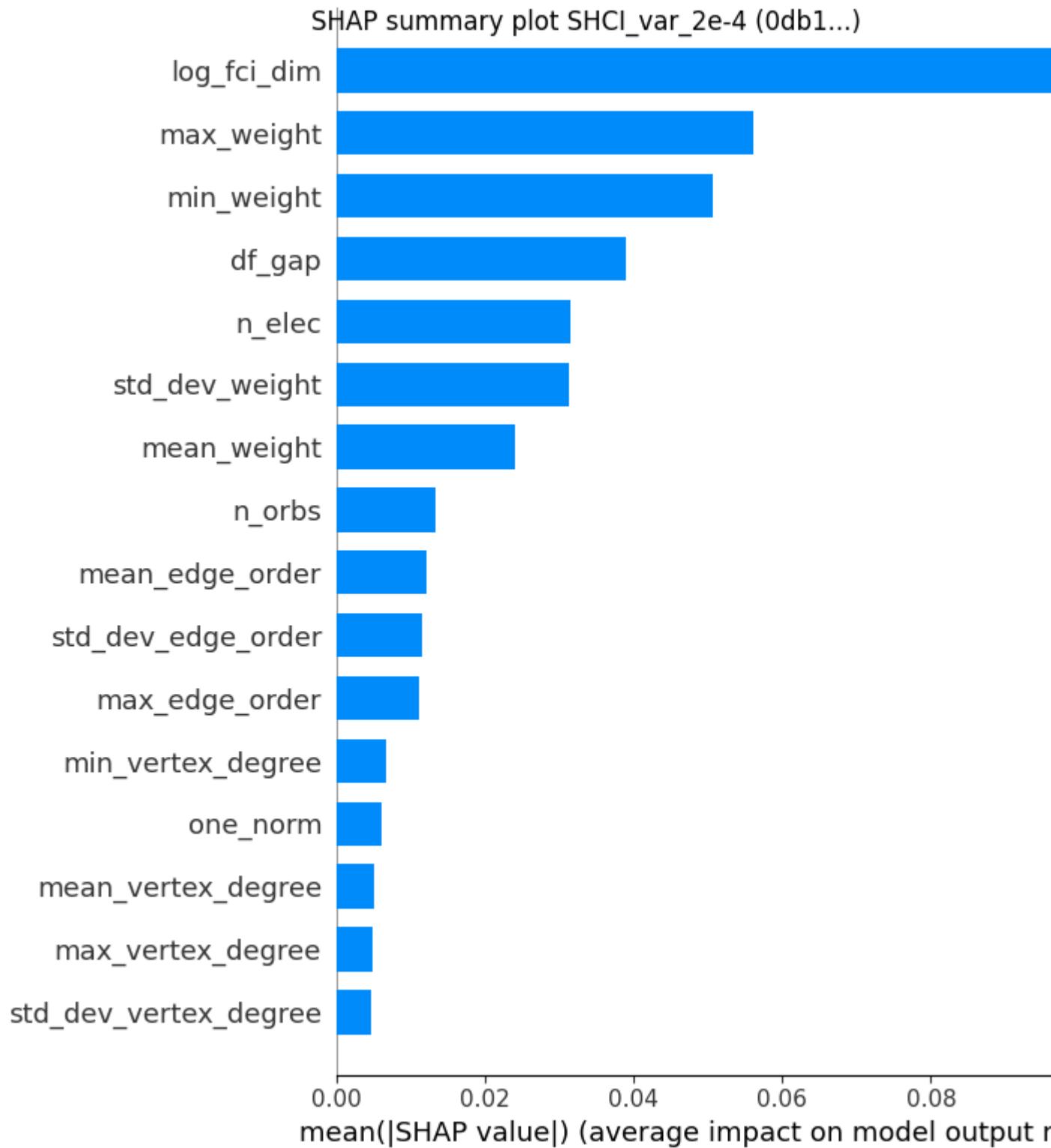
Solver SHCI_var_2e-4 (0db1...)
Embedding: PCA



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.

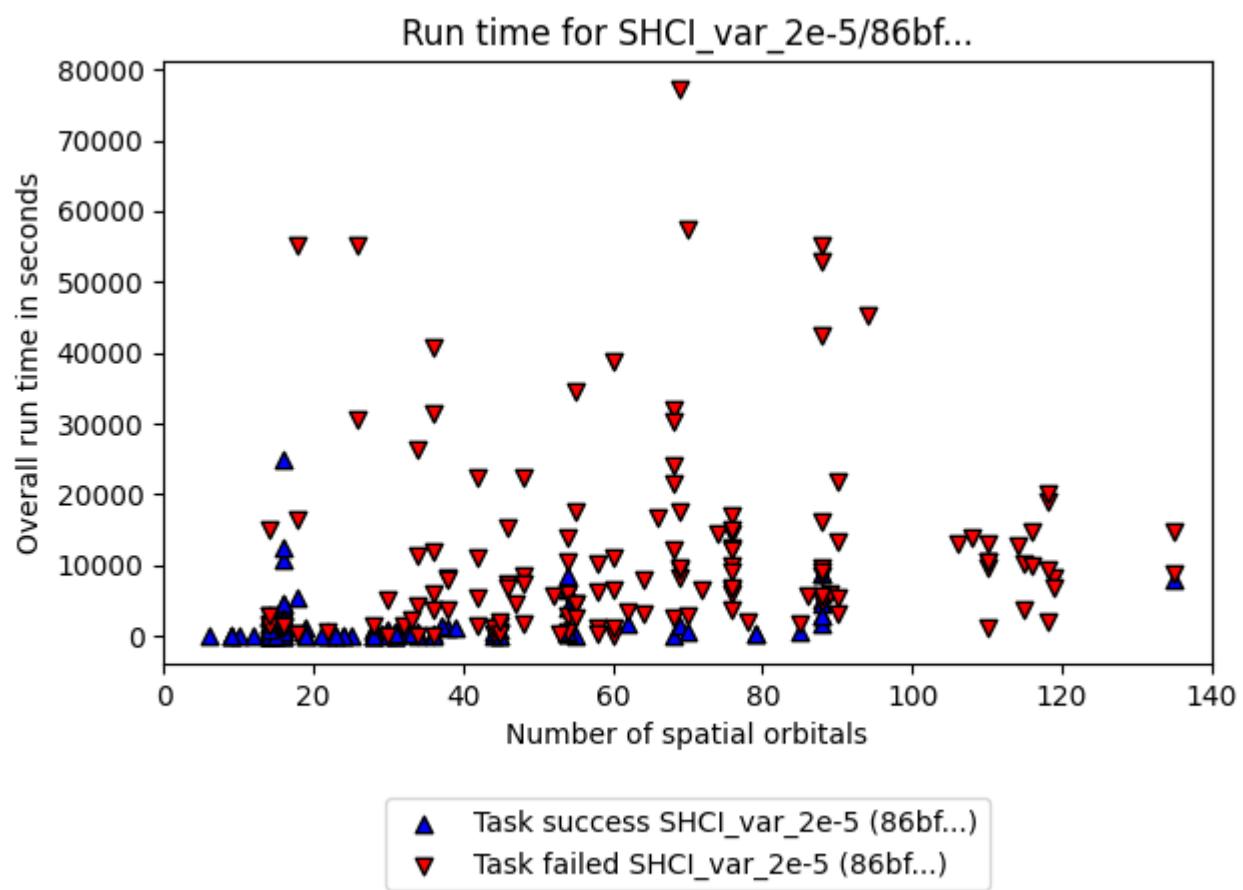


Solver SHCI_var_2e-5, 86bfe50c-9342-4d54-bb68-abc8abd95688

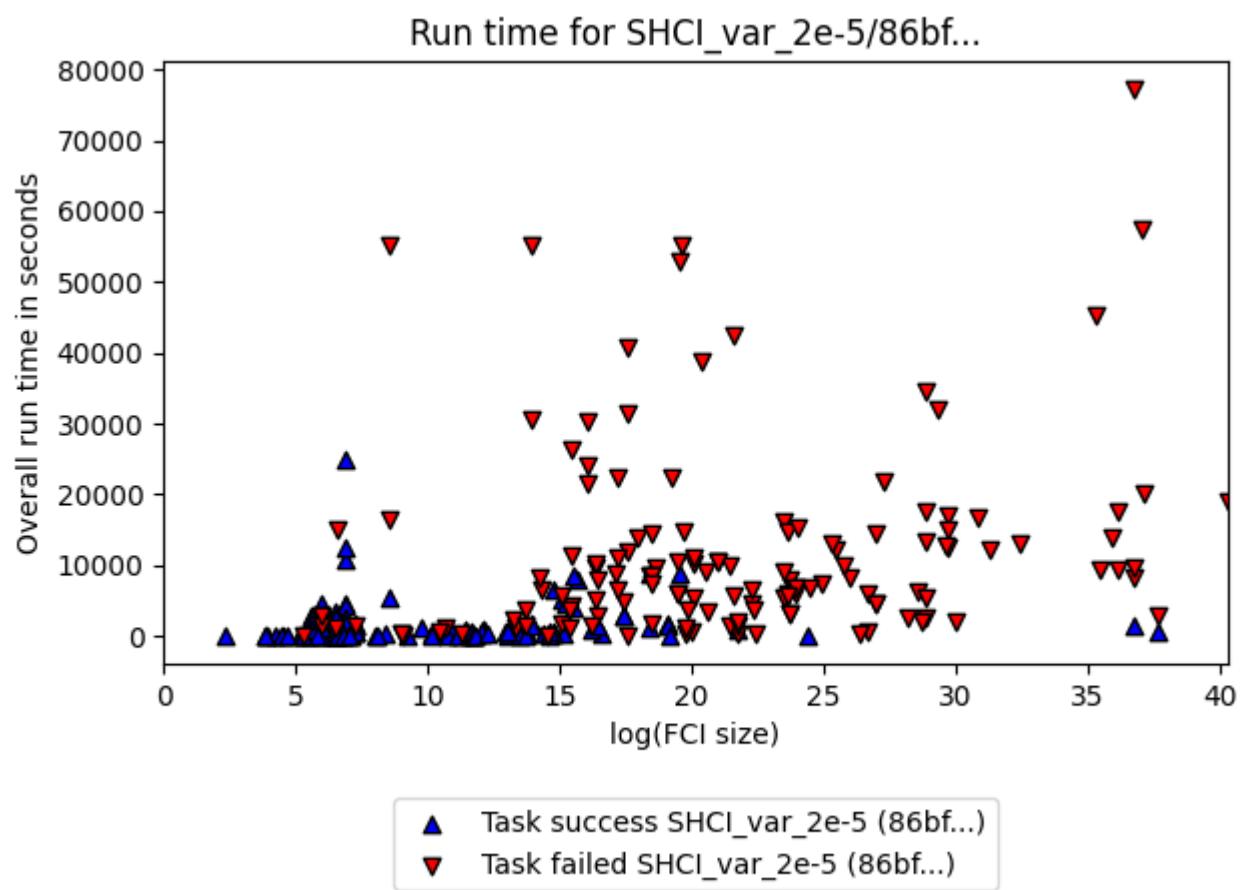
solver_uuid:86bfe50c-9342-4d54-bb68-abc8abd95688

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: 23b952fc-495e-4ea8-be36-60eca9777f9c
creation.timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 18
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 133
number_of_tasks_solved_within_run_time_limit: 275
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: 0.5812
comment: solvability ratio based on PCA embedding.
f1_score: [0.8627450980392157, 0.9735849056603774]
ml.metrics_calculator_version: 1



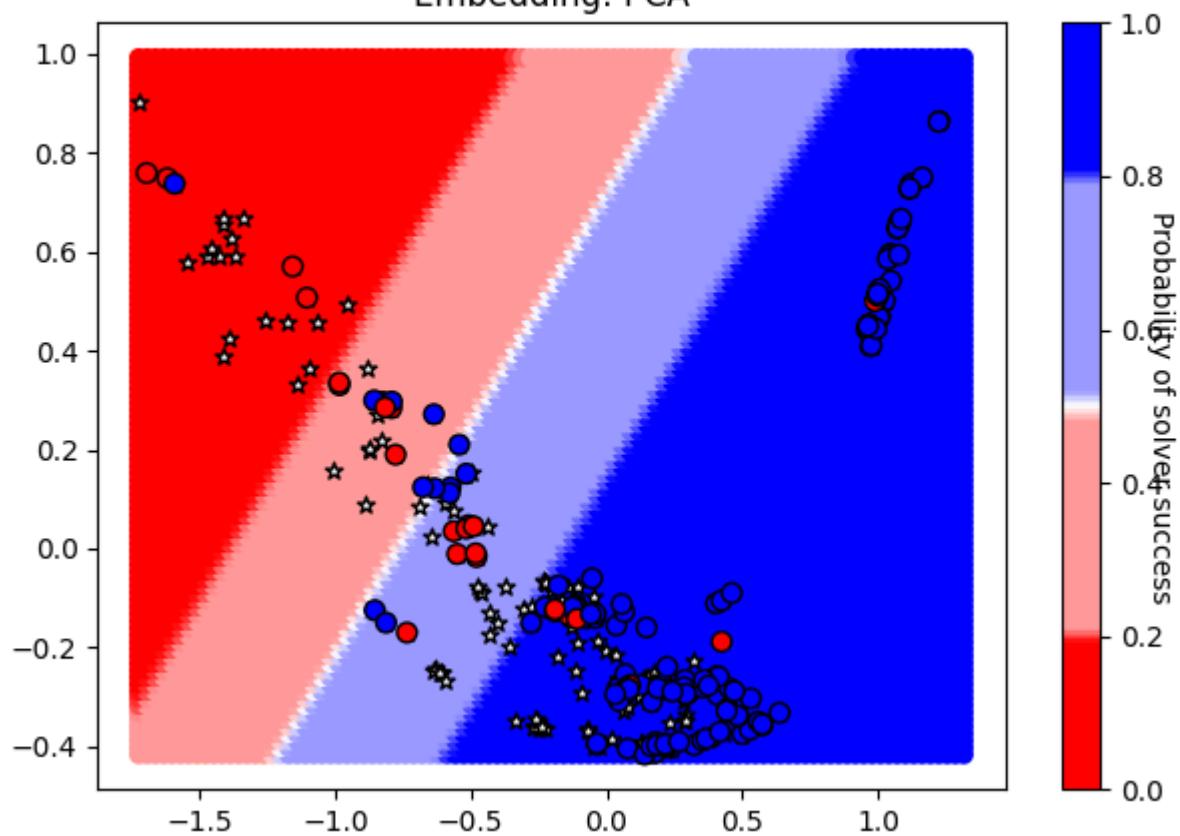
Note: plot only contains attempted tasks.



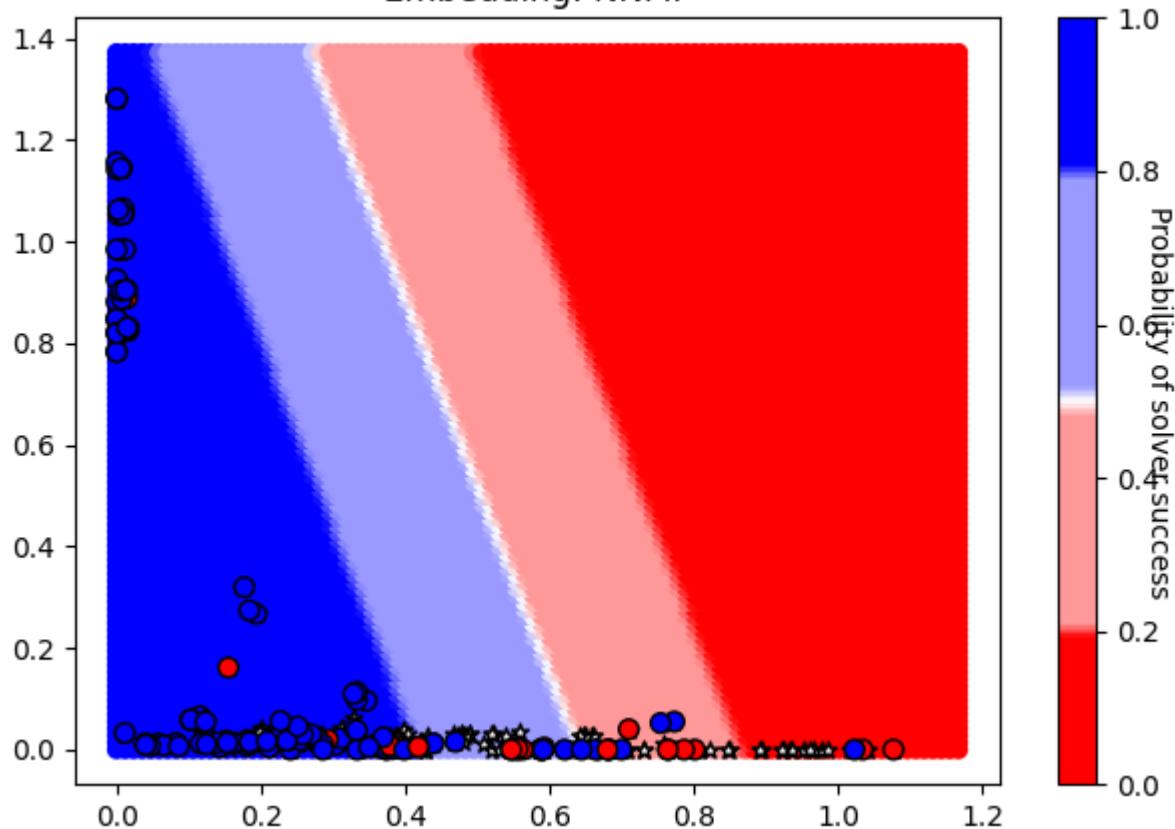
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_86bfe50c-9342-4d54-bb68-abc8abd95688_utility_capture_plot.png)

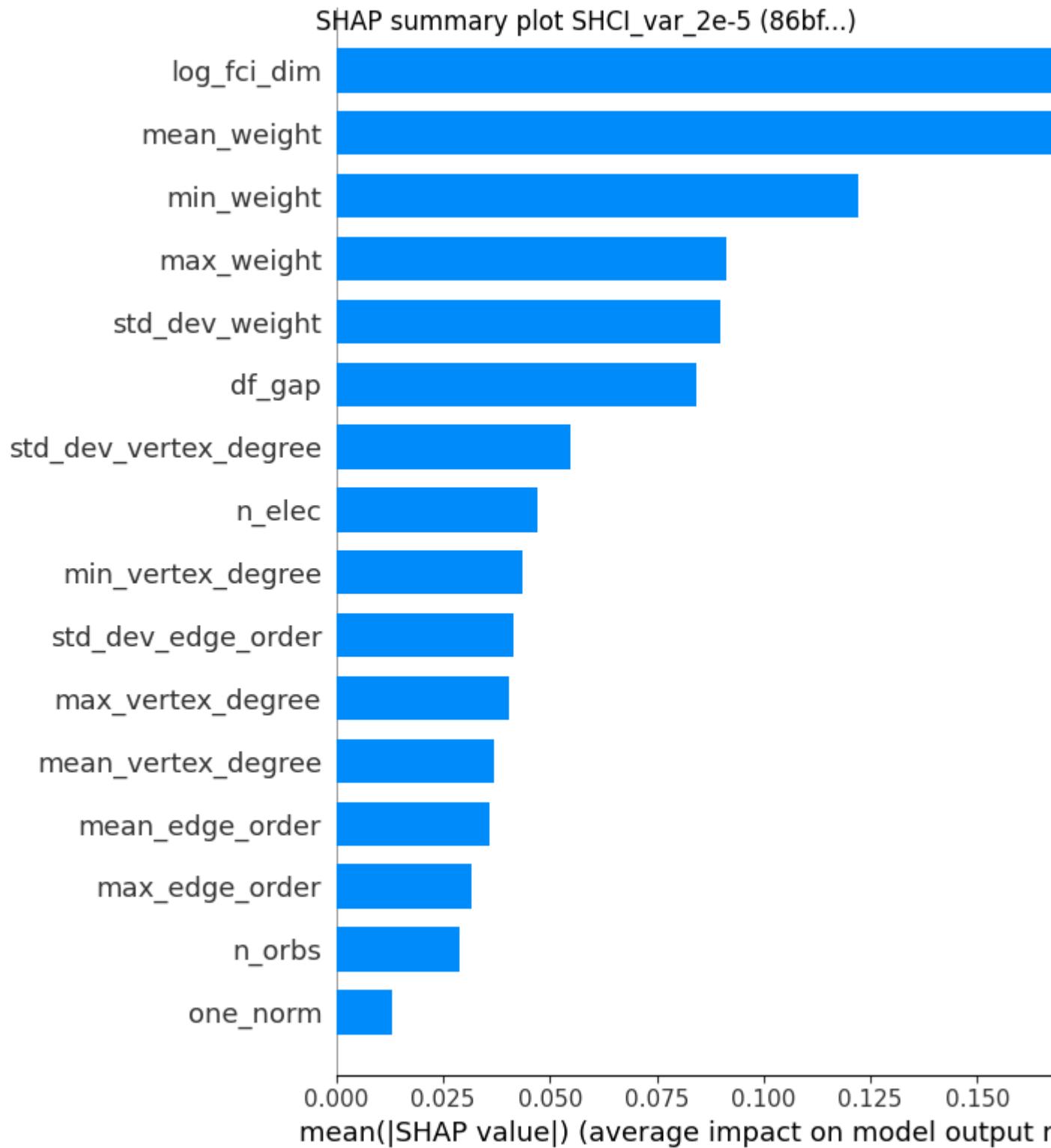
Solver SHCI_var_2e-5 (86bf...)
Embedding: PCA



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.

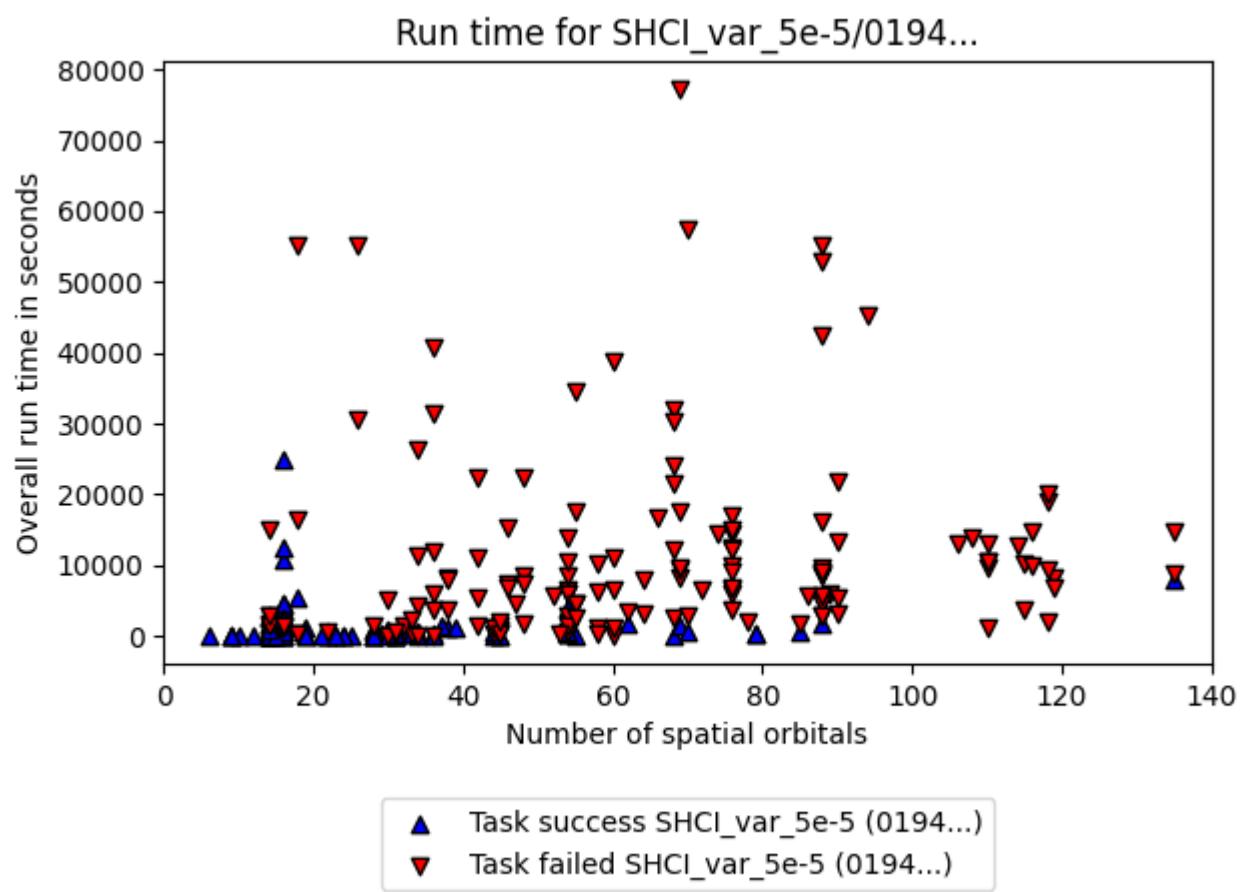


Solver SHCI_var_5e-5, 01949b95-c427-4693-9134-01f47f688c09

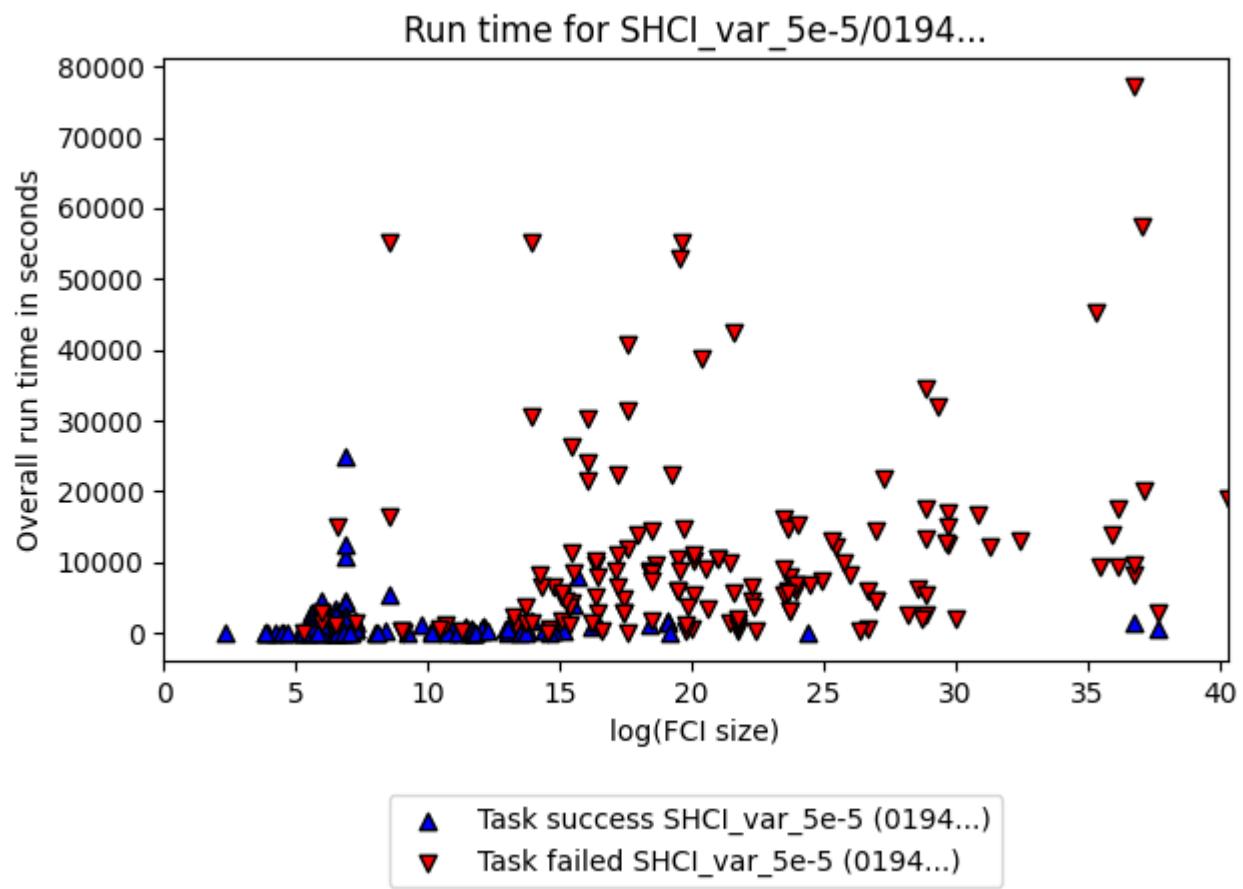
solver_uuid:01949b95-c427-4693-9134-01f47f688c09

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: 8ff27cfa-5bd7-4482-b712-d4f6c7a01439
creation.timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 83
number_of_problem_instances_solved: 14
number_of_tasks: 276
number_of_tasks_attempted: 275
number_of_tasks_solved: 120
number_of_tasks_solved_within_run_time_limit: 275
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: 0.6393
comment: solvability ratio based on PCA embedding.
f1_score: [0.8395061728395061, 0.9446808510638298]
ml.metrics_calculator_version: 1



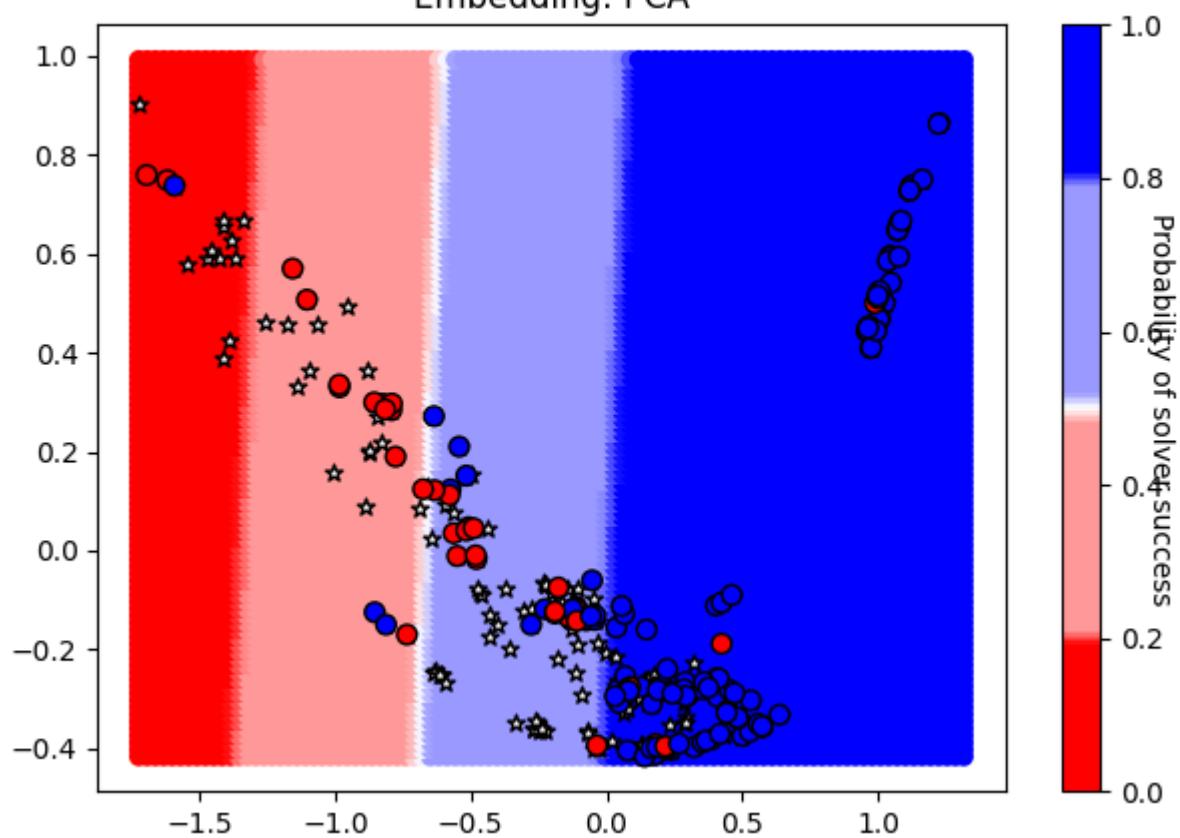
Note: plot only contains attempted tasks.



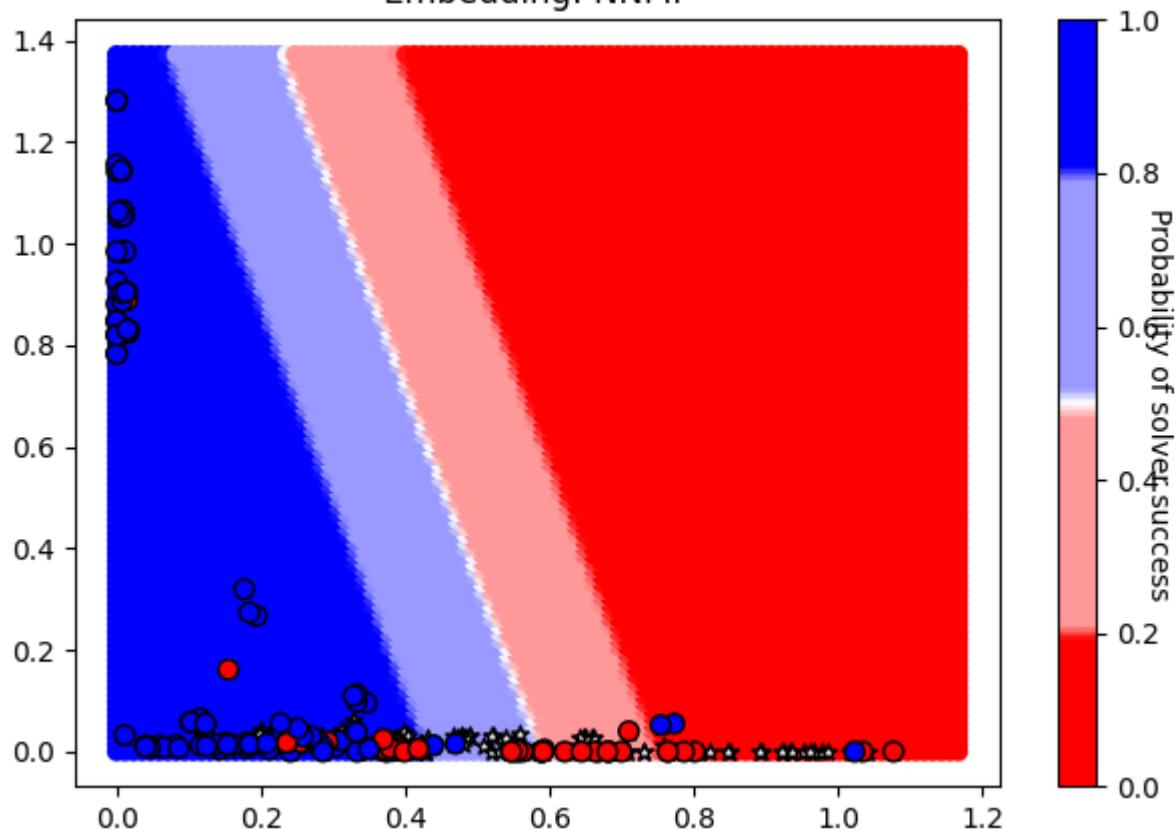
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_01949b95-c427-4693-9134-01f47f688c09_utility_capture_plot.png)

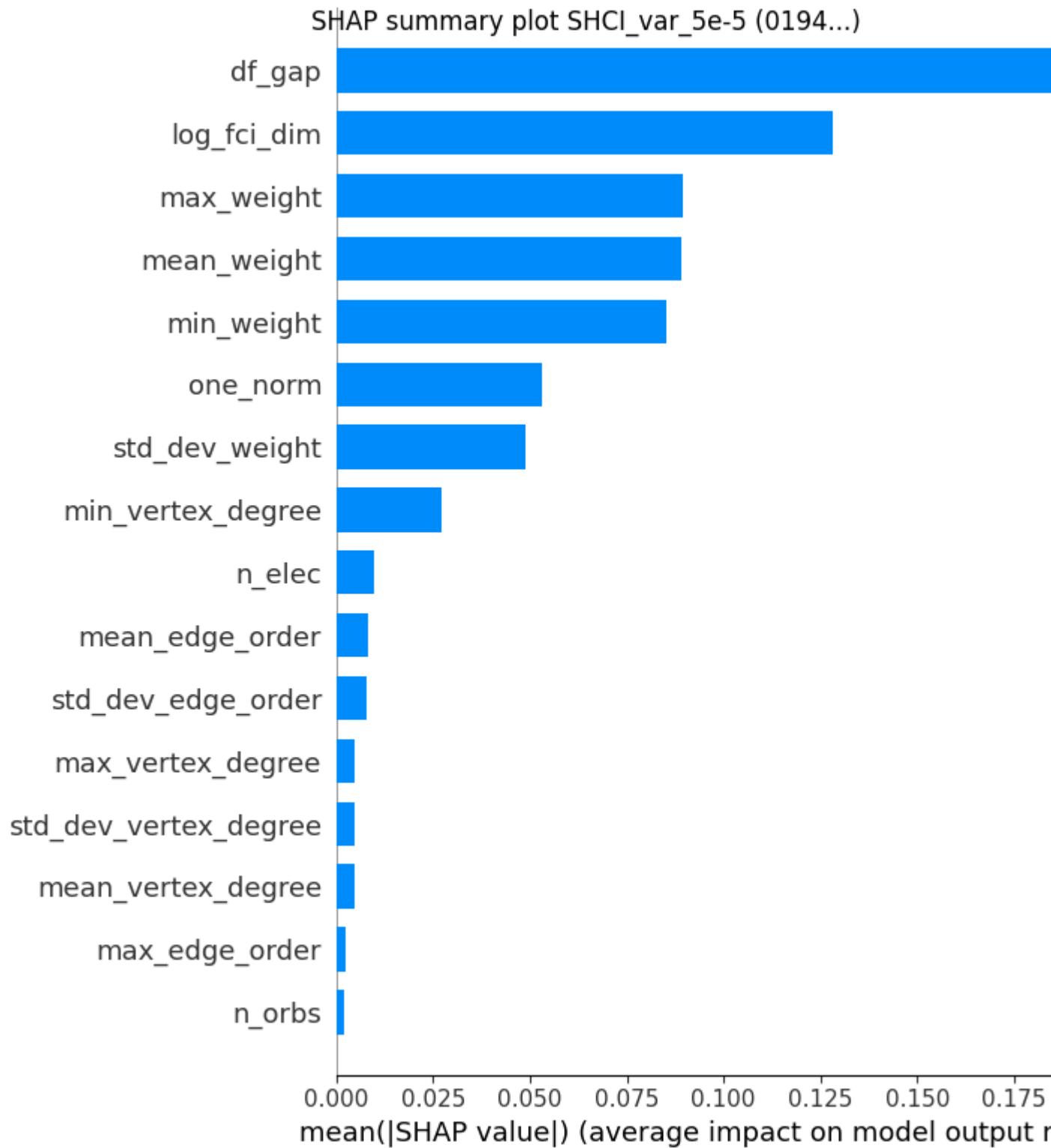
Solver SHCI_var_5e-5 (0194...)
Embedding: PCA



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



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



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

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

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

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

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

logical_resource_estimate_solution_uuid:fc17e113-d2e0-49ab-955a-6fc08c6eb2f9

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

performance_metrics_uuid: a874f899-b02a-4a83-8590-9aae0fbe0179

creation_timestamp: 2025-01-30T17:45:00.466432+00:00

number_of_problem_instances: 84

number_of_problem_instances_attempted: 22

number_of_problem_instances_solved: 0

number_of_tasks: 276

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

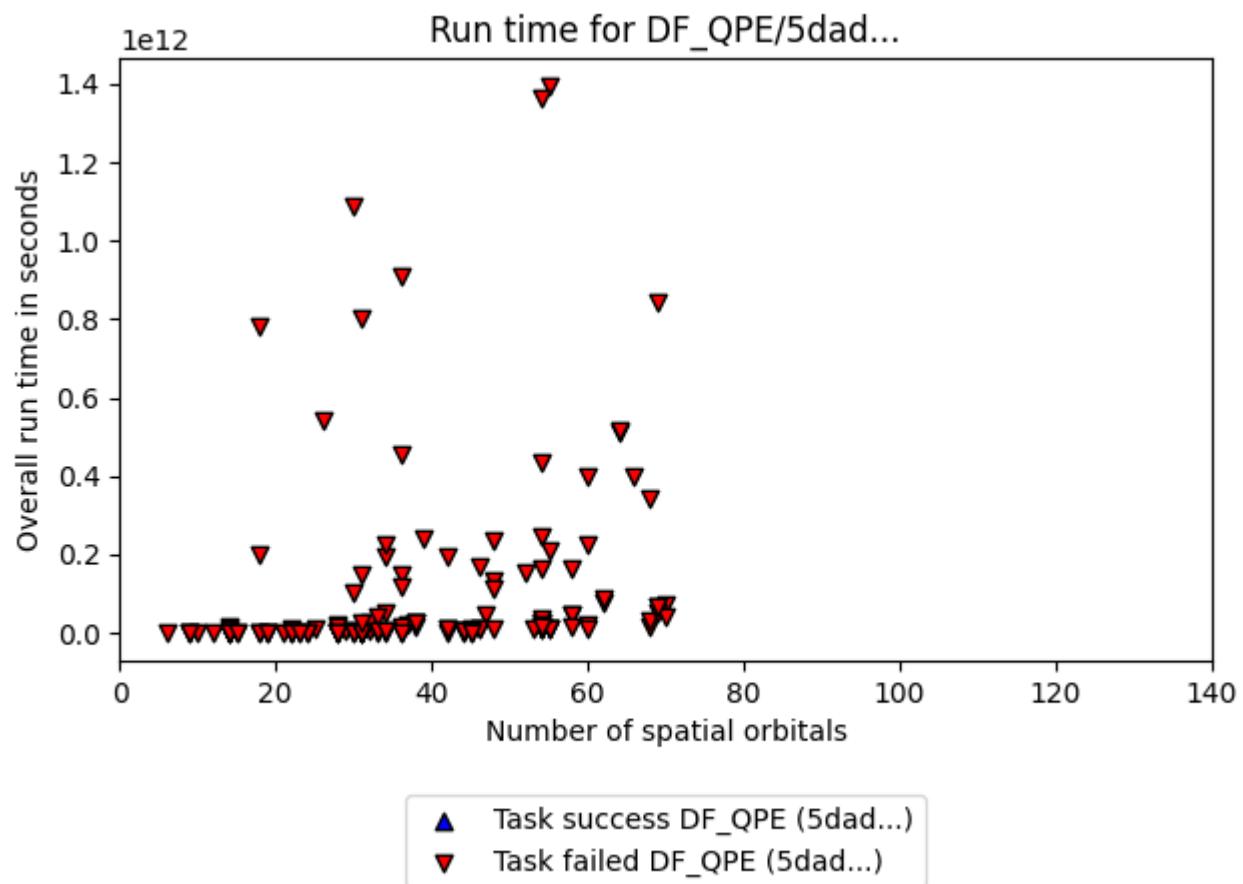
sum_of_run_time_of_attempted_tasks: 15652541022388.93

solvability_ratio: None

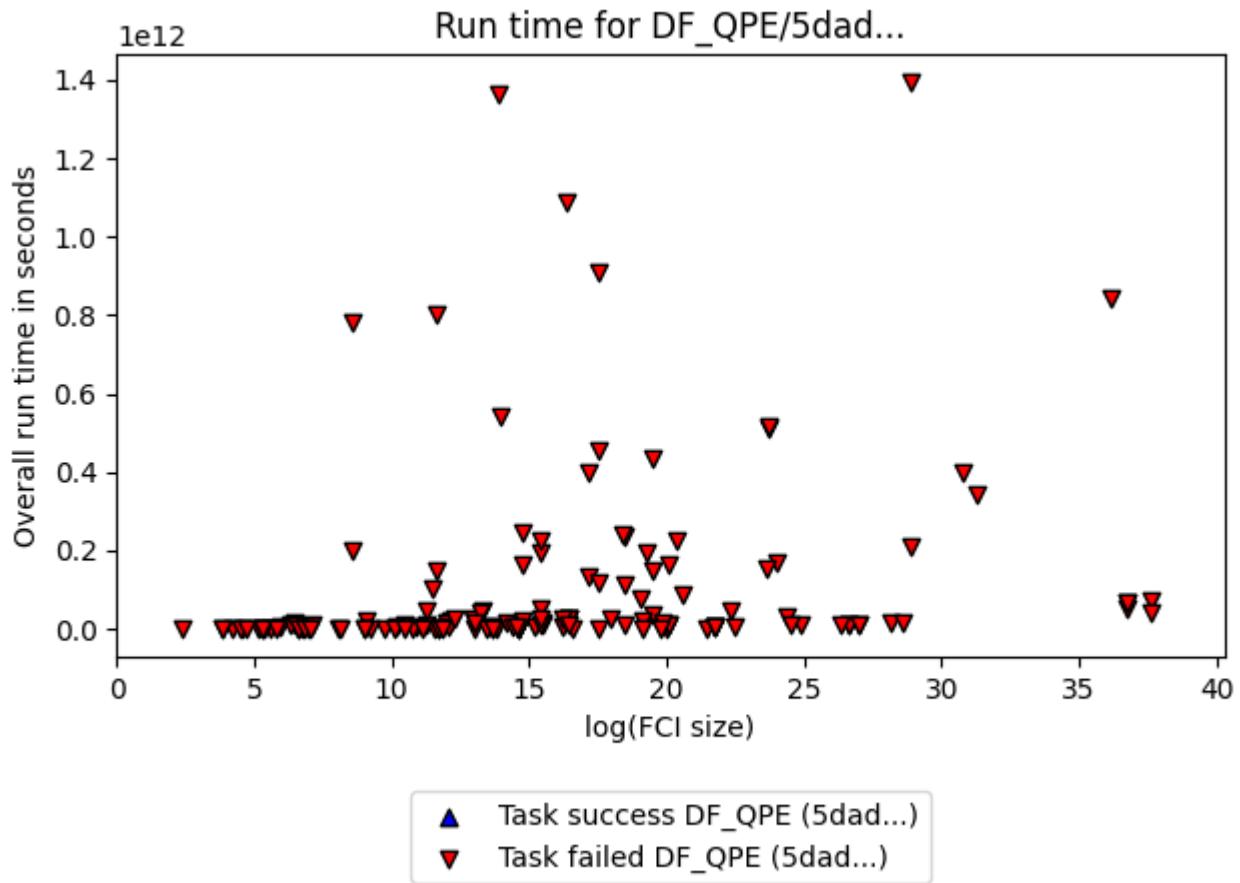
f1_score: None

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.

![Solver utility capture]supporting_artifacts/(solver_5dad4064-
cd11-412f-85cb-d722afe3b3de_utility_capture_plot.png)

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: 8af2957d-4b07-424f-a323-9161d8e16720

creation_timestamp: 2025-01-30T17:45:00.466432+00:00

number_of_problem_instances: 84

number_of_problem_instances_attempted: 84

number_of_problem_instances_solved: 9

number_of_tasks: 276

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

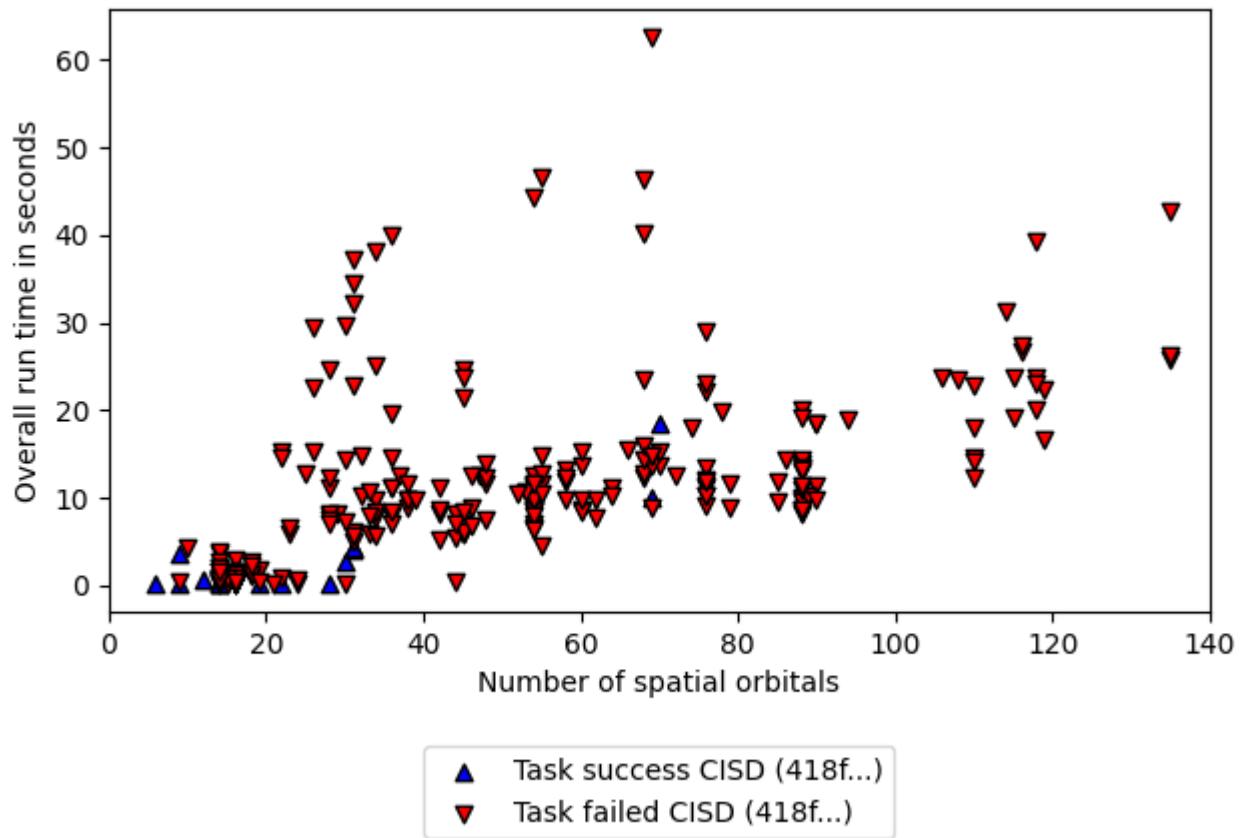
solvability_ratio: 0.0079

comment: solvability ratio based on PCA embedding.

f1_score: [0.9782608695652174, 0.85]

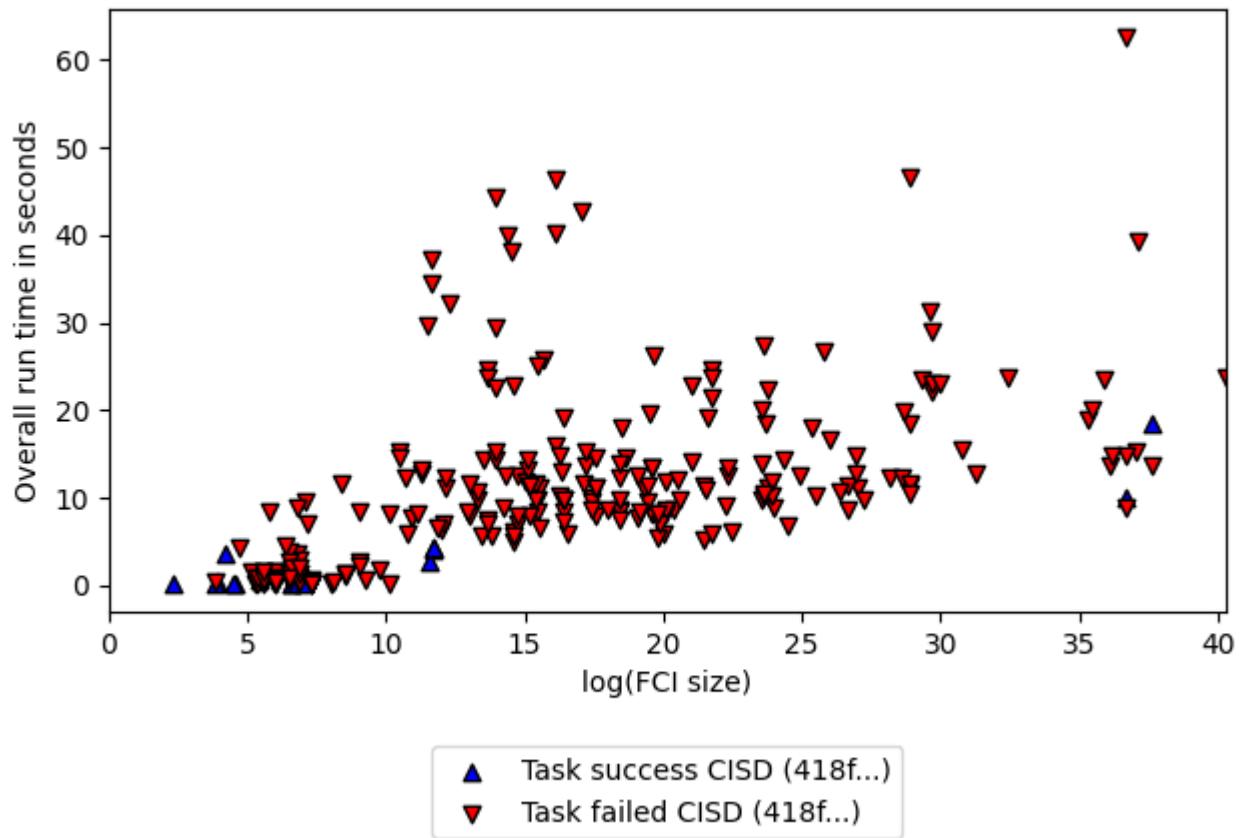
ml_metrics_calculator_version: 1

Run time for CISD/418f...



Note: plot only contains attempted tasks.

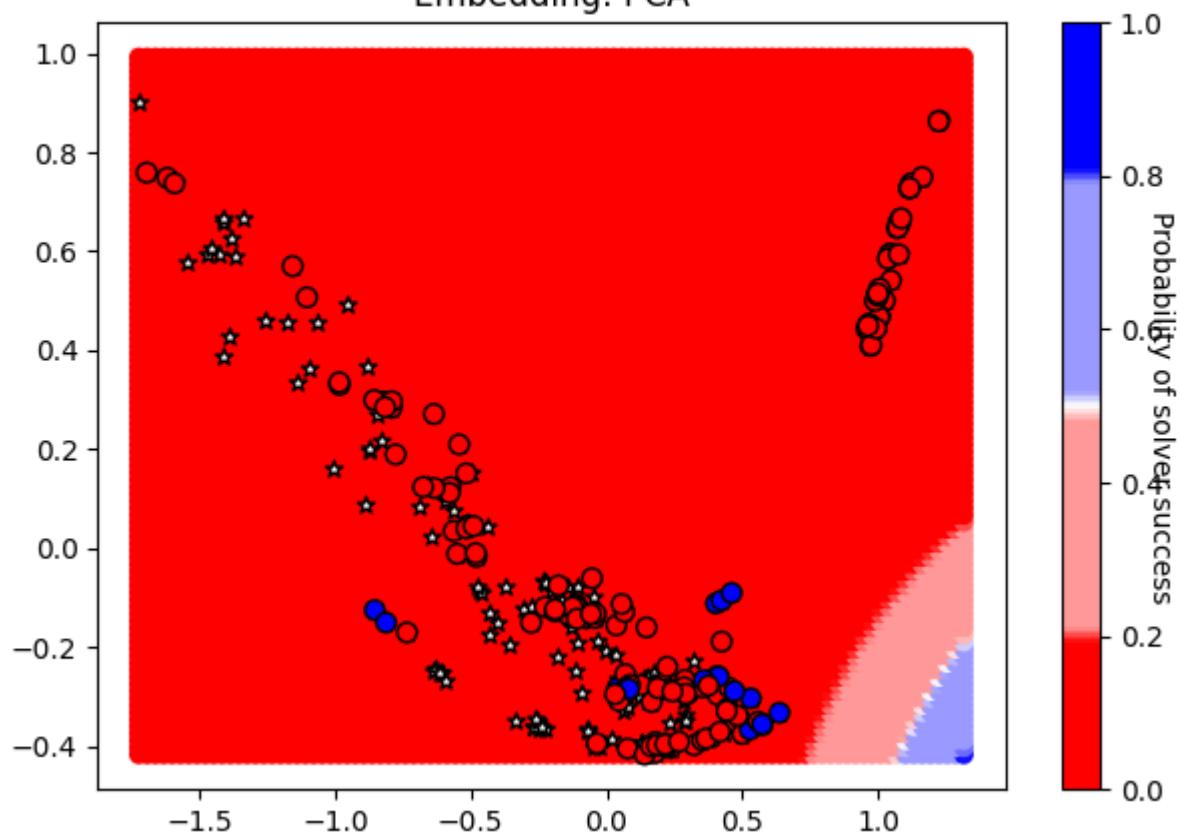
Run time for CISD/418f...



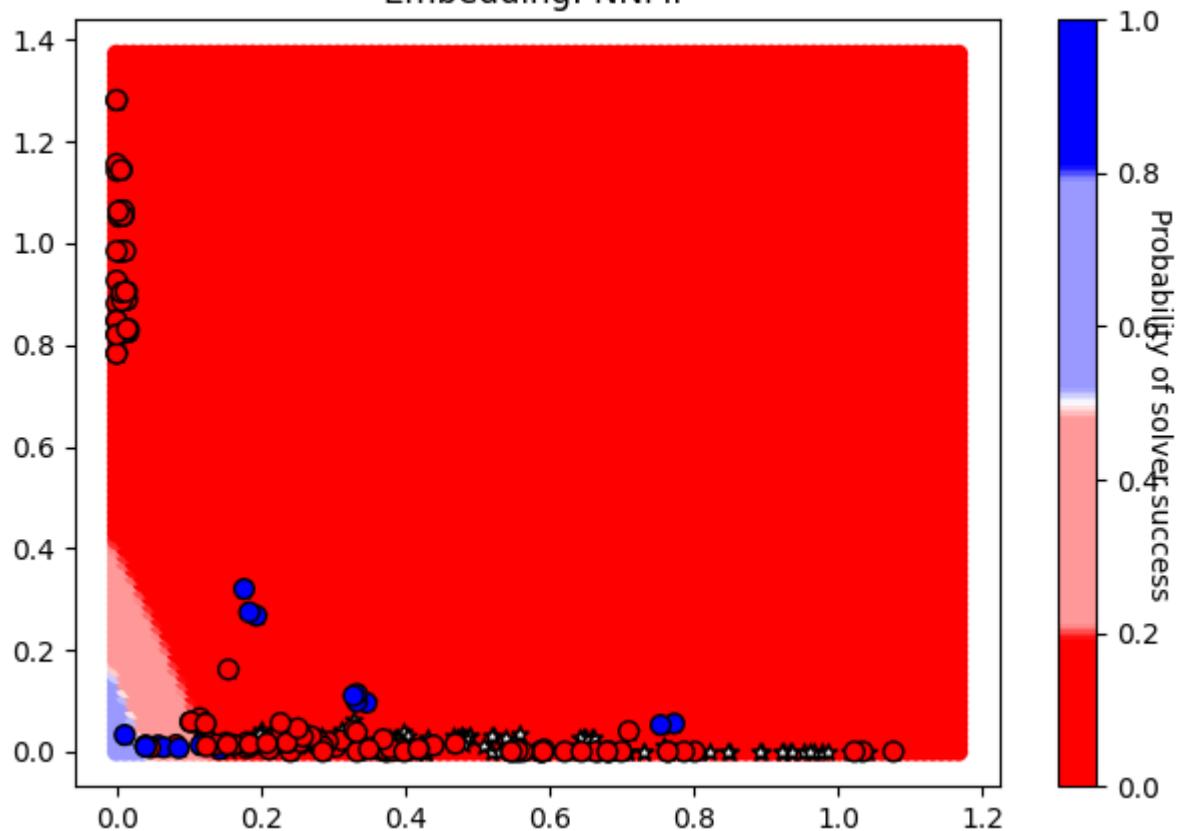
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/
(solver_418f060e-496b-4024-8d2d-9b1f8791e76d_utility_capture_plot.png)

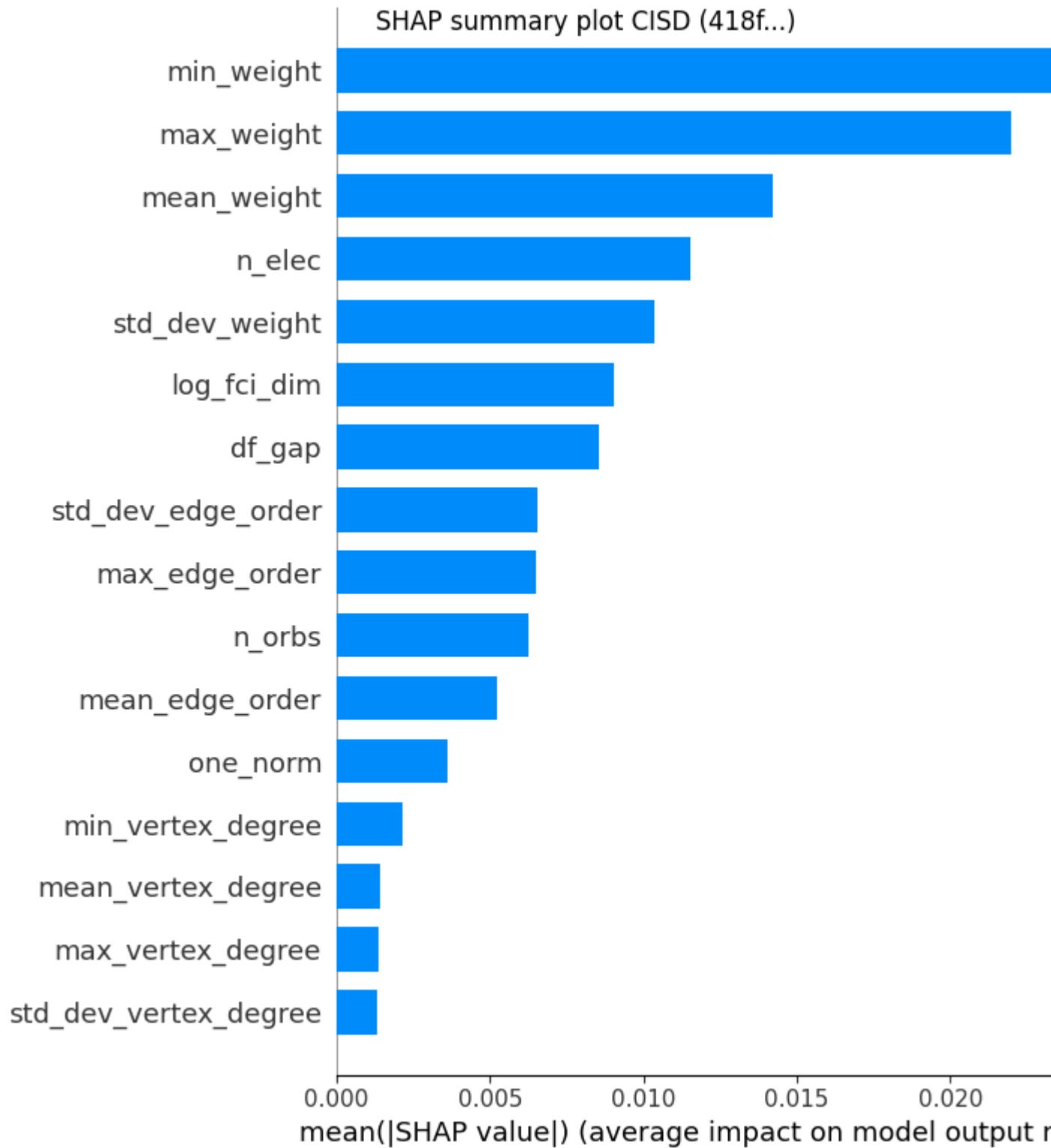
Solver CISD (418f...)
Embedding: PCA



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.



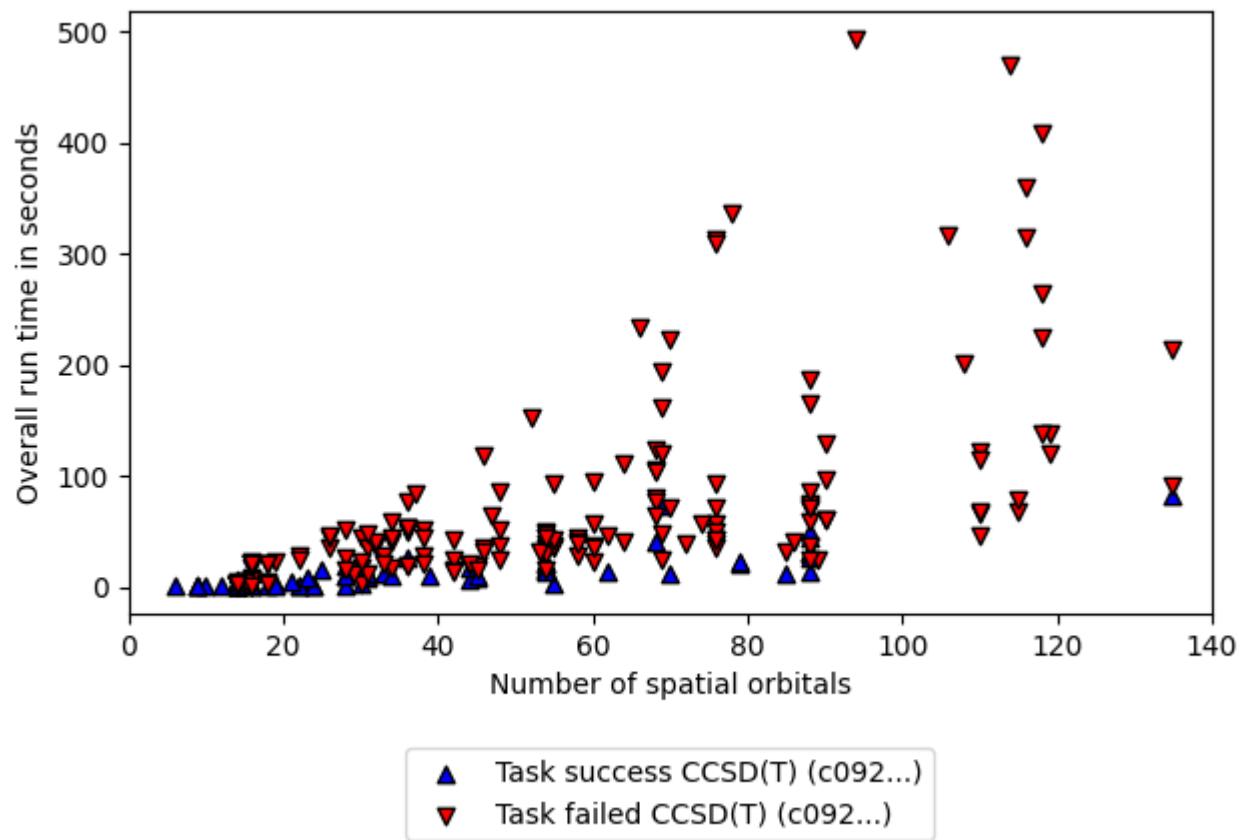
Solver CCSD(T), c09217e6-d0f7-4b0f-81c4-79210b7ac878

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

solver_short_name:CCSD(T)

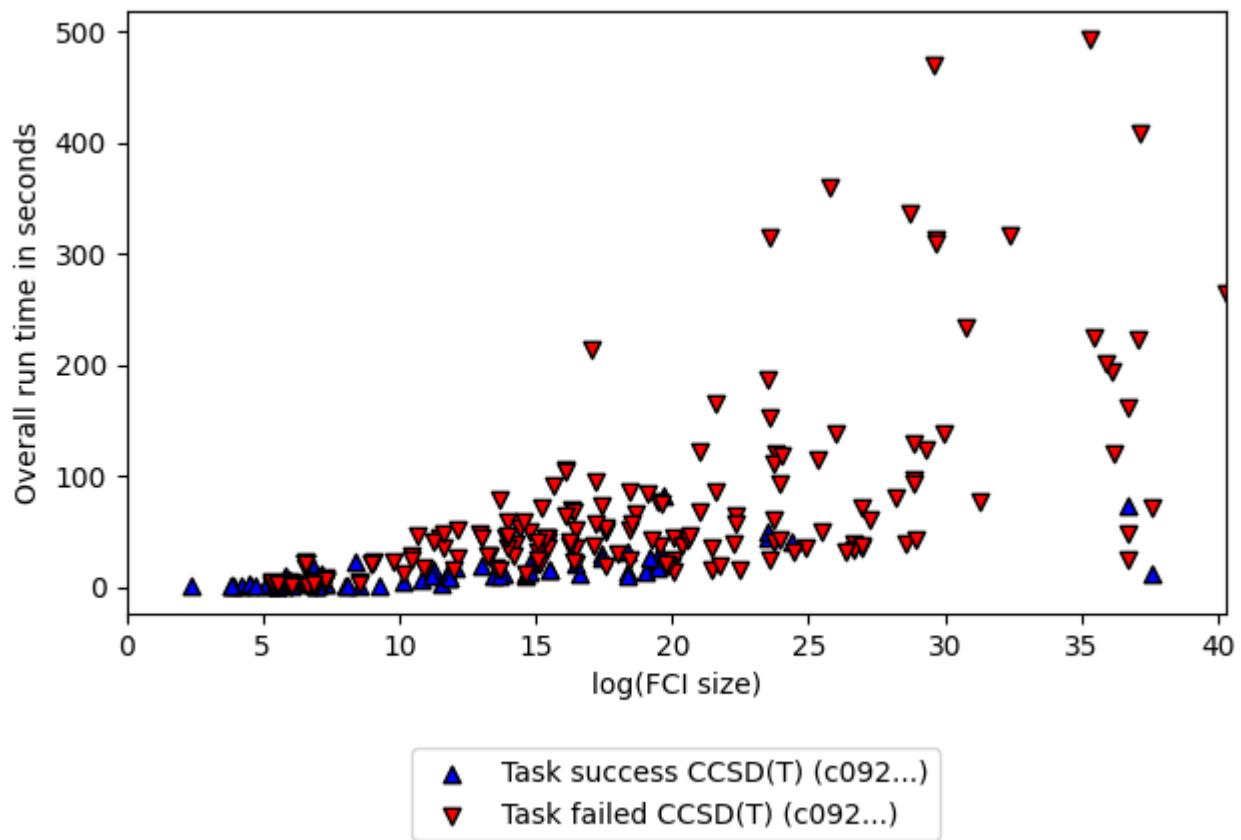
compute.hardware_type:classical_computer
classical.hardware_details:{'computing_environment_name': 'LCRC Improv (per node)', 'cpu_description': '2x AMD EPYC 7713 64C', 'ram_available_gb': '256GB', 'clock_speed': '2 GHz', 'total_num_cores': 128}
algorithm_details:CCSD(T)
software_details:pyscf (<https://github.com/pyscf/pyscf>).
performance_metrics_uuid: 2a64a87c-df90-4c35-9f65-3f73a9572eca
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 79
number_of_problem_instances_solved: 19
number_of_tasks: 276
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: 0.6011
comment: solvability ratio based on PCA embedding.
f1_score: [0.8695652173913043, 0.864516129032258]
ml_metrics_calculator_version: 1

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



Note: plot only contains attempted tasks.

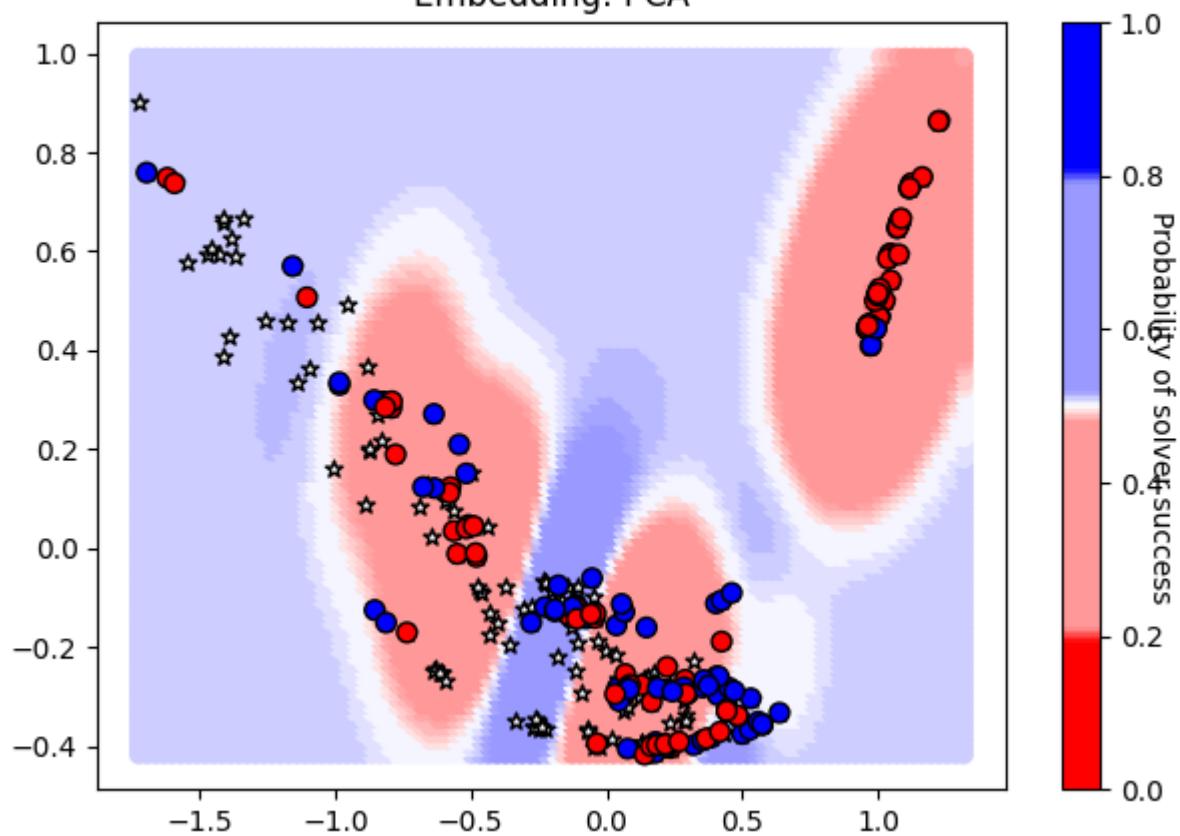
Run time for CCSD(T)/c092...



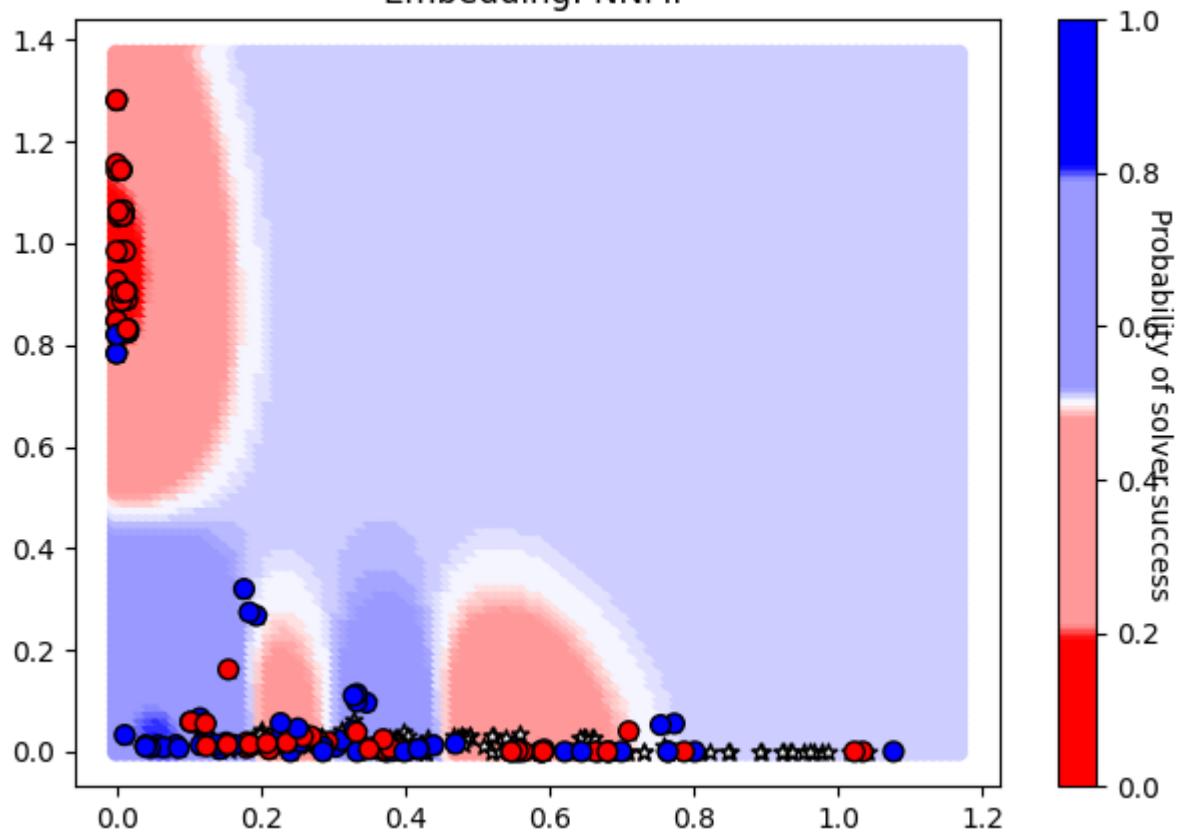
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_c09217e6-d0f7-4b0f-81c4-79210b7ac878_utility_capture_plot.png)

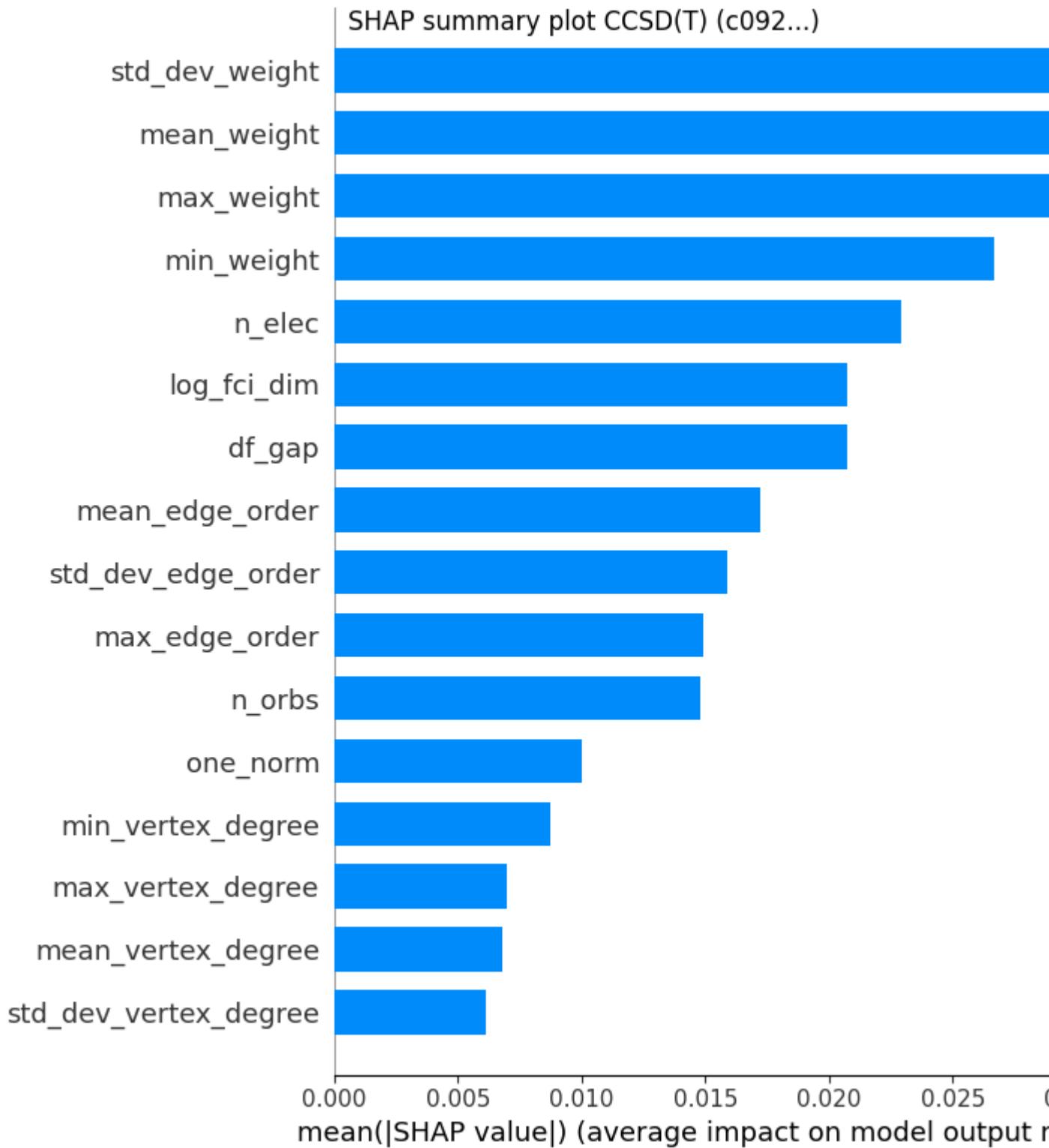
Solver CCSD(T) (c092...)
Embedding: PCA



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.



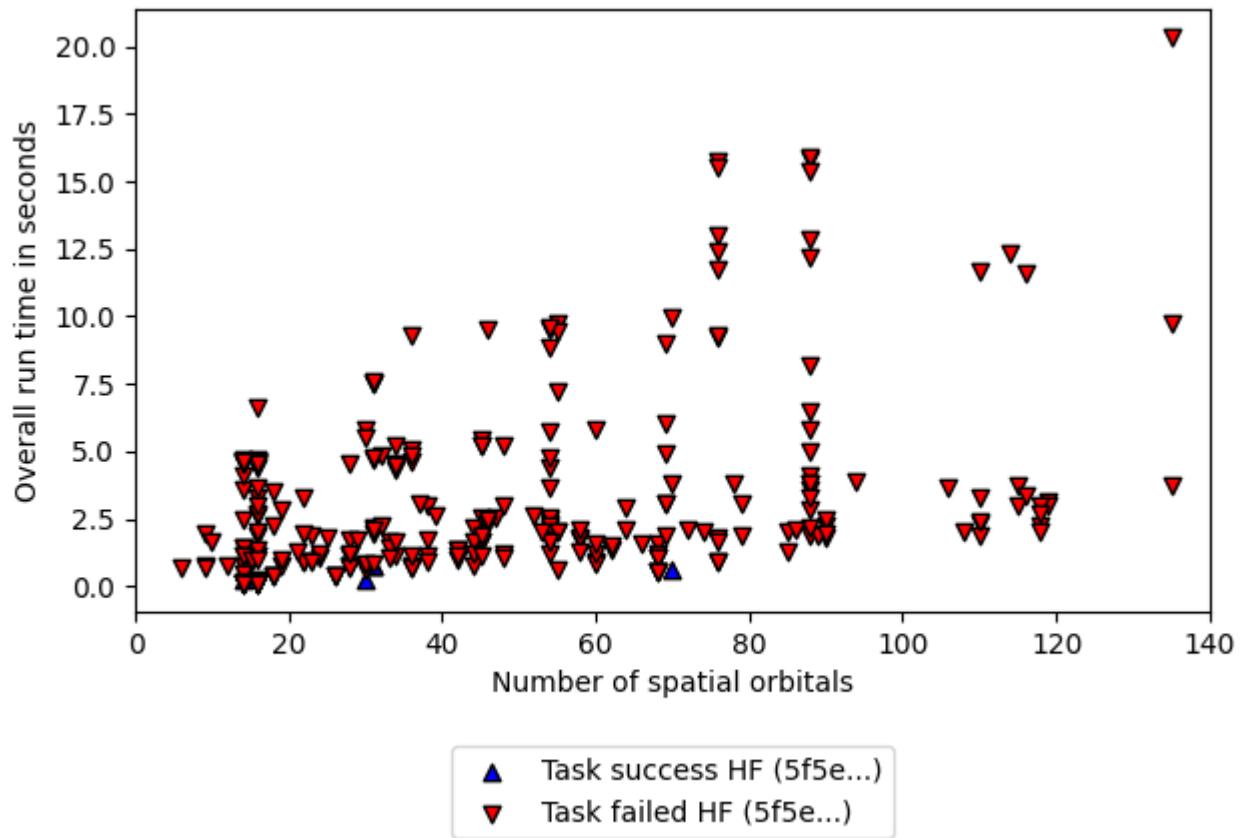
Solver HF, 5f5e617a-19c2-4d82-bebc-b2d6b3dcb012

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

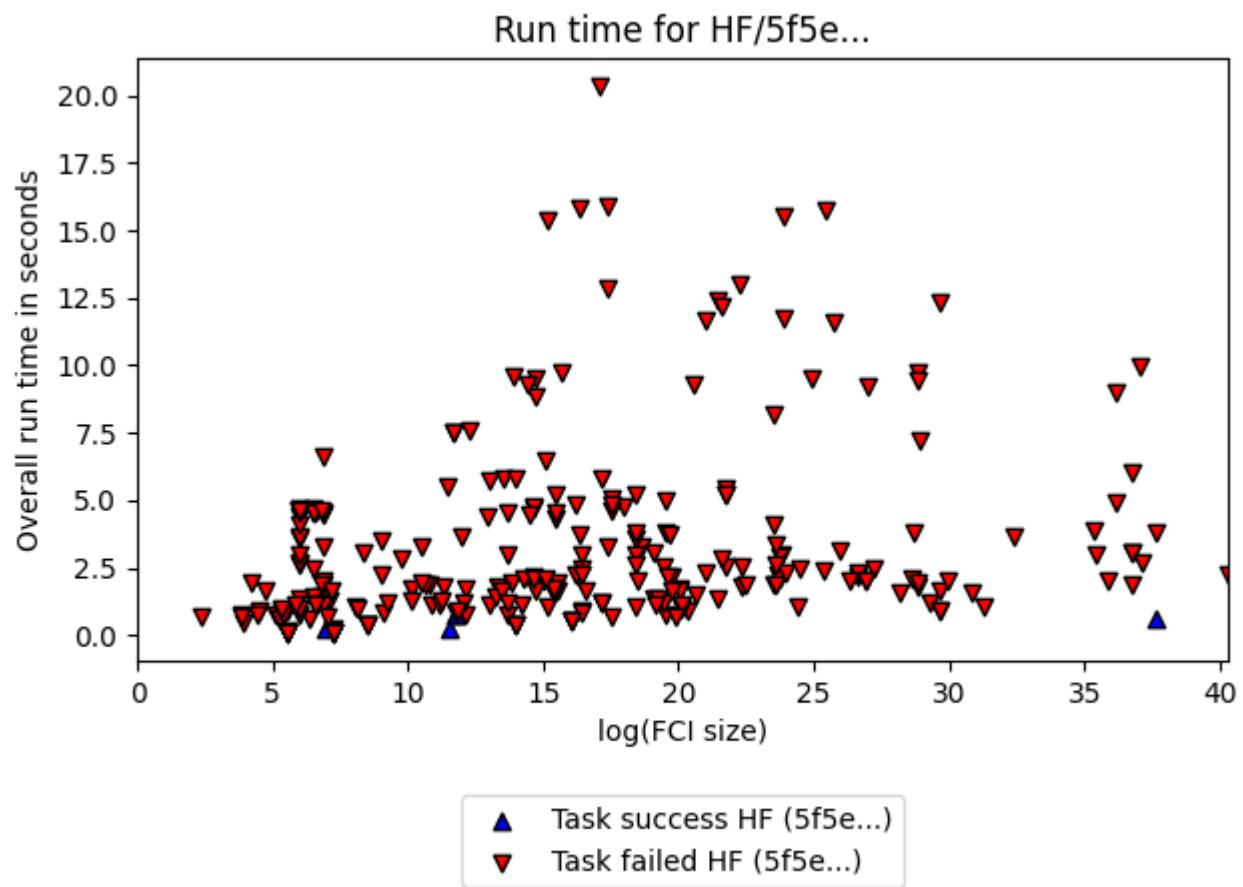
solver_short_name:HF

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: 454c3ce7-6f3b-47b3-b784-f9a2da023c3e
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 84
number_of_problem_instances_solved: 5
number_of_tasks: 276
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: [0.9867549668874173, 0.7142857142857143]
ml_metrics_calculator_version: 1

Run time for HF/5f5e...



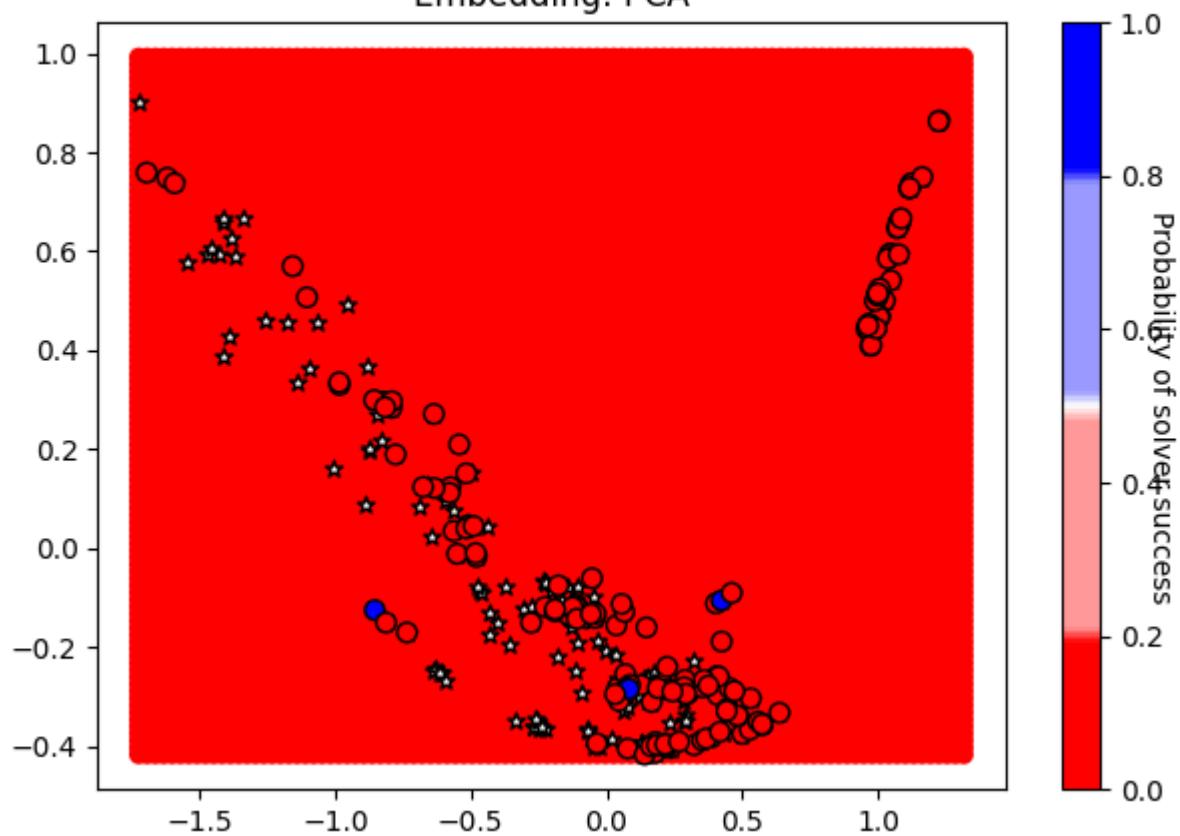
Note: plot only contains attempted tasks.



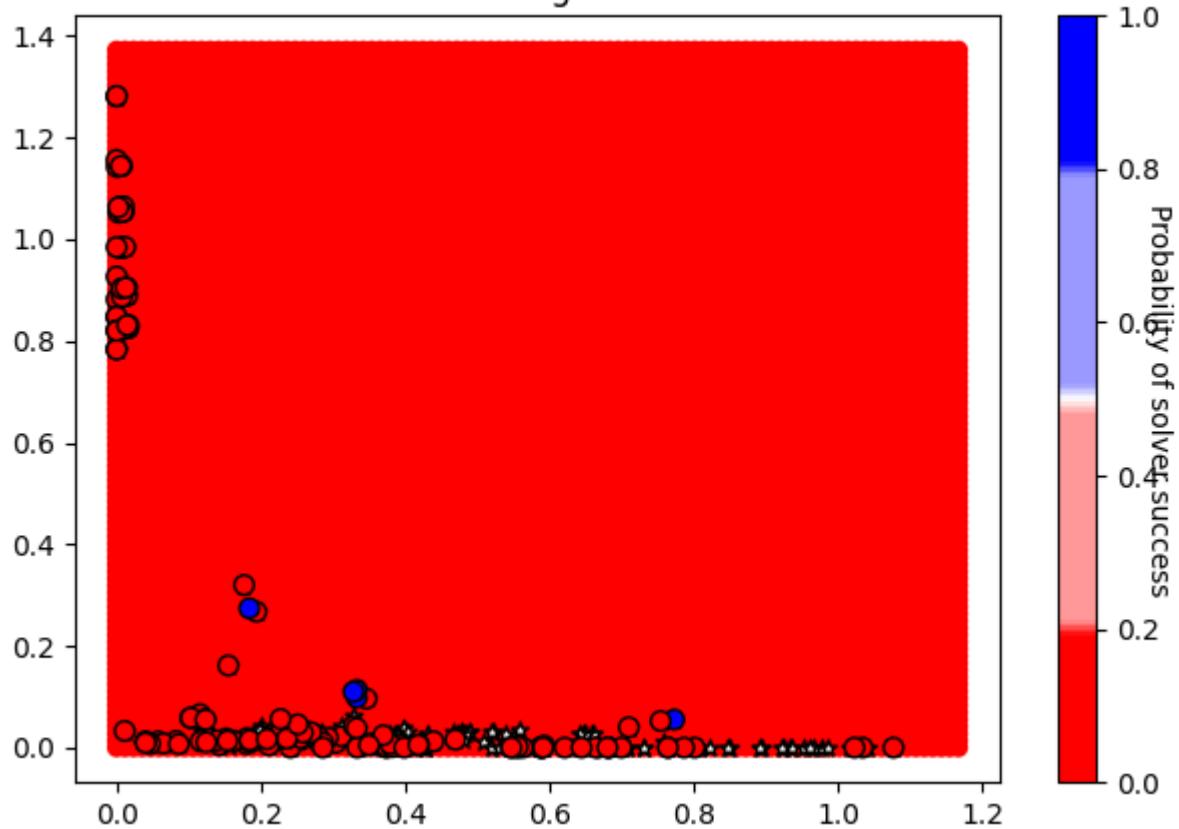
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_5f5e617a-19c2-4d82-bebc-b2d6b3dc012_utility_capture_plot.png)

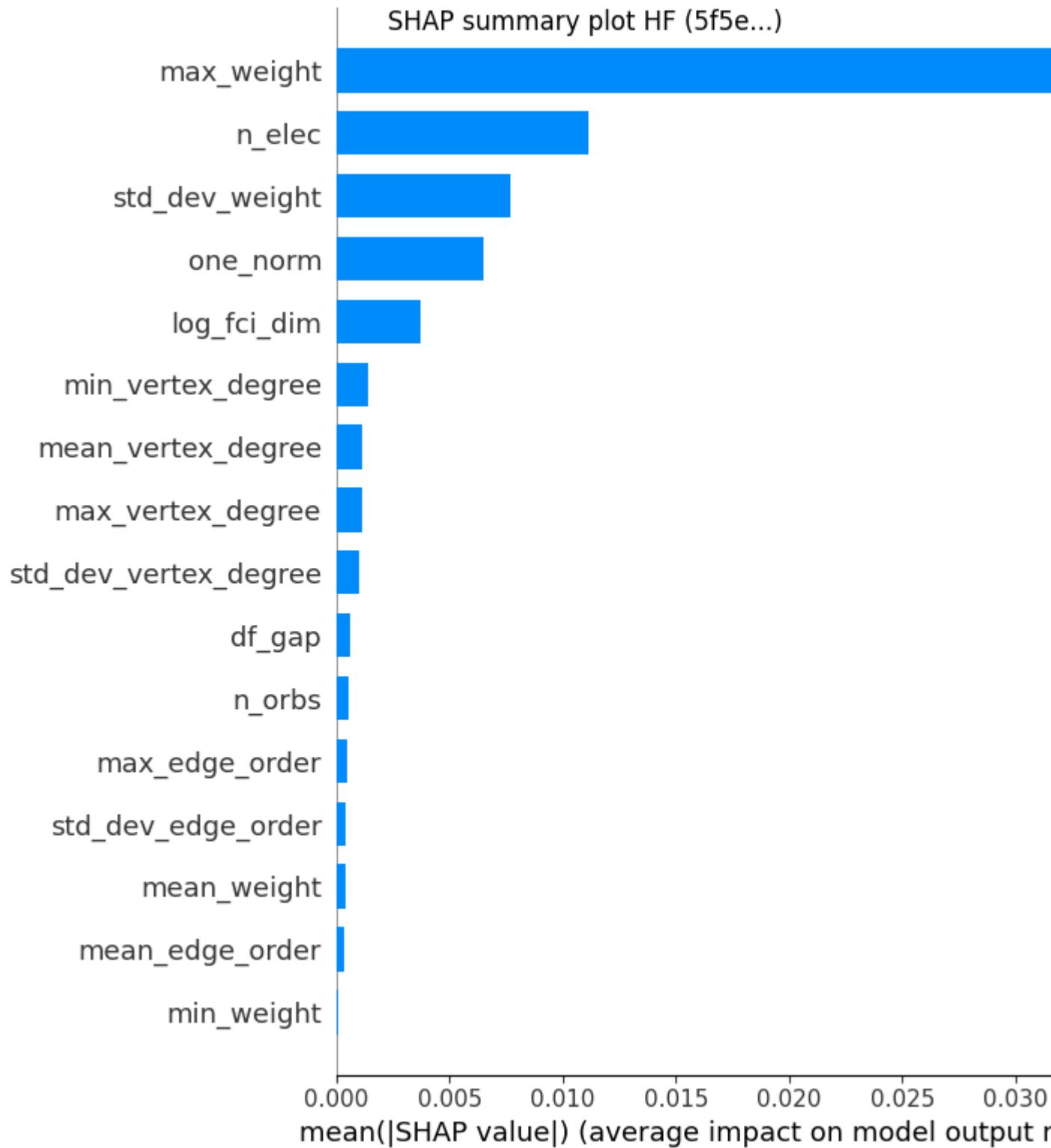
Solver HF (5f5e...)
Embedding: PCA



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.



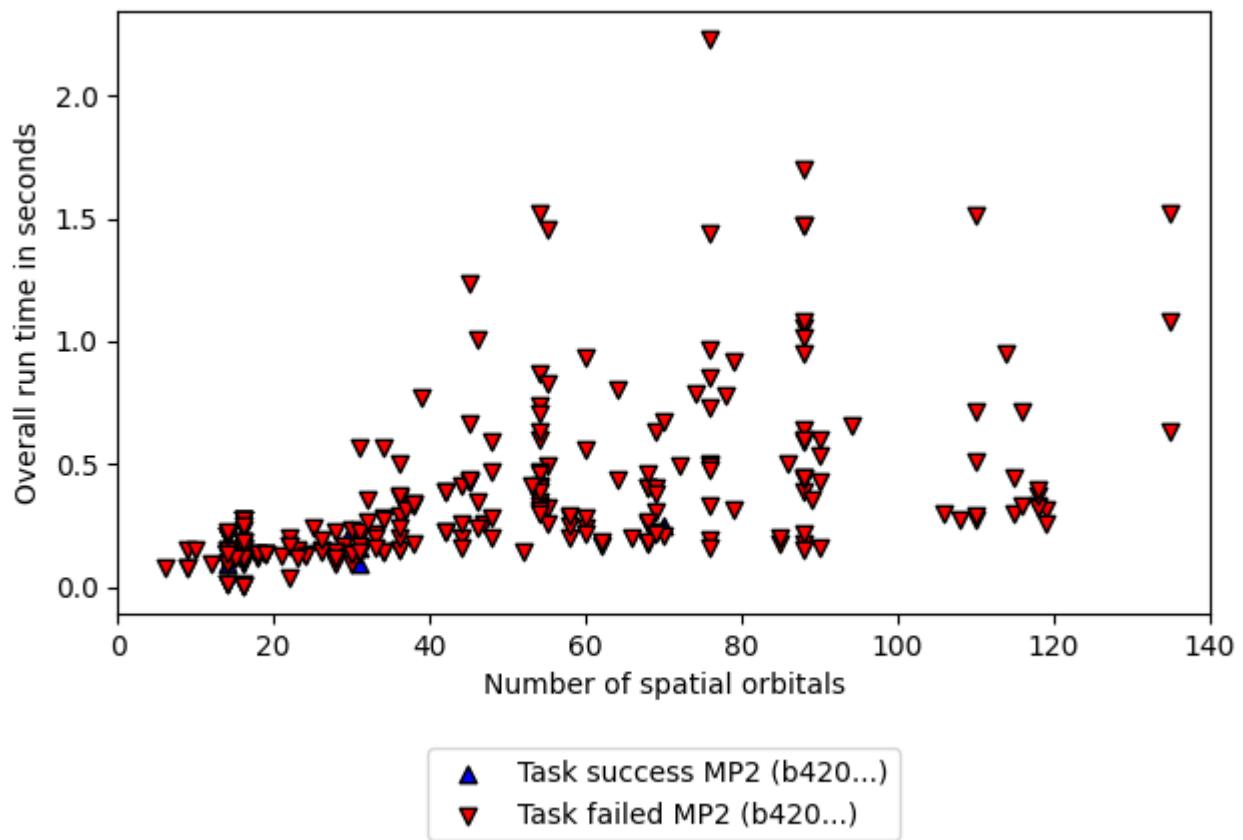
Solver MP2, b420358b-5def-41e6-8c5d-b9d93b6aecd2

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

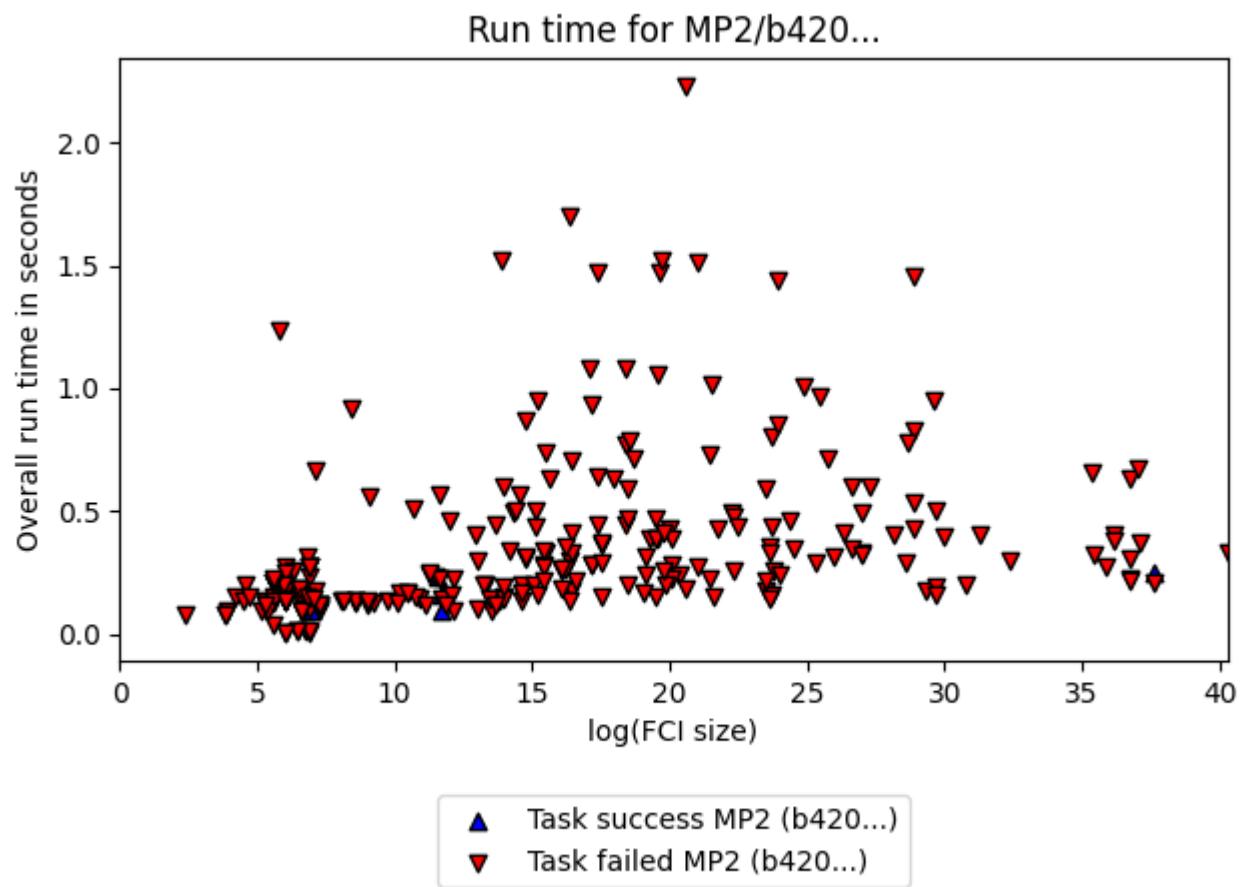
solver_short_name:MP2

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: 31522f8f-1c01-4fec-9bdf-1c12aca7471d
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 81
number_of_problem_instances_solved: 5
number_of_tasks: 276
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: [0.9867549668874173, 0.7142857142857143]
ml_metrics_calculator_version: 1

Run time for MP2/b420...



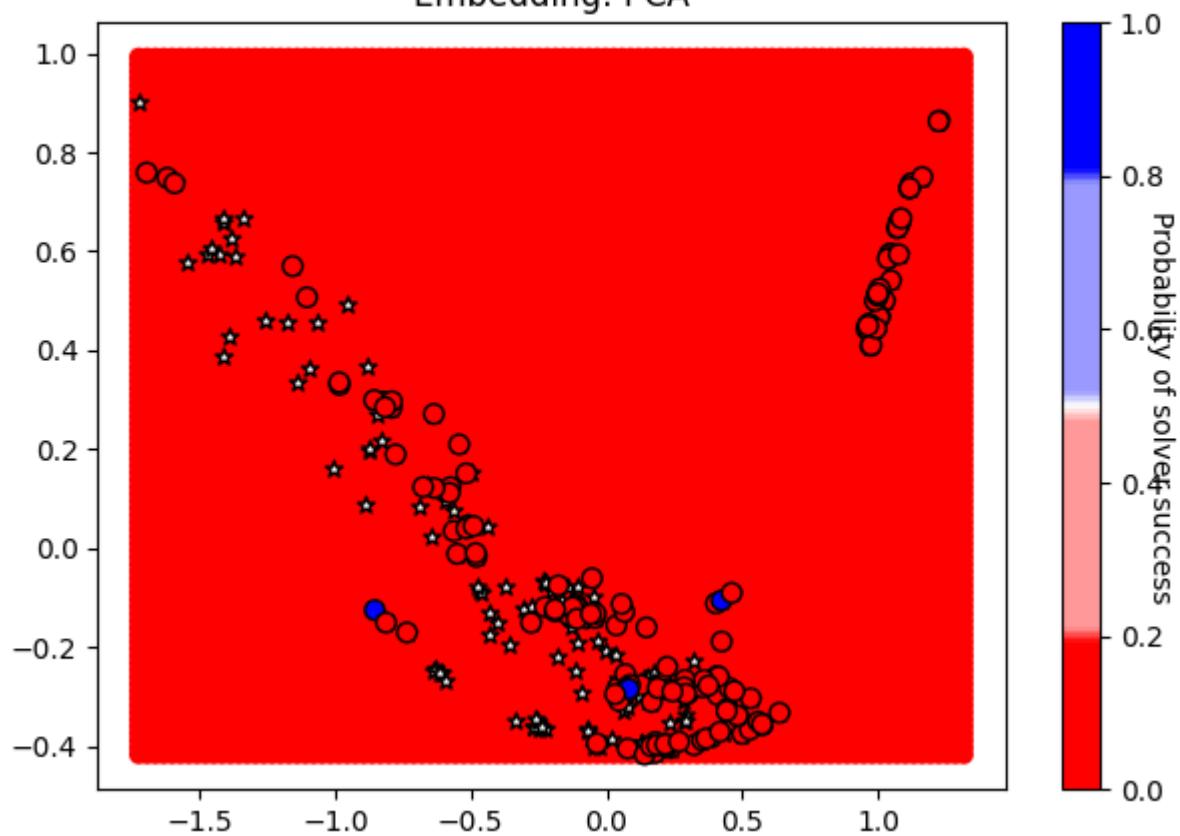
Note: plot only contains attempted tasks.



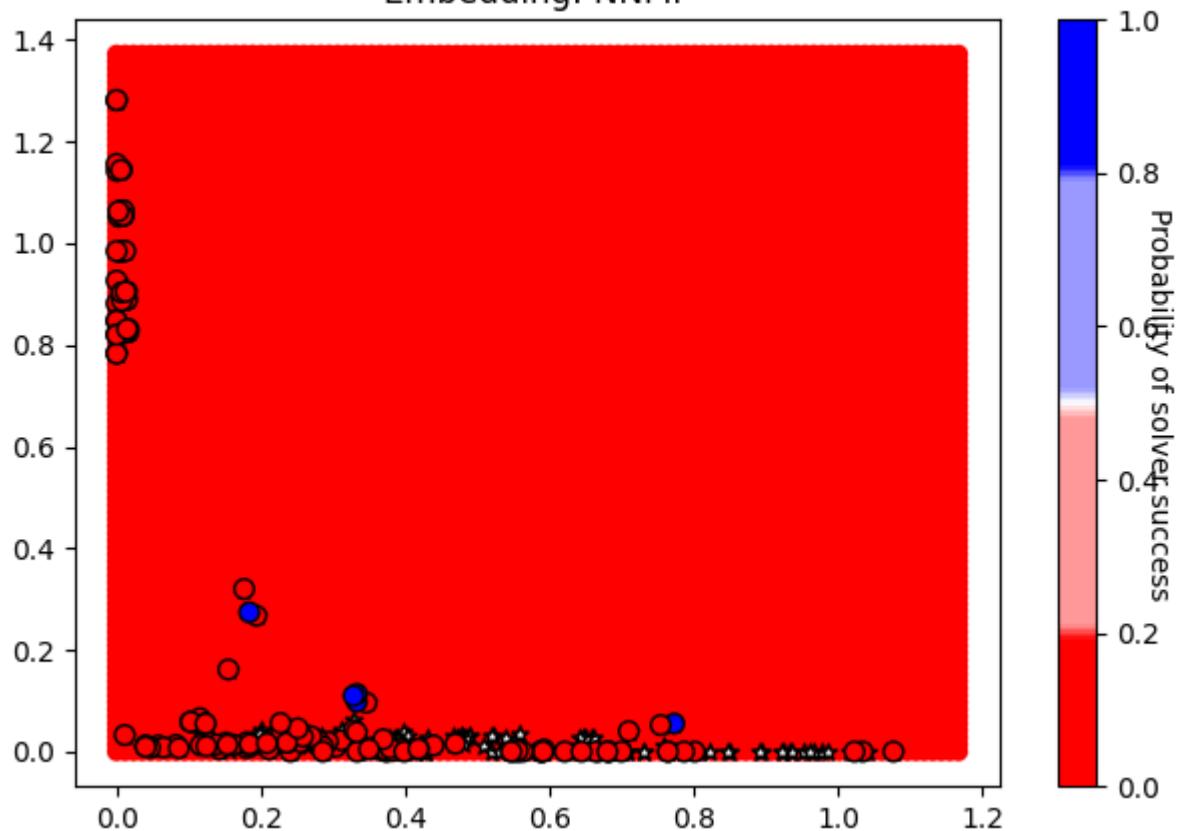
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/
(solver_b420358b-5def-41e6-8c5d-b9d93b6aecf2_utility_capture_plot.png)

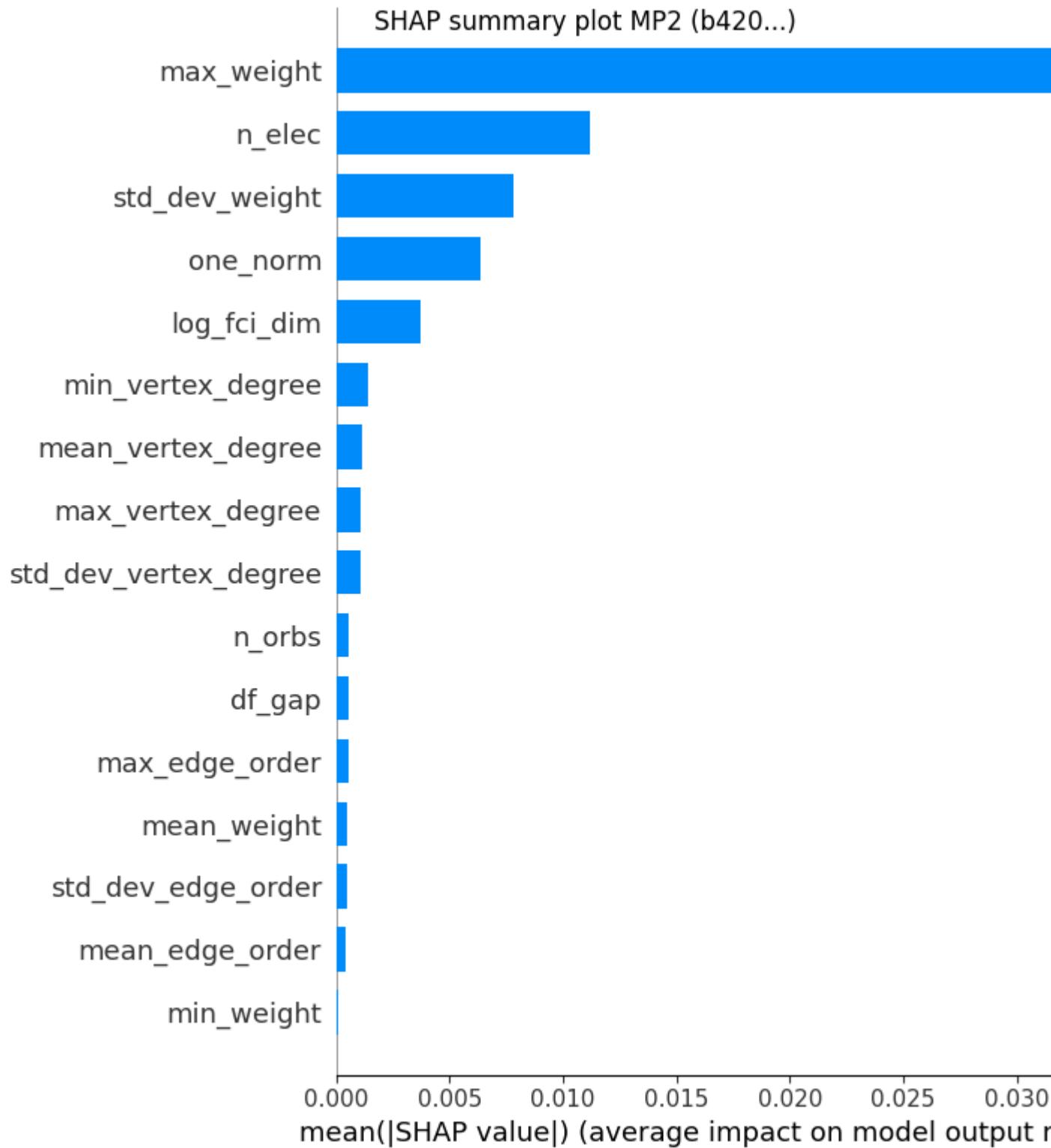
Solver MP2 (b420...)
Embedding: PCA



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.



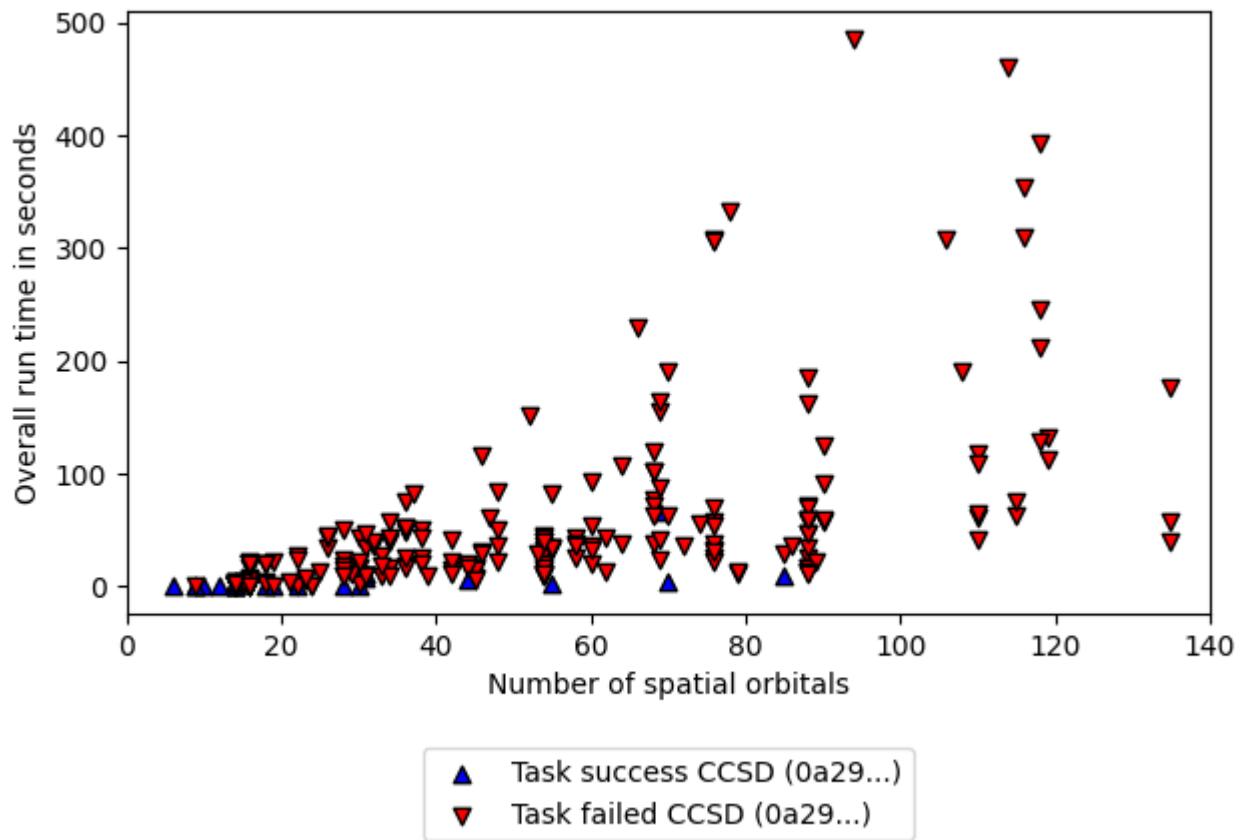
Solver CCSD, 0a29e54f-bef9-4d19-bafa-d94b1c4b37aa

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

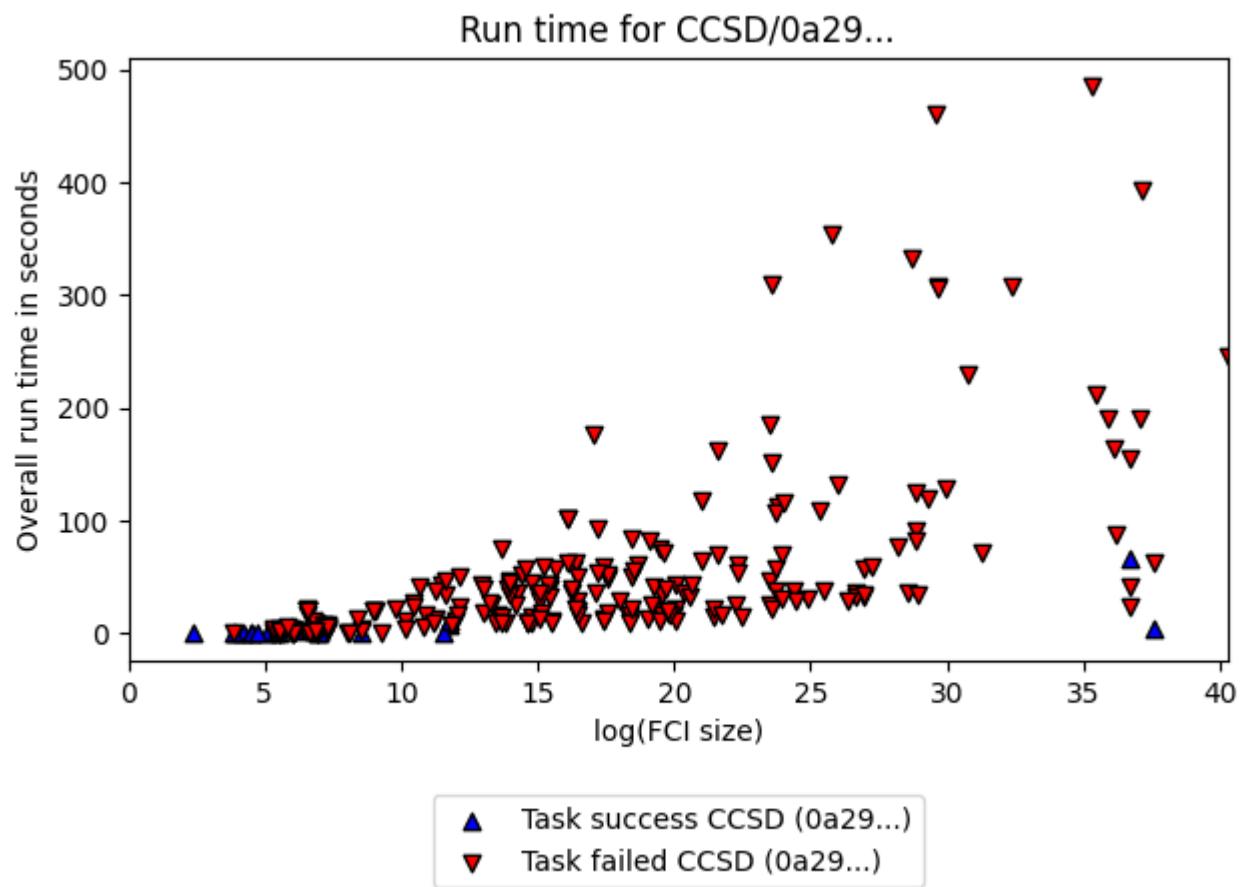
solver_short_name:CCSD

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: 2833f154-b15d-4549-9649-fd2bb6cd7d3b
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 79
number_of_problem_instances_solved: 10
number_of_tasks: 276
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: [0.9886792452830189, 0.9411764705882353]
ml_metrics_calculator_version: 1

Run time for CCSD/0a29...



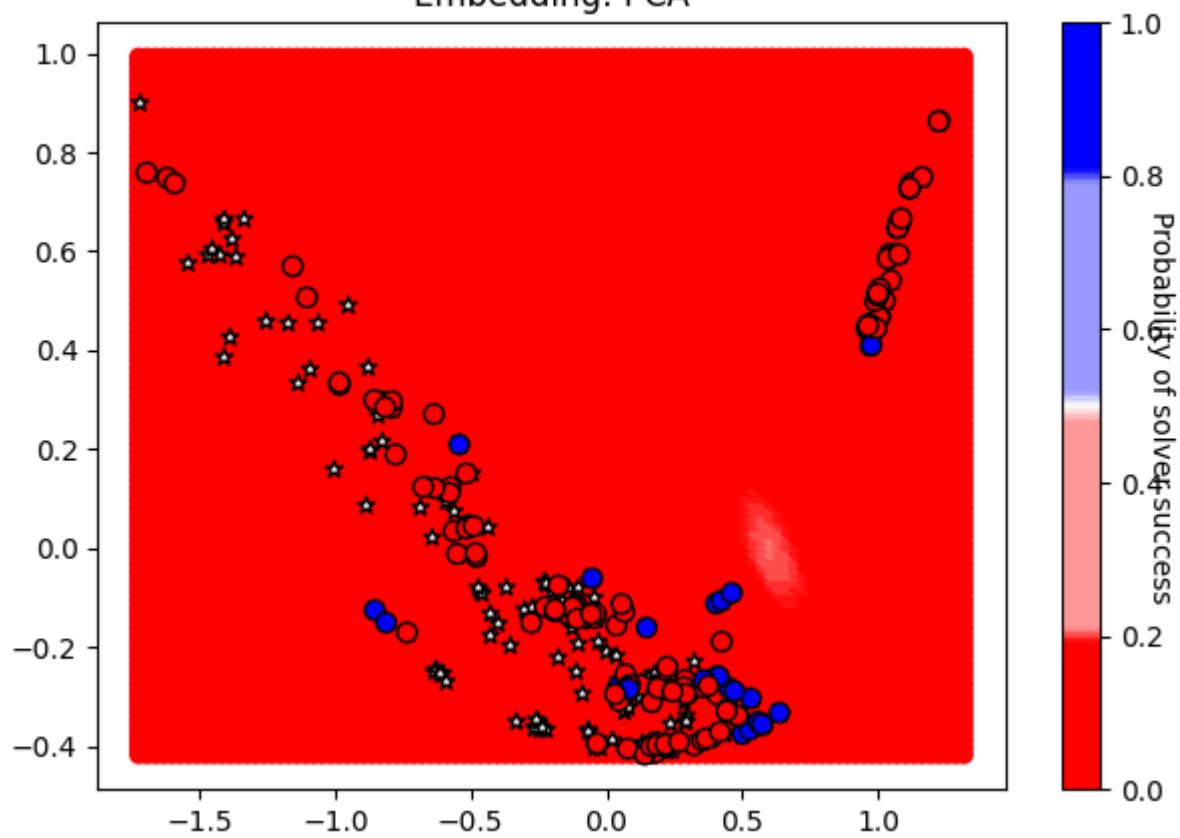
Note: plot only contains attempted tasks.



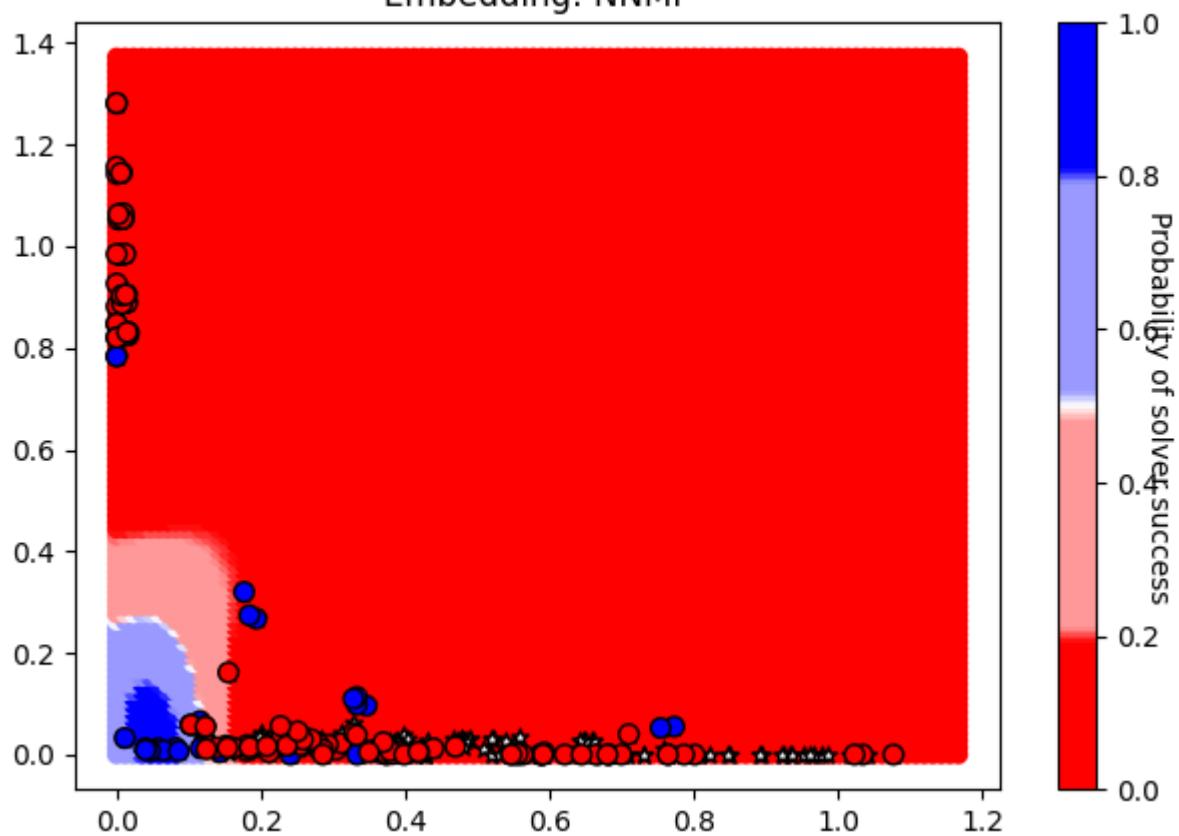
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_0a29e54f-bef9-4d19-bafa-d94b1c4b37aa_utility_capture_plot.png)

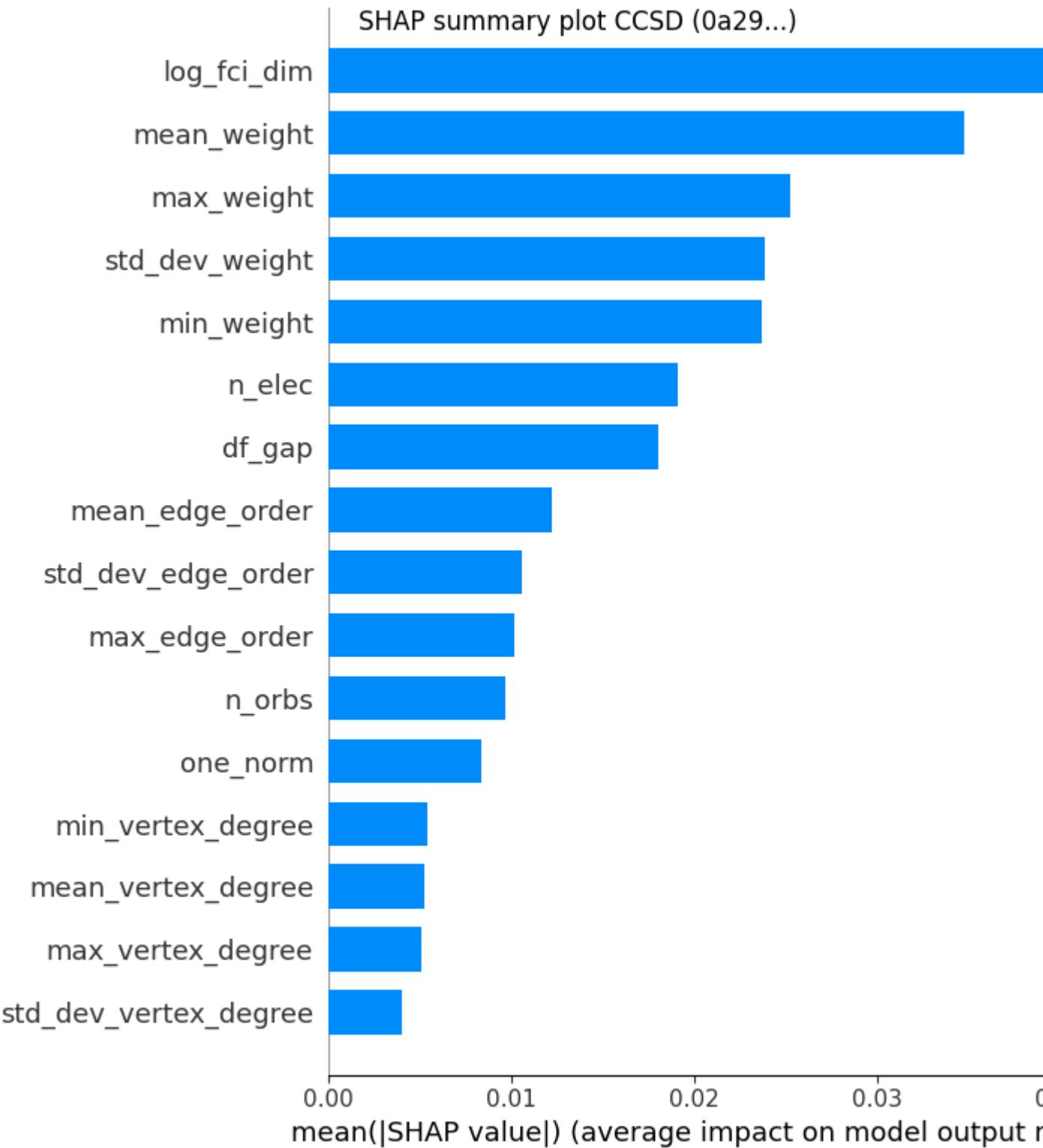
Solver CCSD (0a29...)
Embedding: PCA



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



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

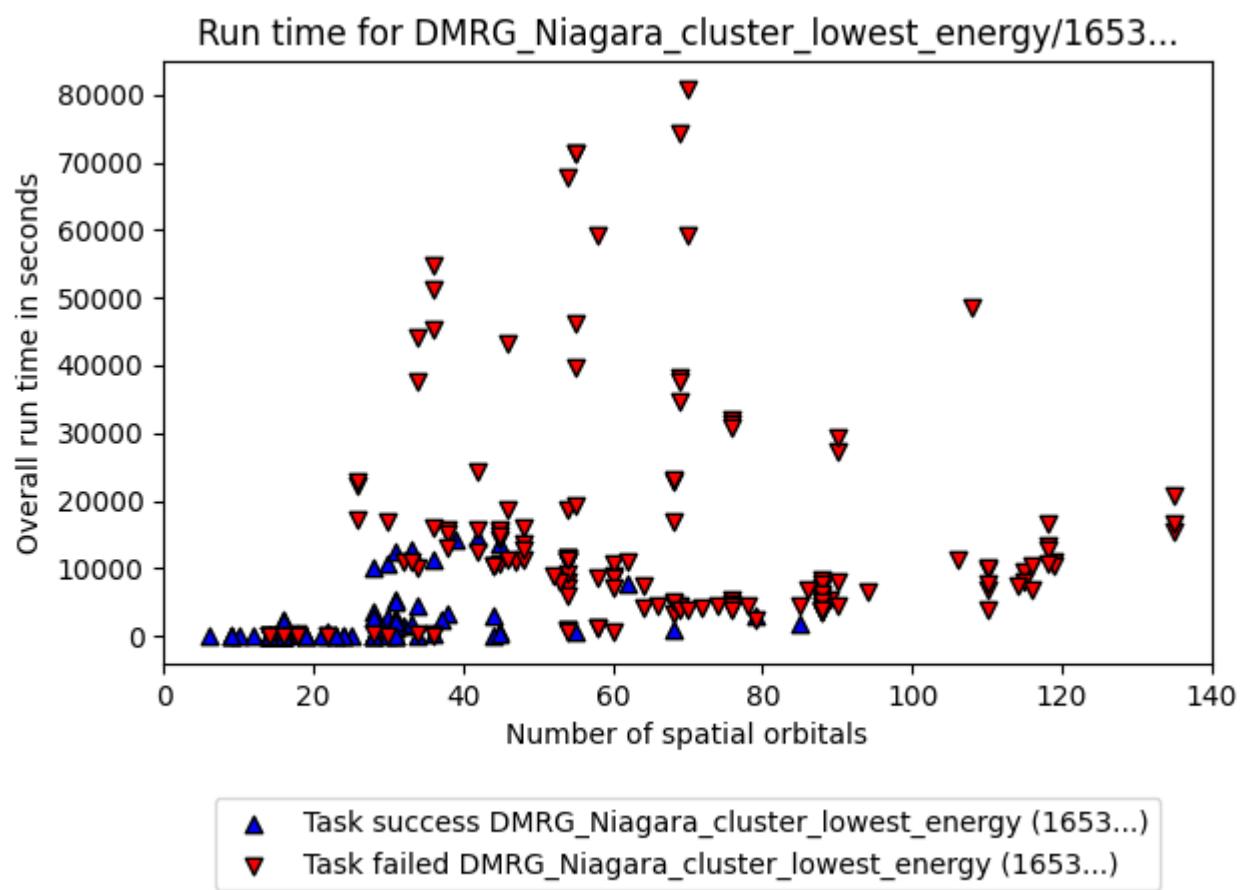


Solver DMRG_Niagara_cluster_lowest_energy, 16537433-9f4c-4eae-a65d-787dc3b35b59

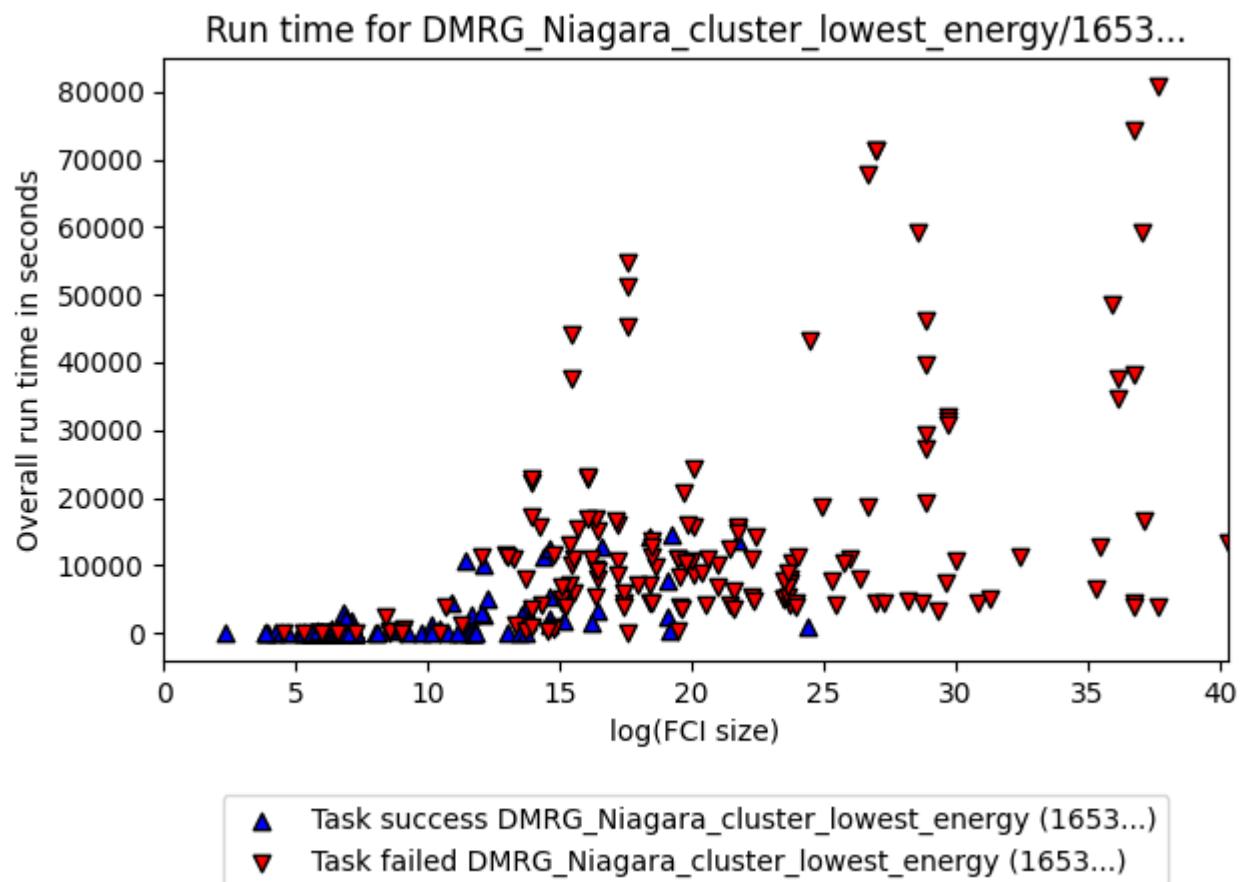
solver_uuid:16537433-9f4c-4eae-a65d-787dc3b35b59

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: ba1f55ba-aa5a-406a-9405-8c62ee76c00a
creation_timestamp: 2025-01-30T17:45:00.466432+00:00
number_of_problem_instances: 84
number_of_problem_instances_attempted: 84
number_of_problem_instances_solved: 9
number_of_tasks: 276
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: 0.5461
comment: solvability ratio based on PCA embedding.
f1_score: [0.9662921348314607, 0.986784140969163]
ml_metrics_calculator_version: 1



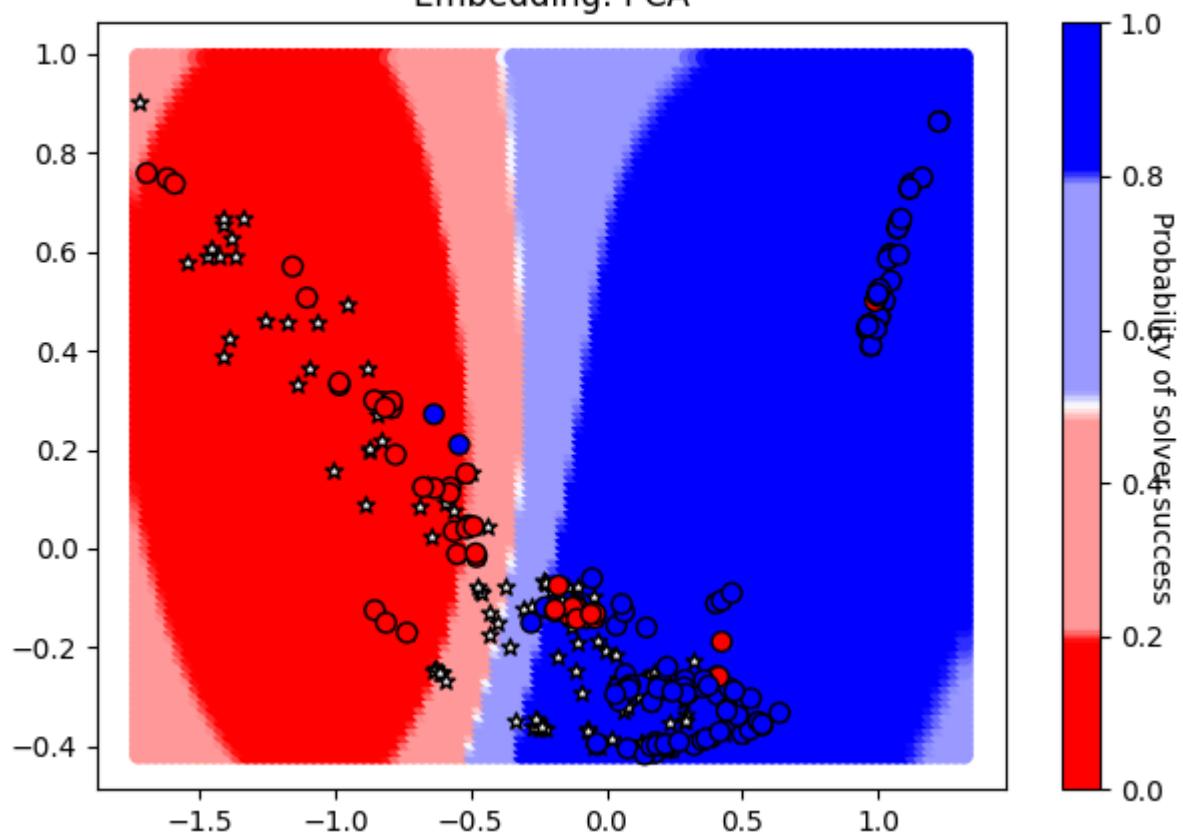
Note: plot only contains attempted tasks.



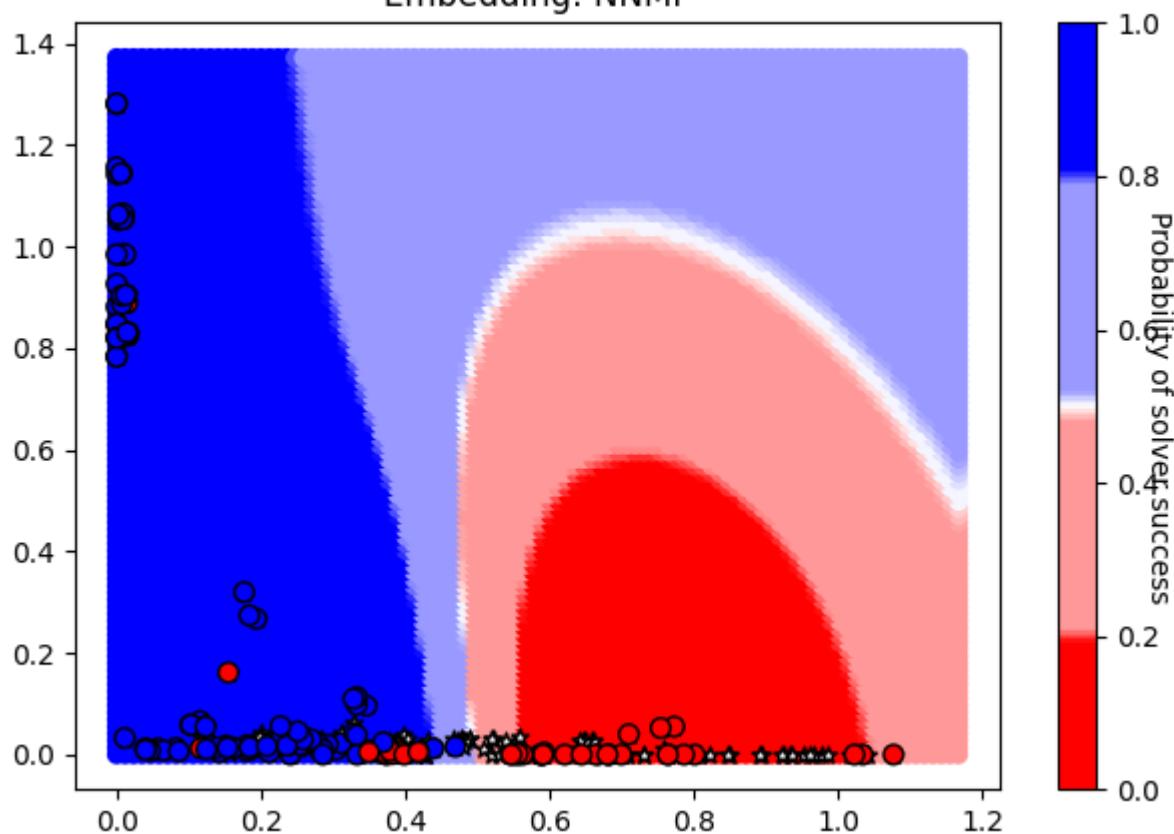
Note: plot only contains attempted tasks.

![Solver utility capture]supporting_artifacts/(solver_16537433-9f4c-4eae-a65d-787dc3b35b59_utility_capture_plot.png)

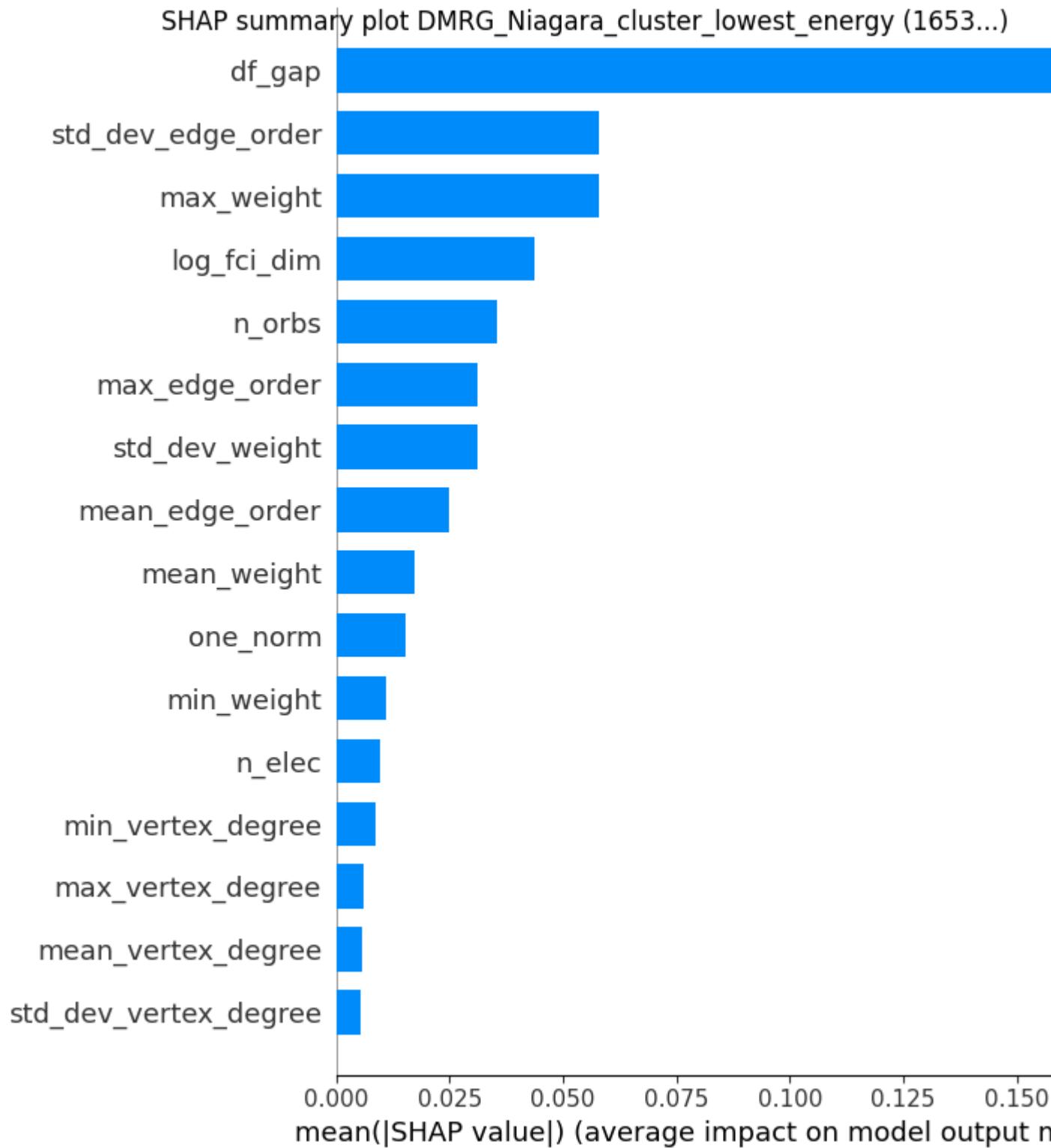
Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: PCA



Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: NMF



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



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

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

solver_short_name:DF_QPE

compute.hardware_type:quantum_computer

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

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

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

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

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

performance_metrics_uuid: ee63a8ee-17b5-4e7f-bf29-176ee801c905

creation_timestamp: 2025-01-30T17:45:00.466432+00:00

number_of_problem_instances: 84

number_of_problem_instances_attempted: 3

number_of_problem_instances_solved: 0

number_of_tasks: 276

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

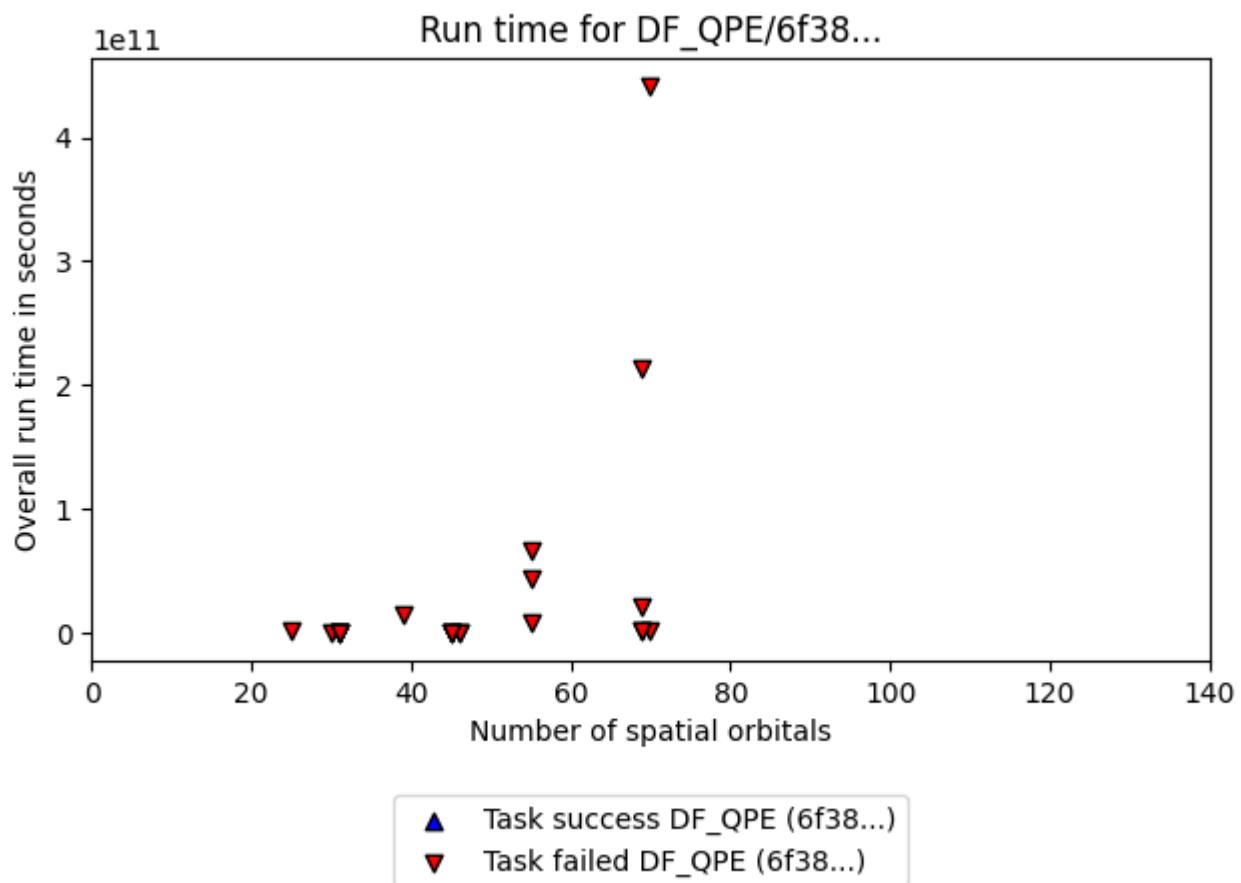
sum_of_run_time_of_attempted_tasks: 819346667619.2955

solvability_ratio: None

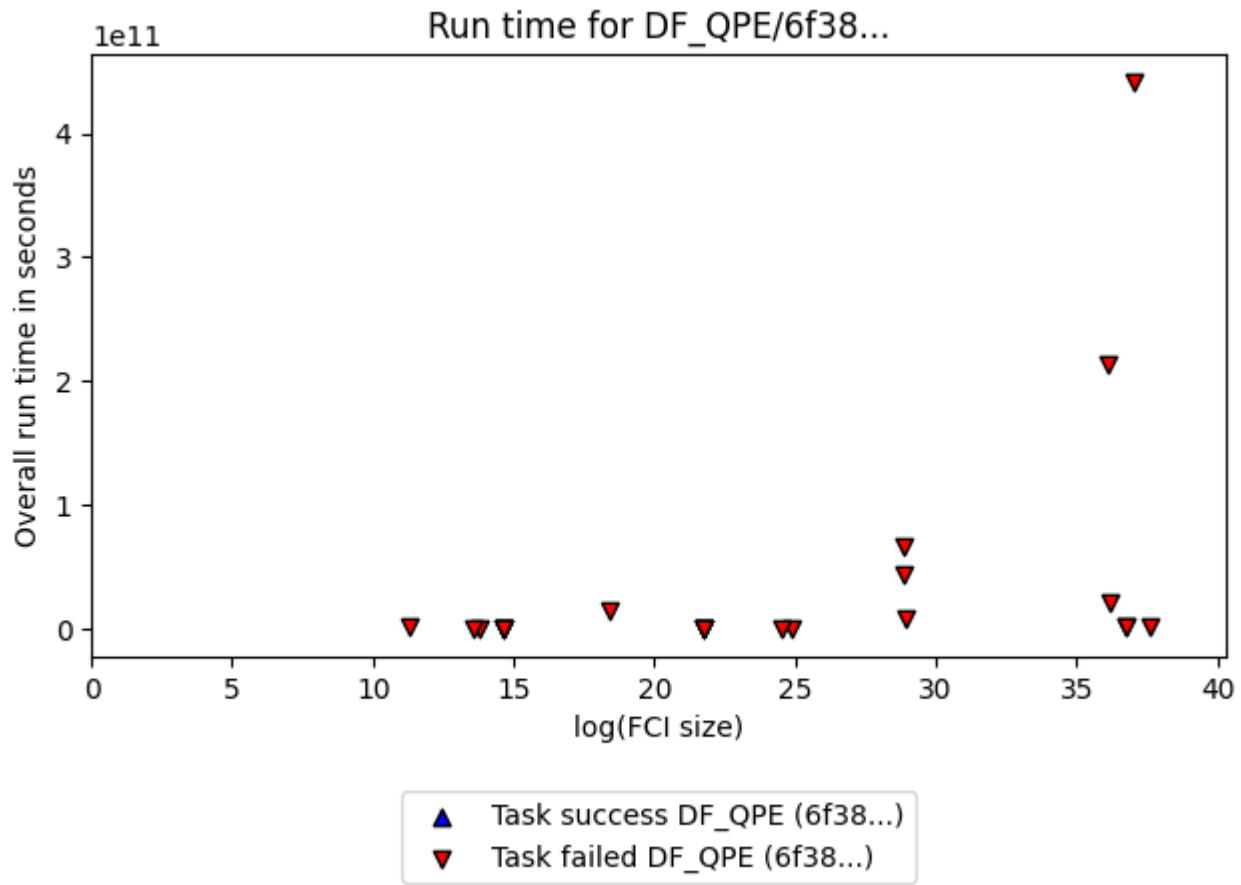
f1_score: None

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.

![Solver utility capture]supporting_artifacts/(solver_6f385080-934b-4cbb-b813-39c2cb61349e_utility_capture_plot.png)

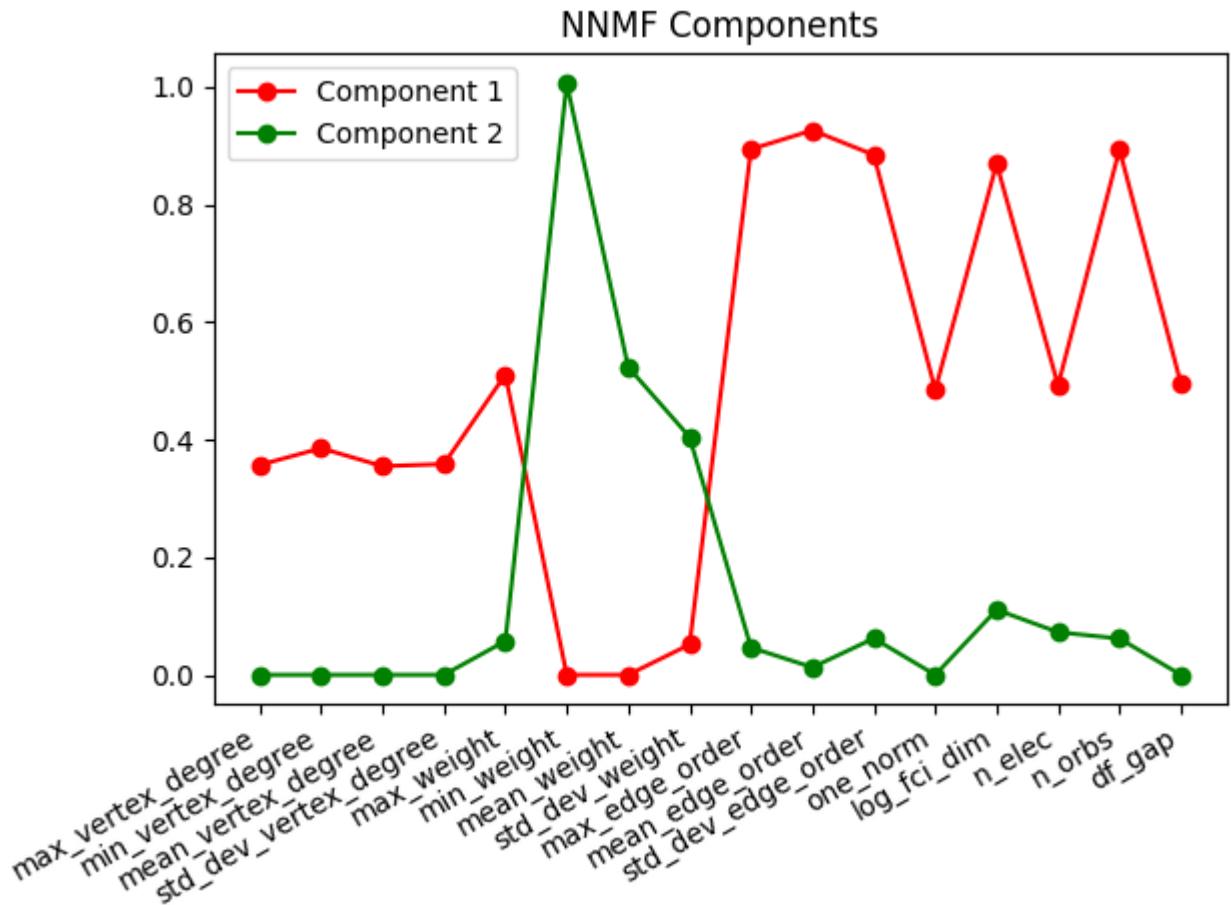
Solver PCA plot

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

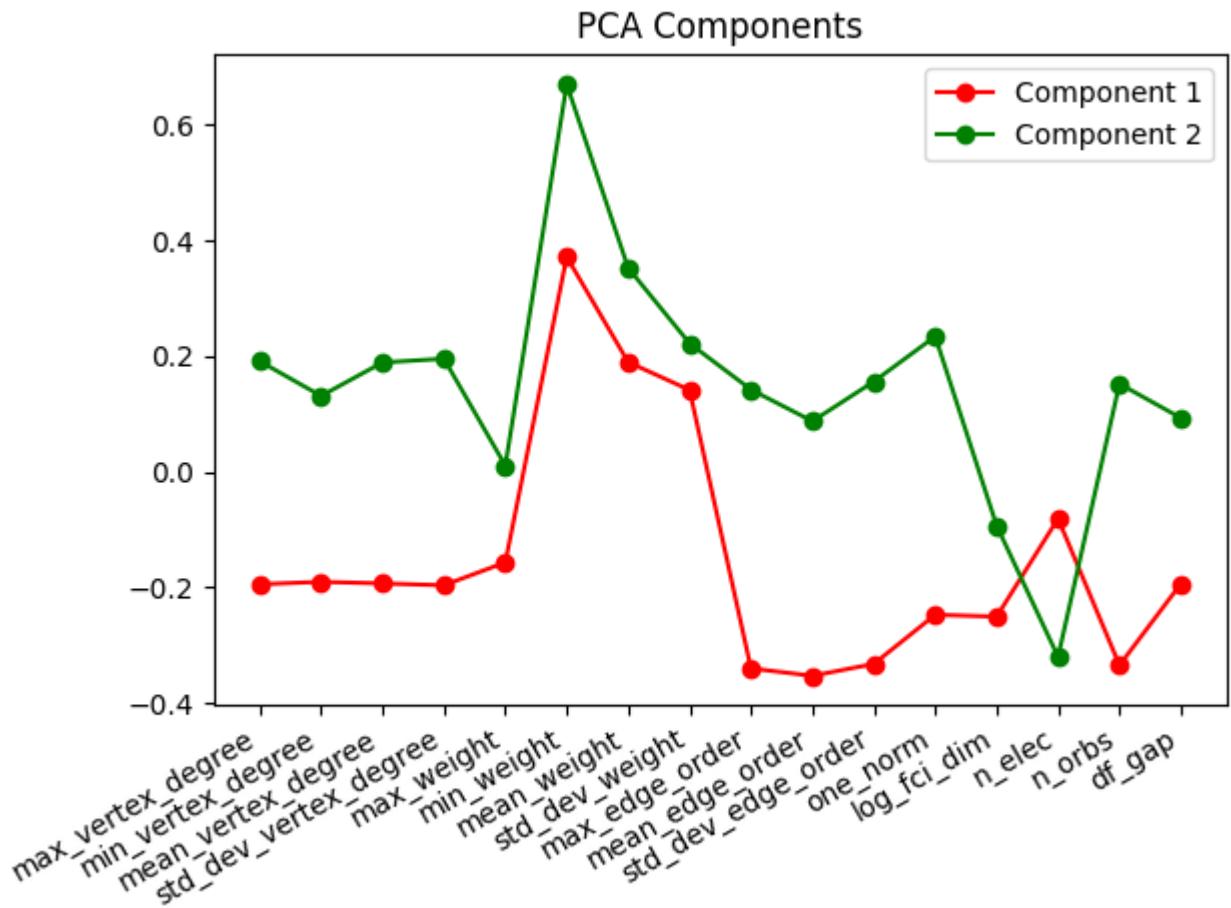
ML Feature Analysis



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: [0.35690922 0.38545468 0.35487749 0.35852601
0.51063391 0.0 0.0515893 0.89395573 0.92611292 0.88423213
0.48450204 0.86941452 0.49234596 0.89376327 0.49515561]

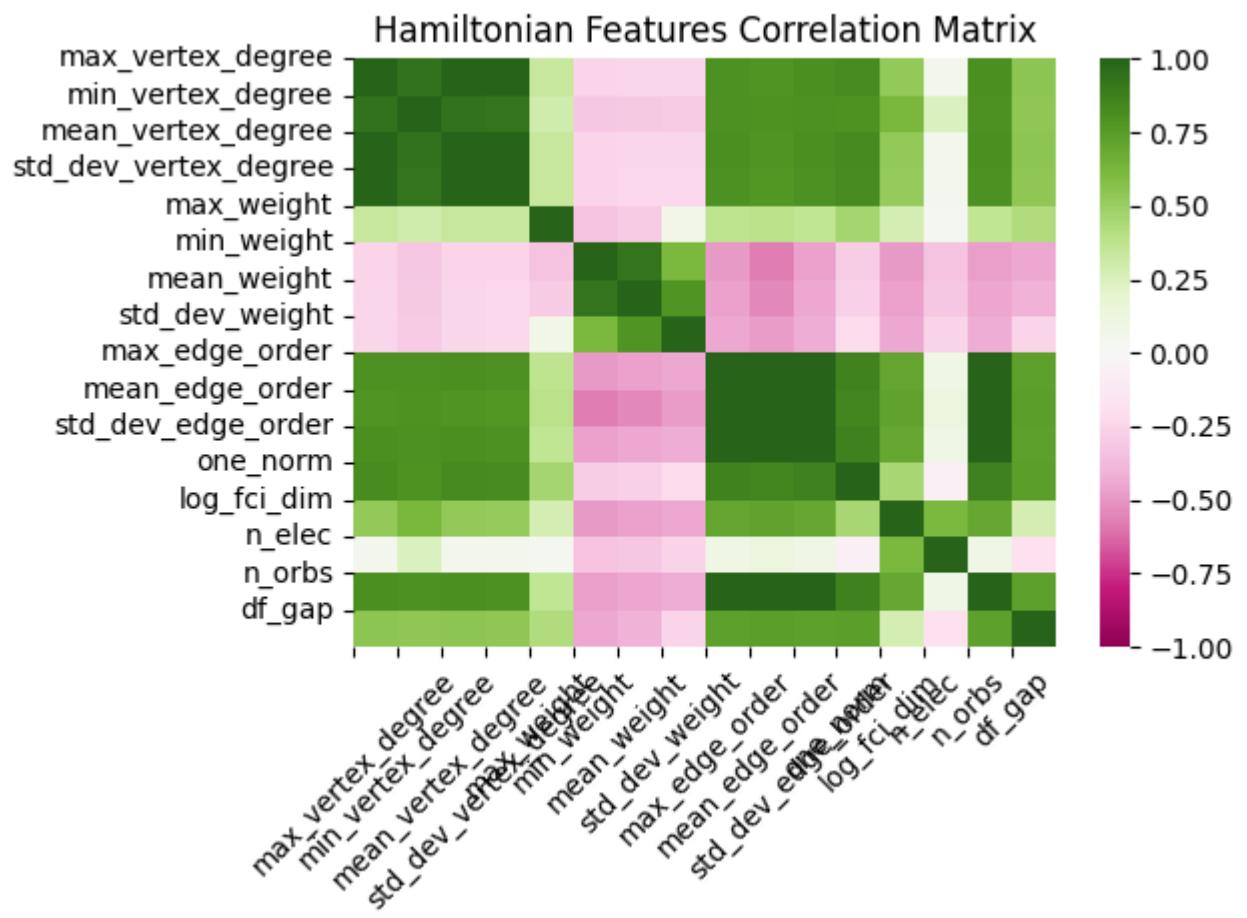
NNMF Component 2: [0. 0. 0. 0. 0.05747991 1.00601694 0.52355998
0.4045106 0.04642006 0.0127596 0.06203818 0. 0.11068966 0.07250786
0.06174321 0.]



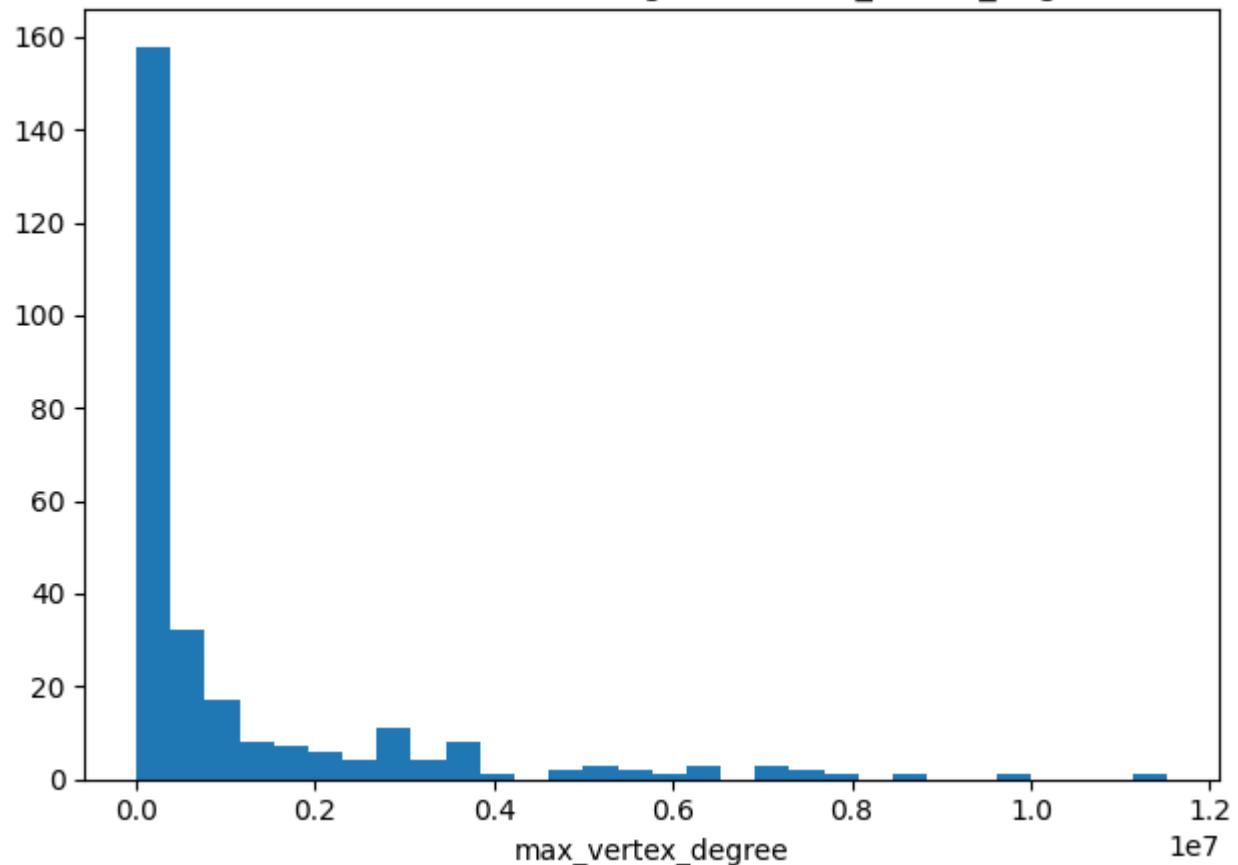
Features: ['max_vertex_degree', 'min_vertex_degree', 'mean_vertex_degree', 'std_dev_vertex_degree', 'max_weight', 'min_weight', 'mean_weight', 'std_dev_weight', 'max_edge_order', 'mean_edge_order', 'std_dev_edge_order', 'one_norm', 'log_fci_dim', 'n_elec', 'n_orbs', 'df_gap']

PCA Component 1: [-0.19469875 -0.1905585 -0.19330939 -0.19648849
 -0.15688445 0.37161153 0.18959114 0.14129338 -0.34024927 -0.35312811
 -0.33247843 -0.24744499 -0.25069969 -0.08107924 -0.33468266
 -0.19367631]

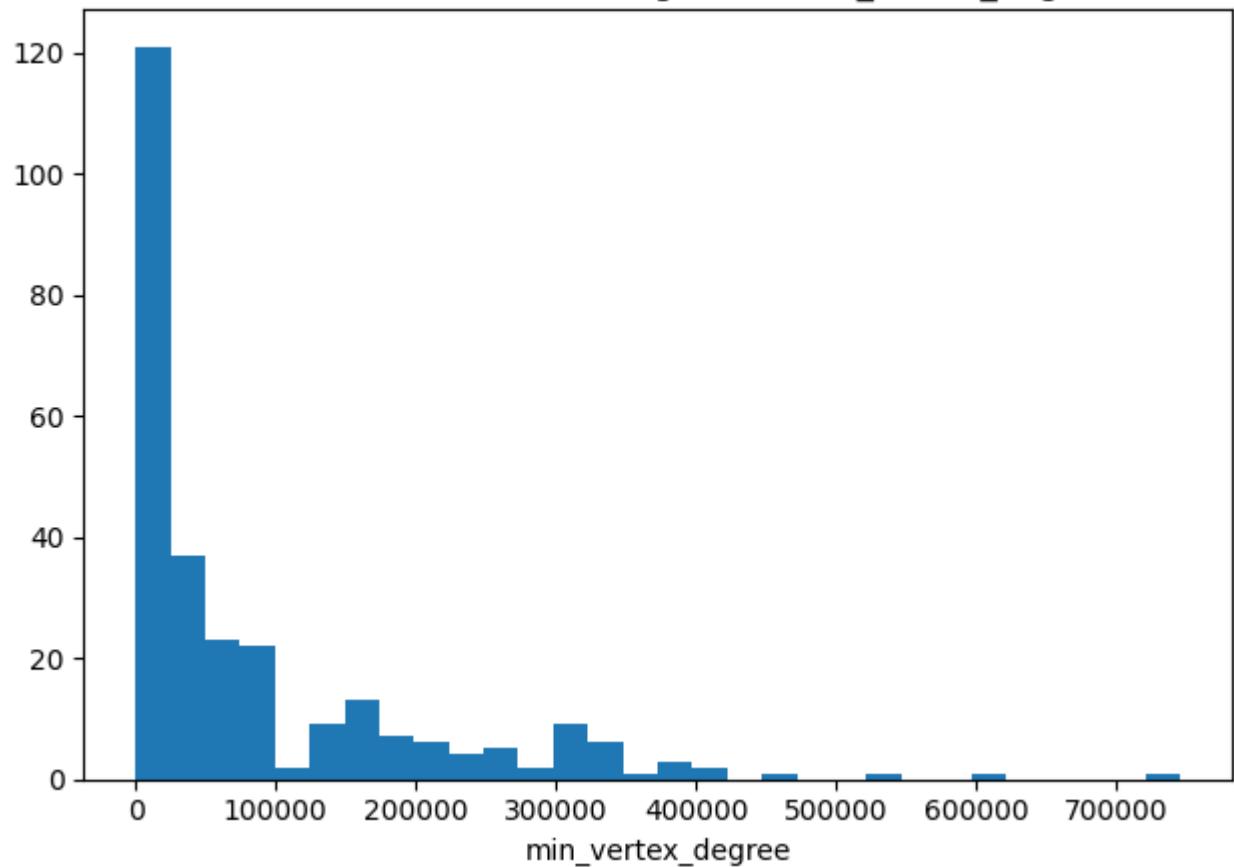
PCA Component 2: [0.19114047 0.13109532 0.18894197 0.19538013
 0.01054327 0.67004575 0.35245706 0.22194563 0.141961 0.08731617
 0.15593002 0.23400049 -0.09326605 -0.32024179 0.15208325 0.0928356]



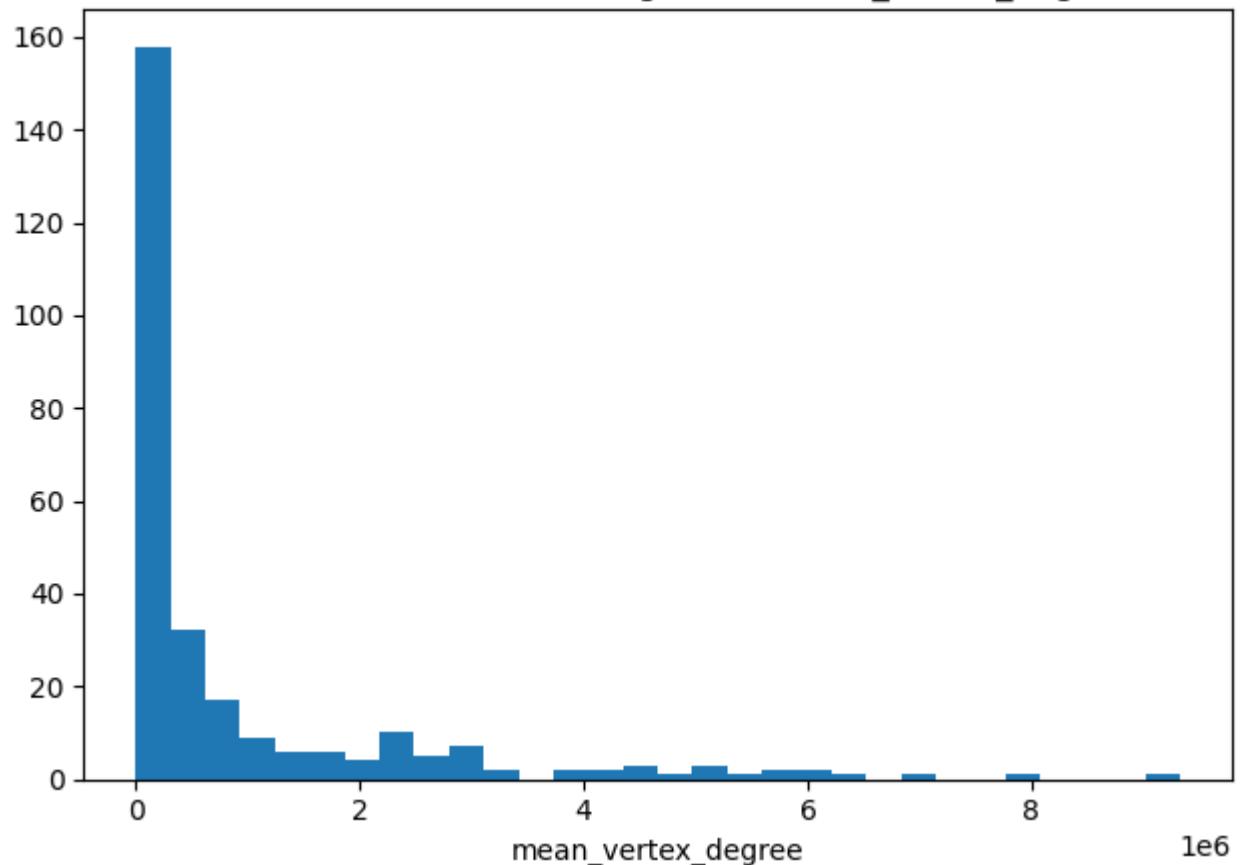
Hamiltonian features: histogram of max_vertex_degree



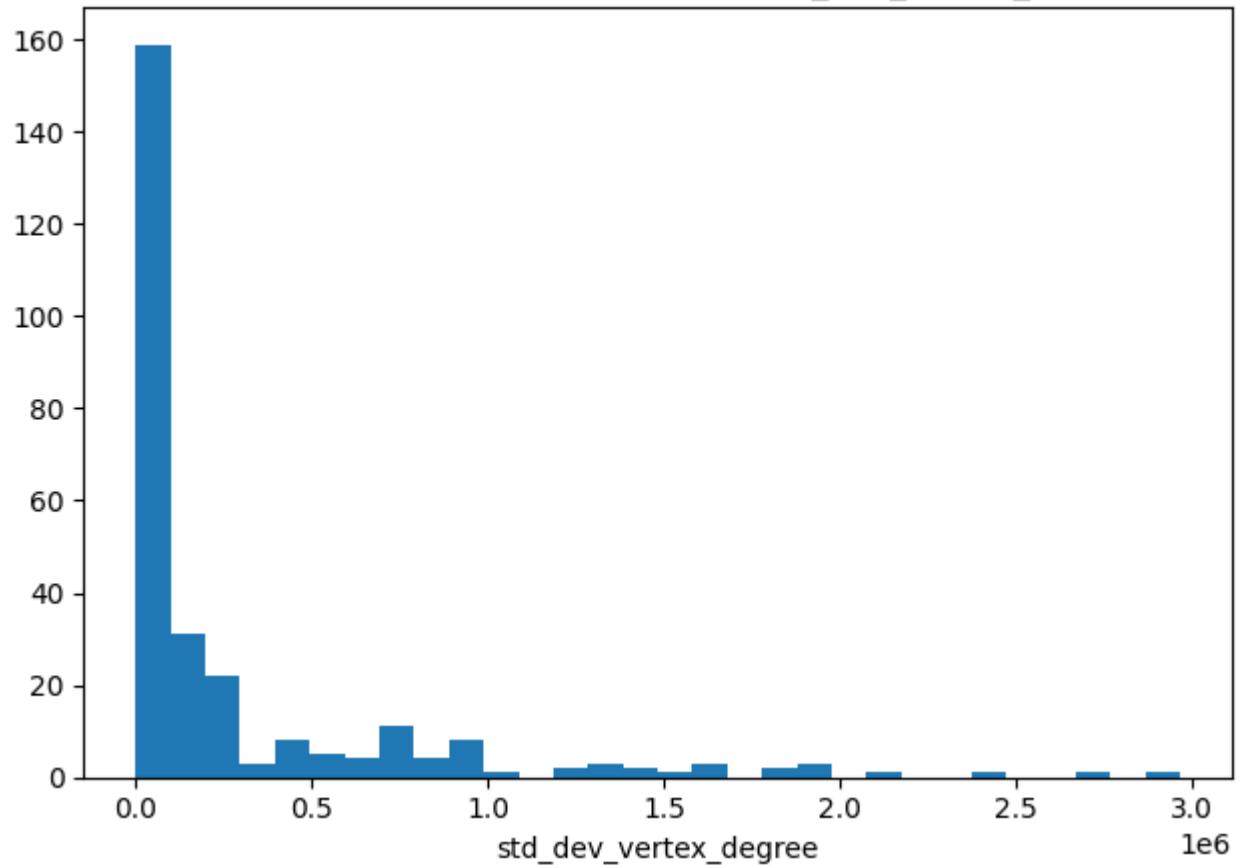
Hamiltonian features: histogram of min_vertex_degree



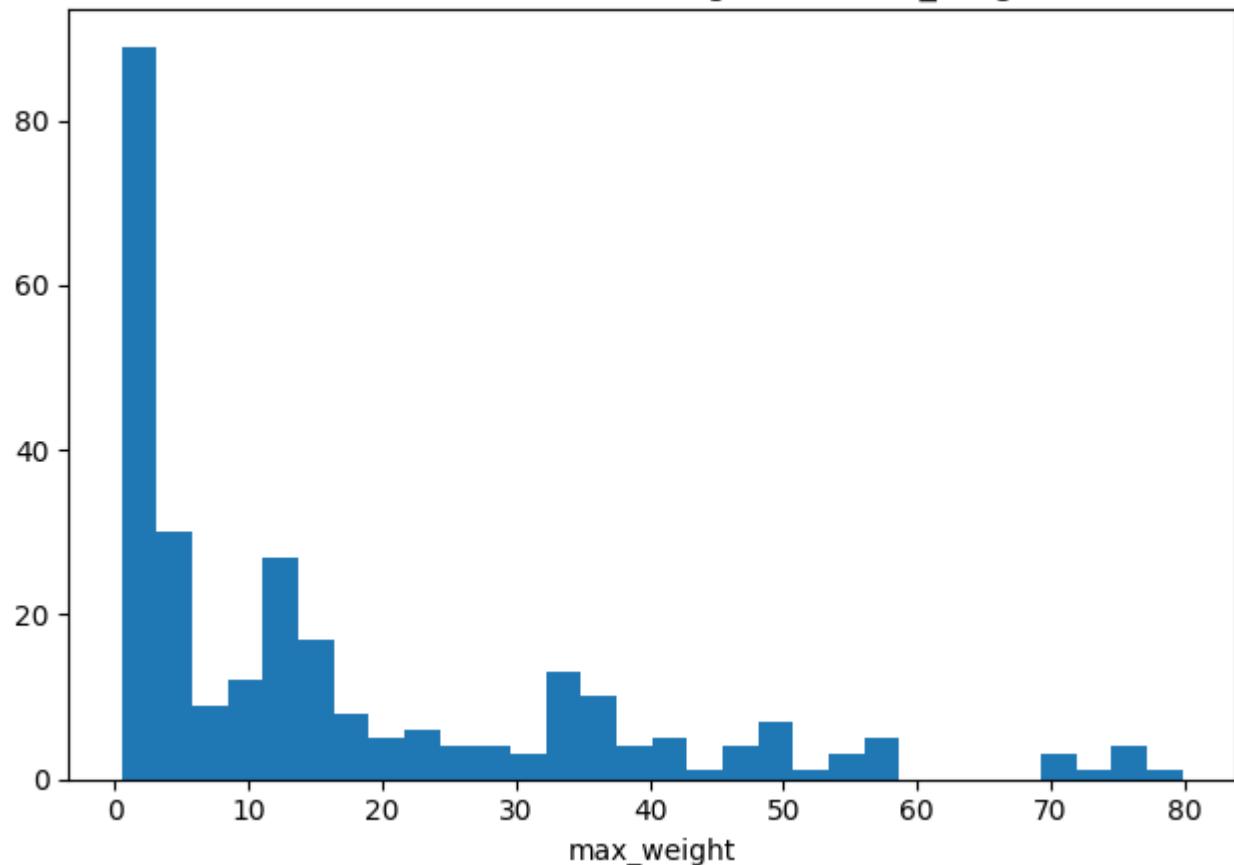
Hamiltonian features: histogram of mean_vertex_degree



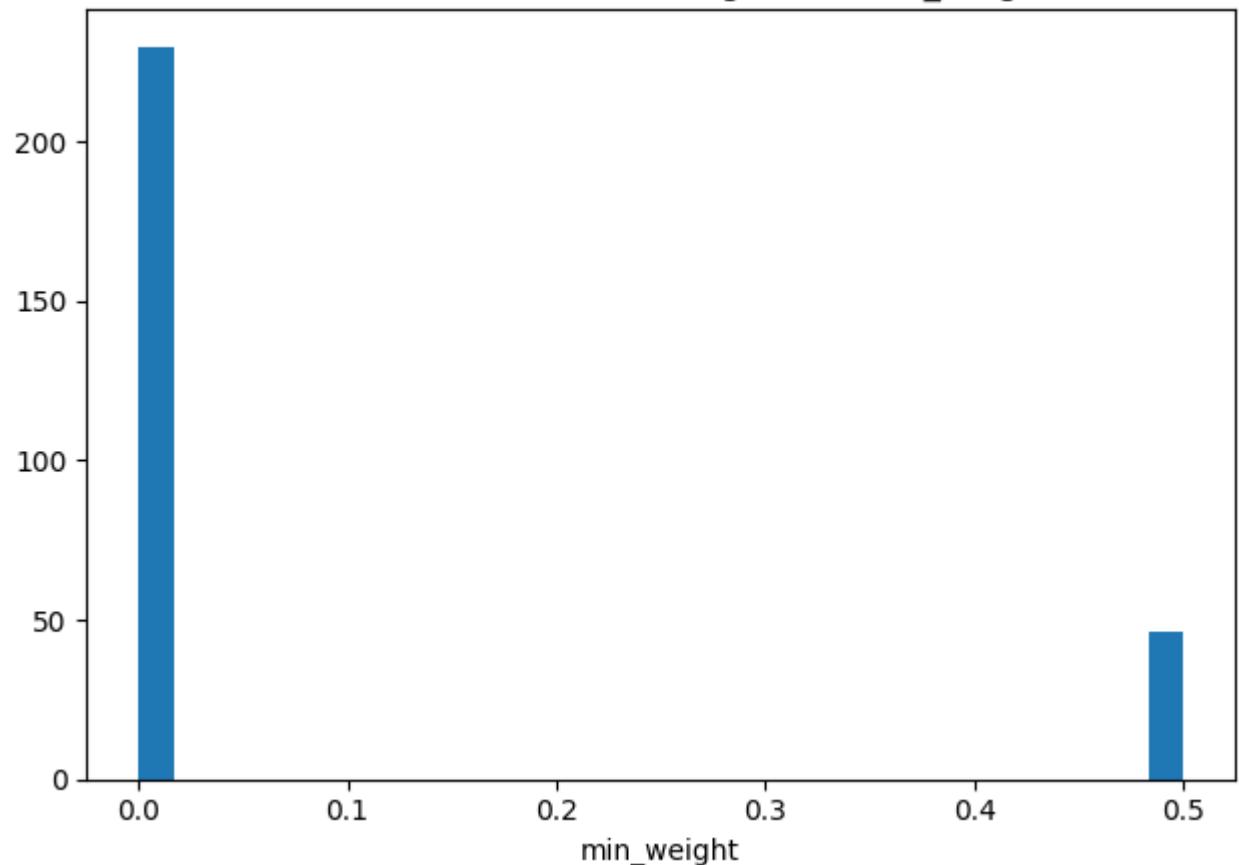
Hamiltonian features: histogram of std_dev_vertex_degree



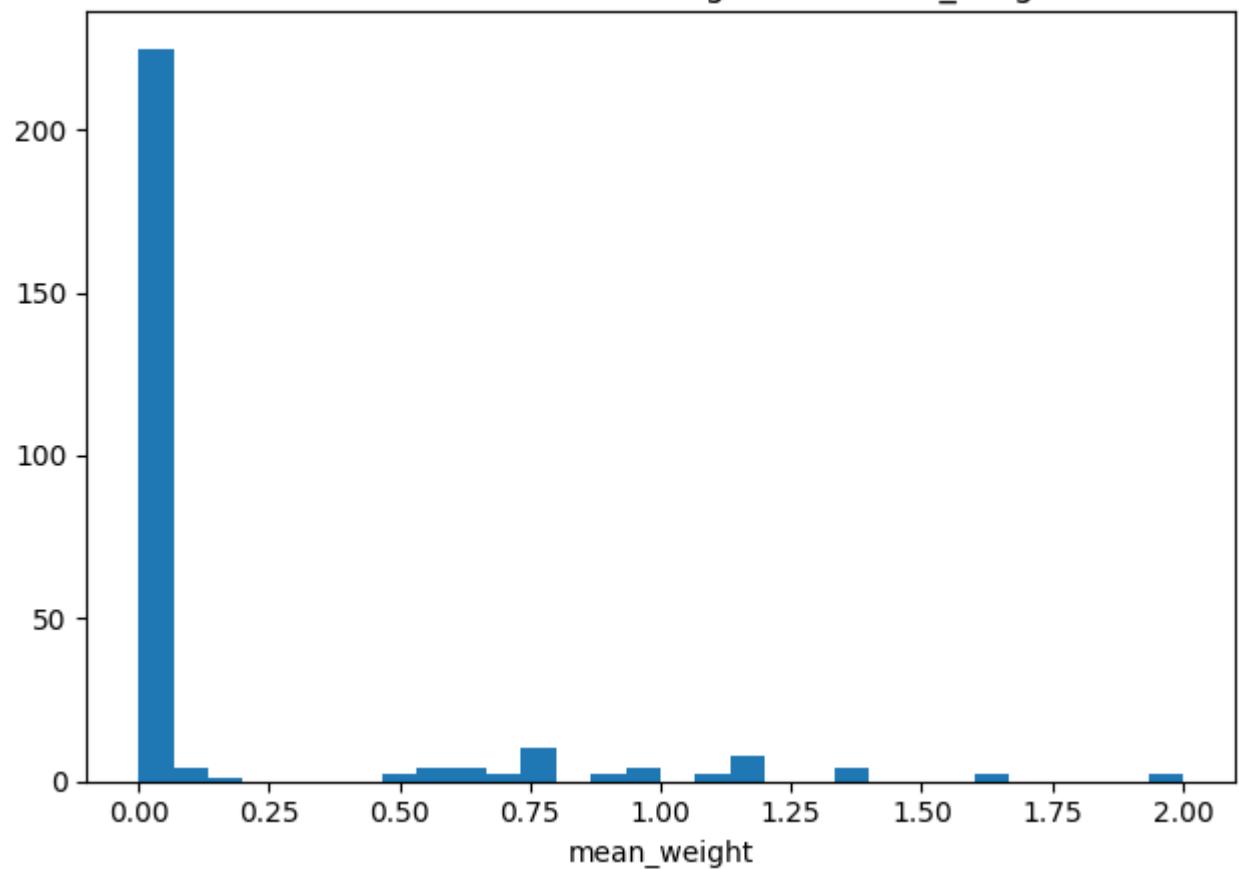
Hamiltonian features: histogram of max_weight



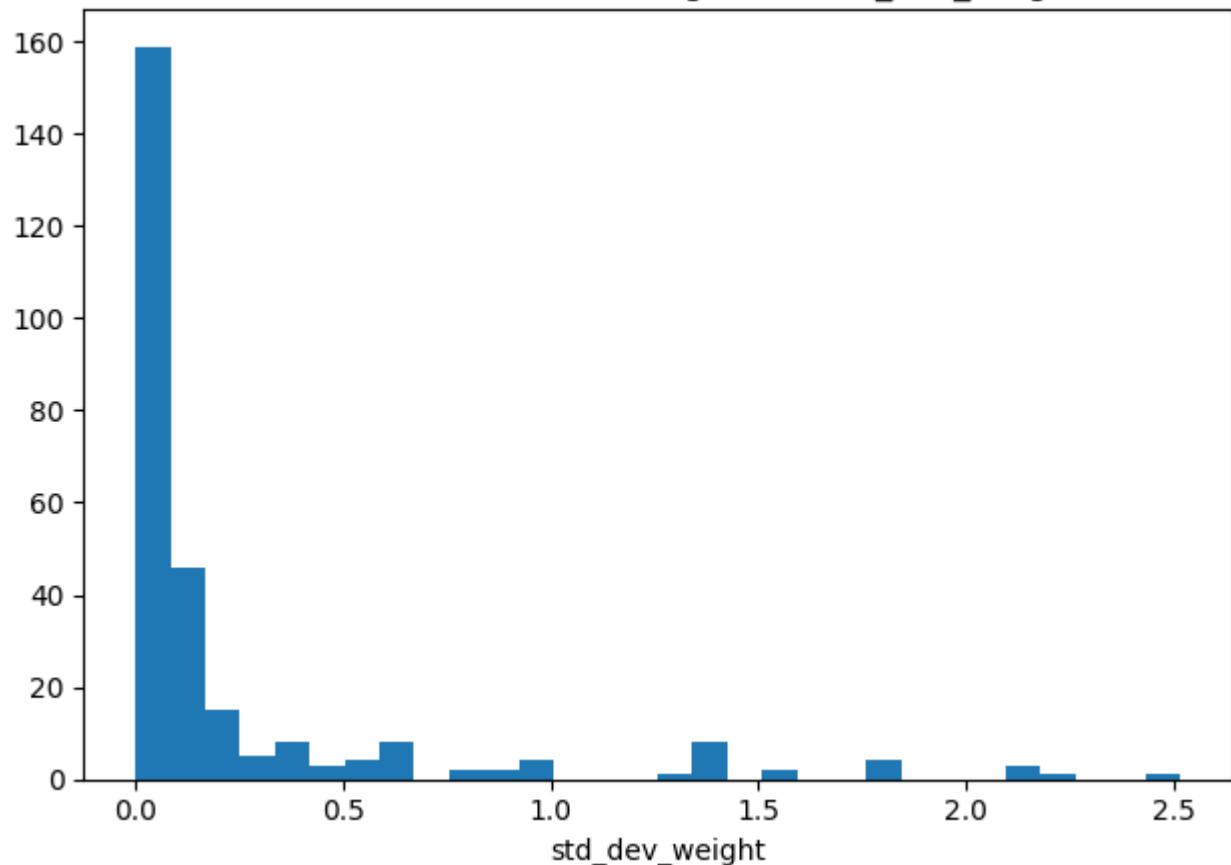
Hamiltonian features: histogram of min_weight



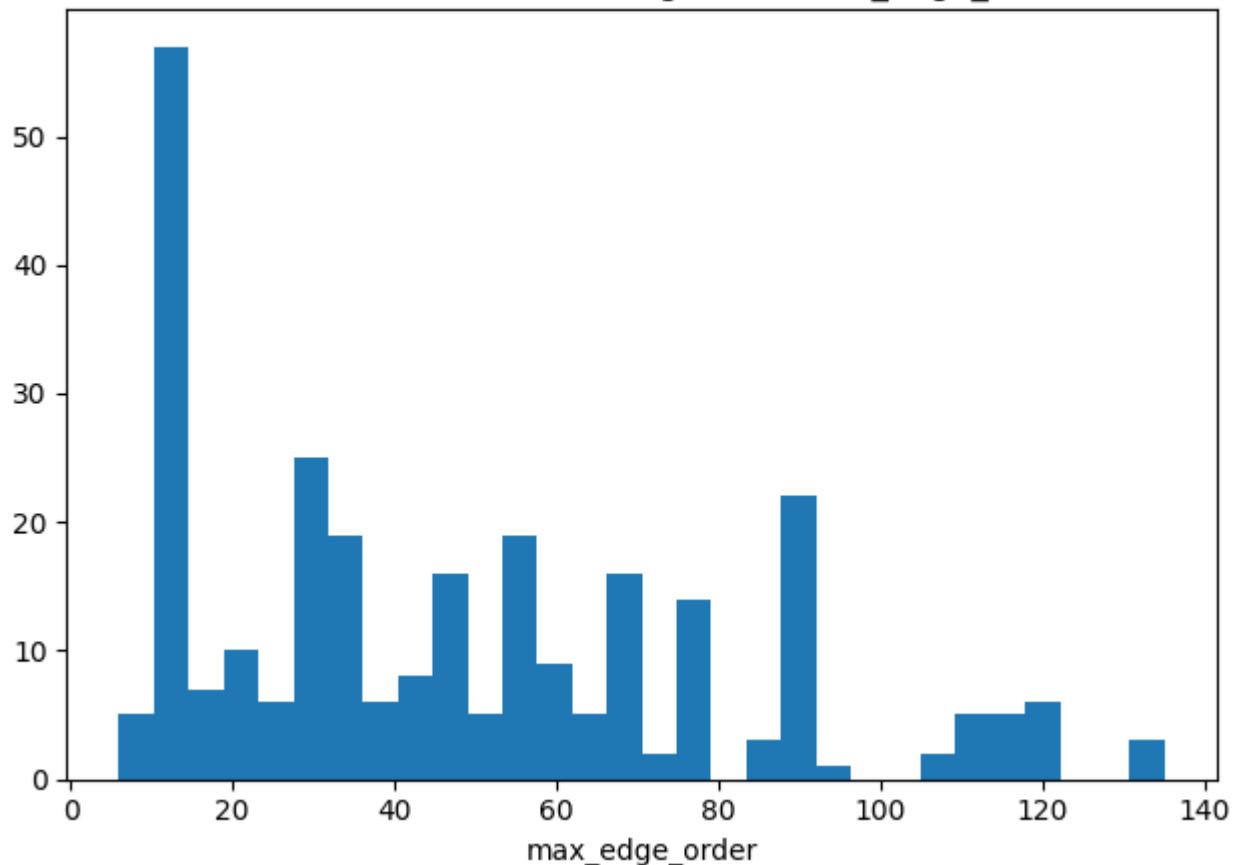
Hamiltonian features: histogram of mean_weight



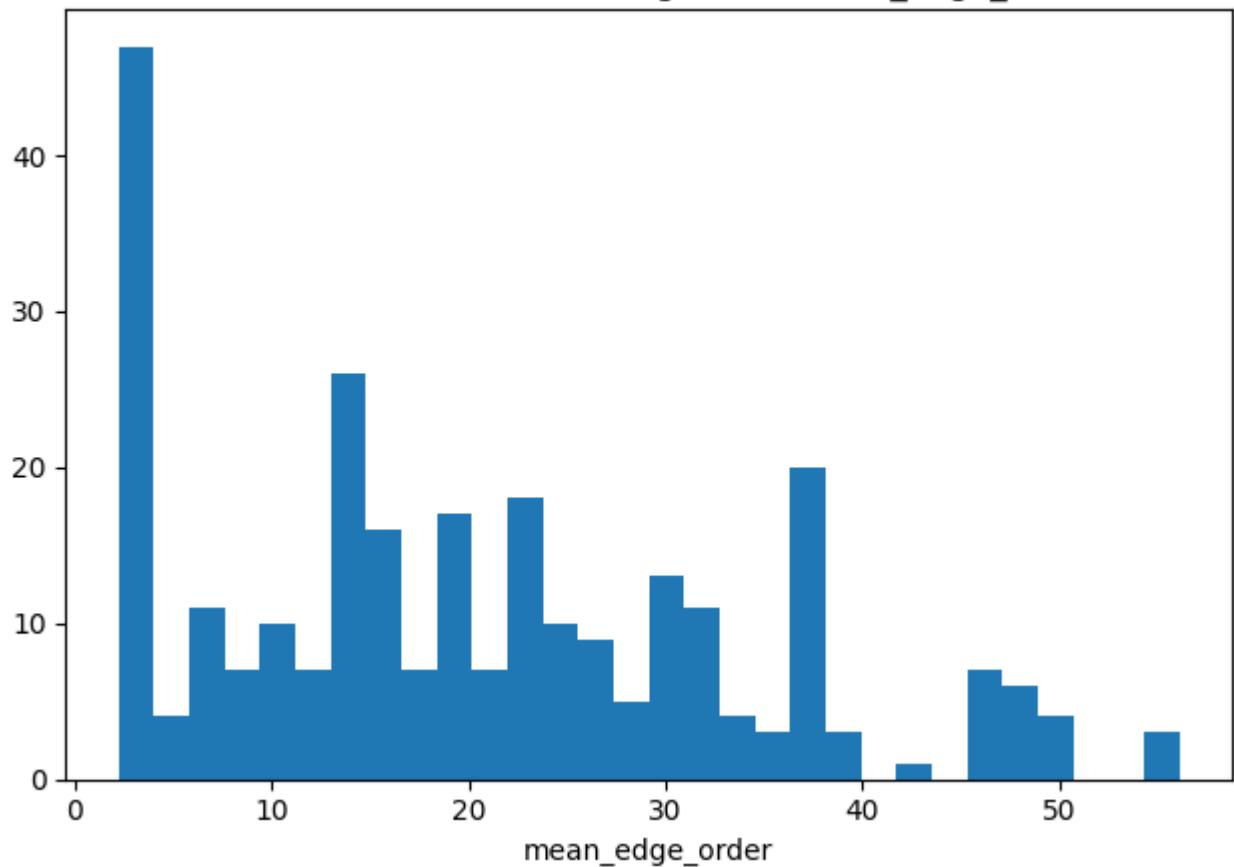
Hamiltonian features: histogram of std_dev_weight



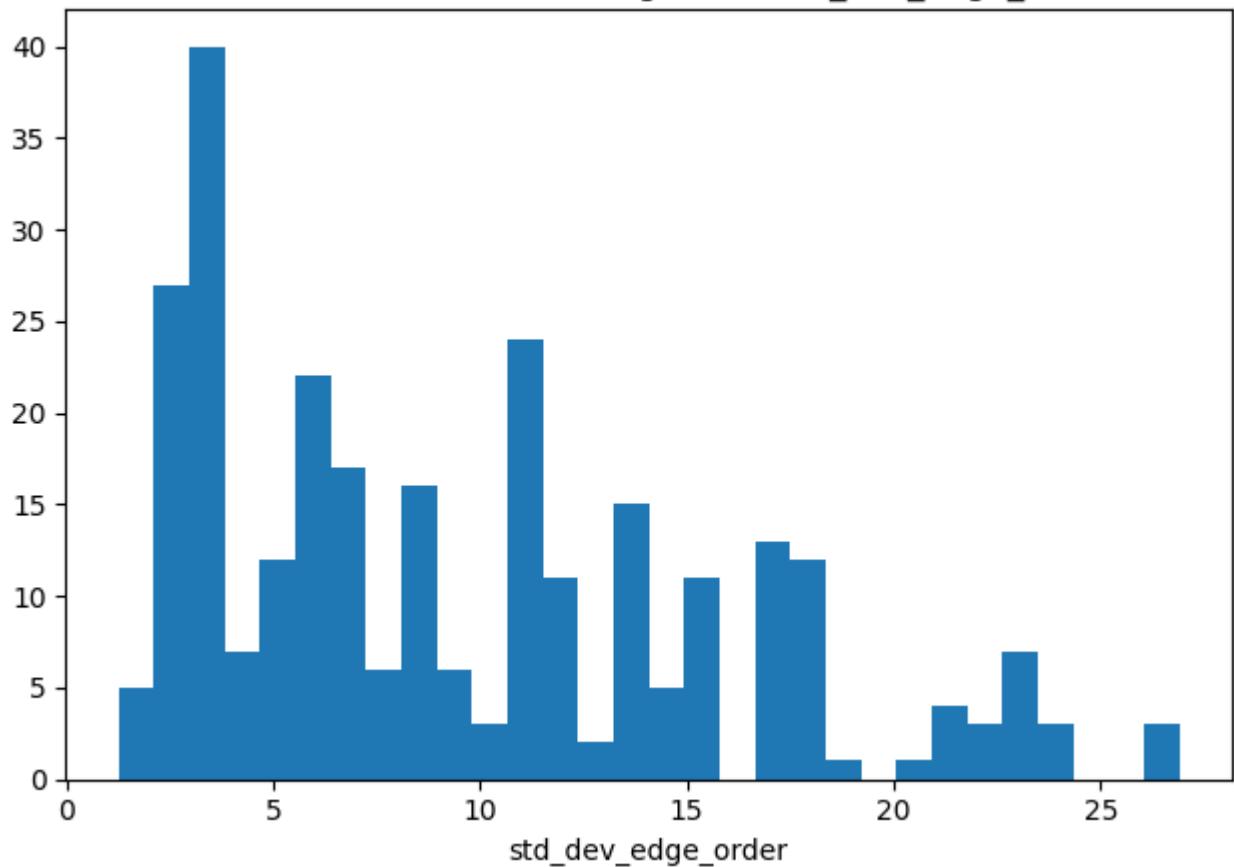
Hamiltonian features: histogram of max_edge_order



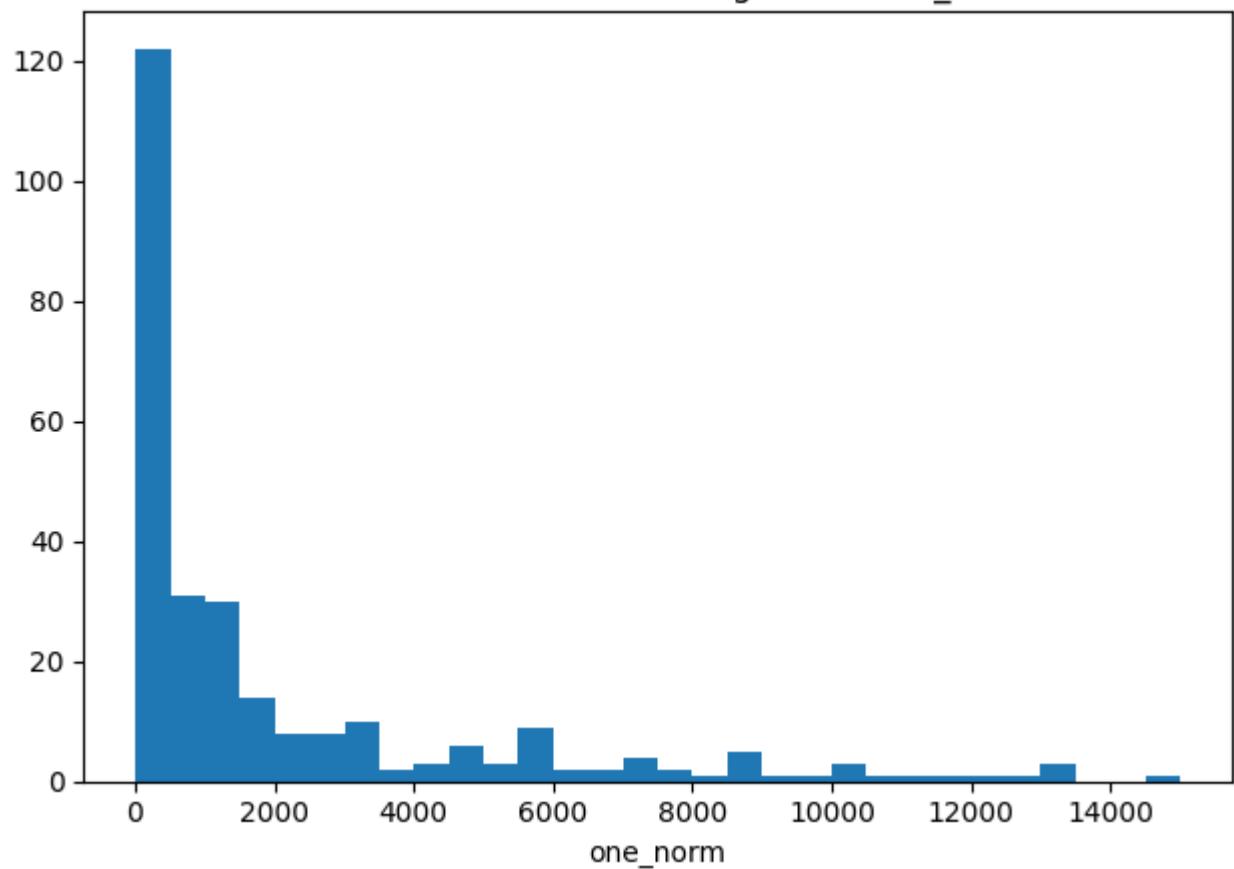
Hamiltonian features: histogram of mean_edge_order



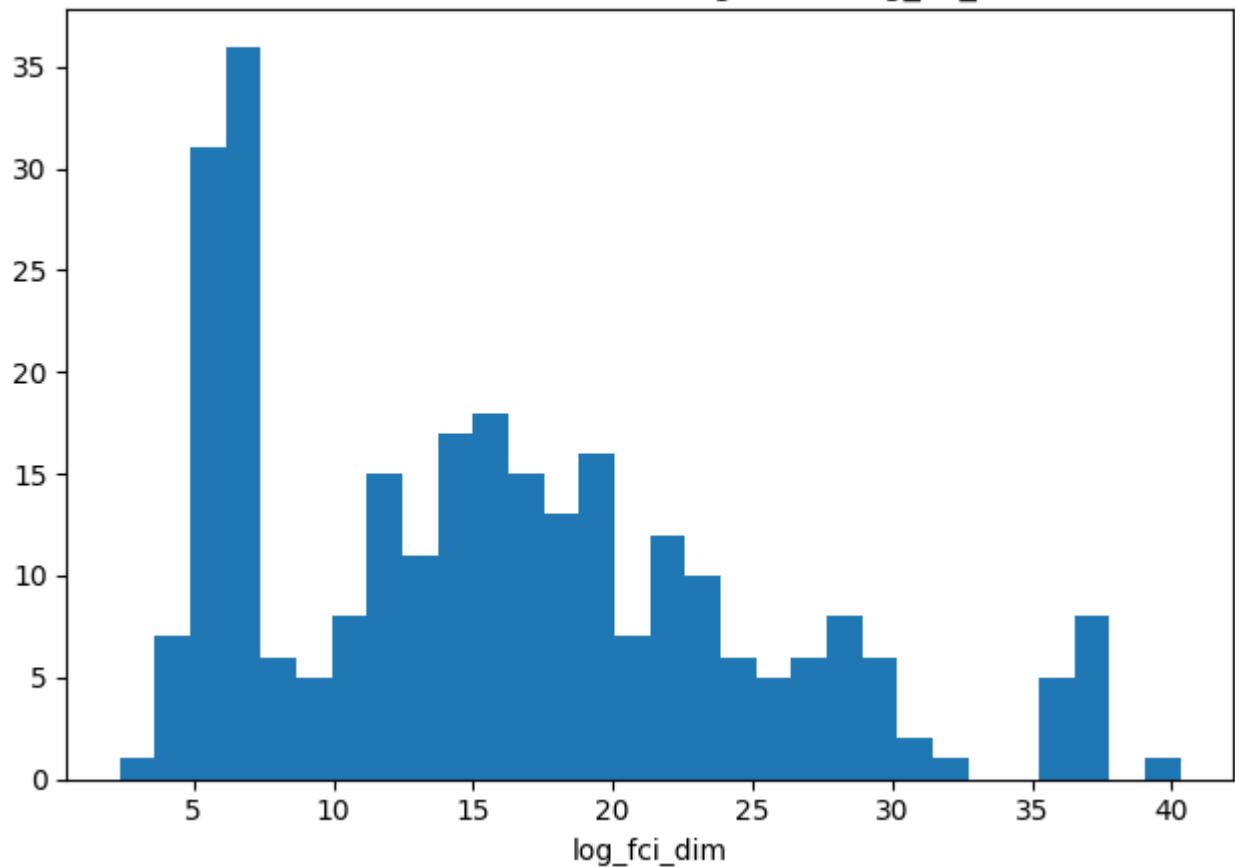
Hamiltonian features: histogram of std_dev_edge_order



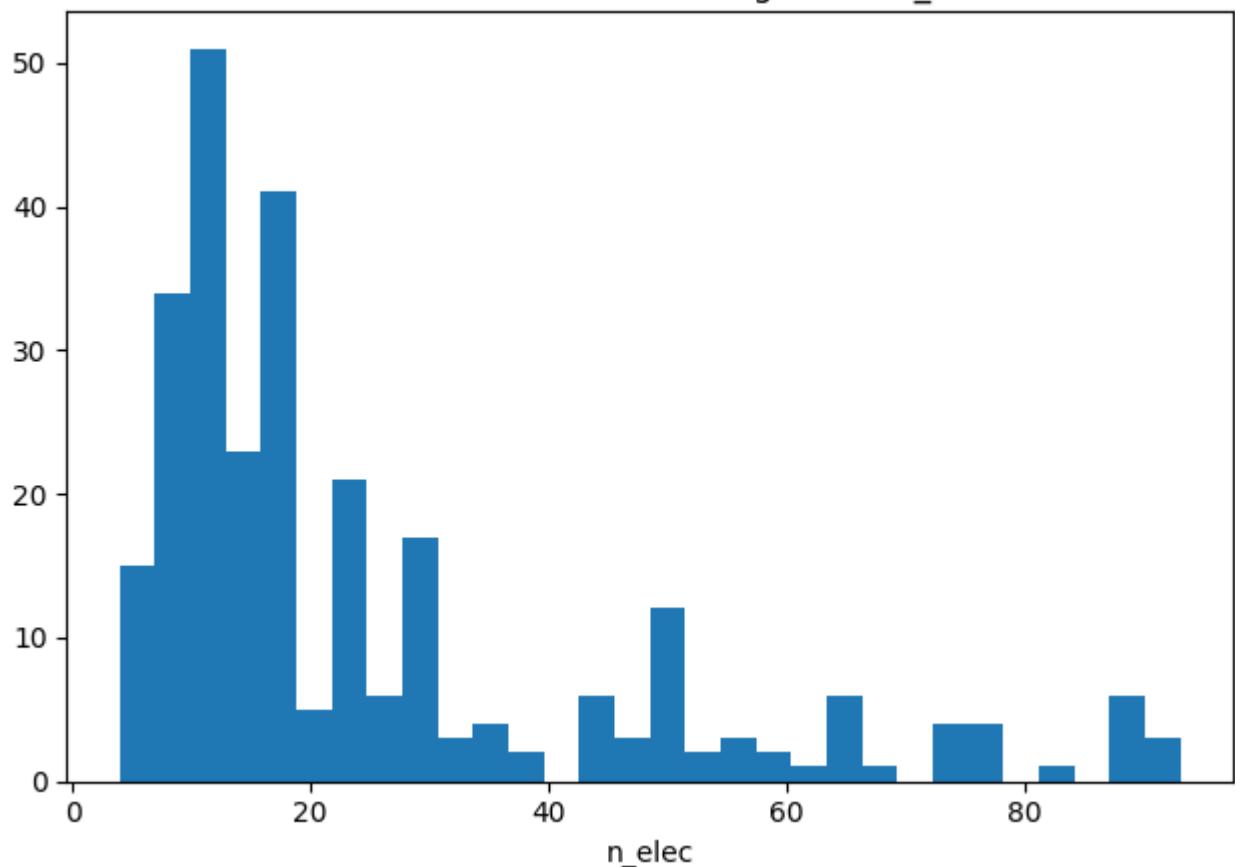
Hamiltonian features: histogram of one_norm



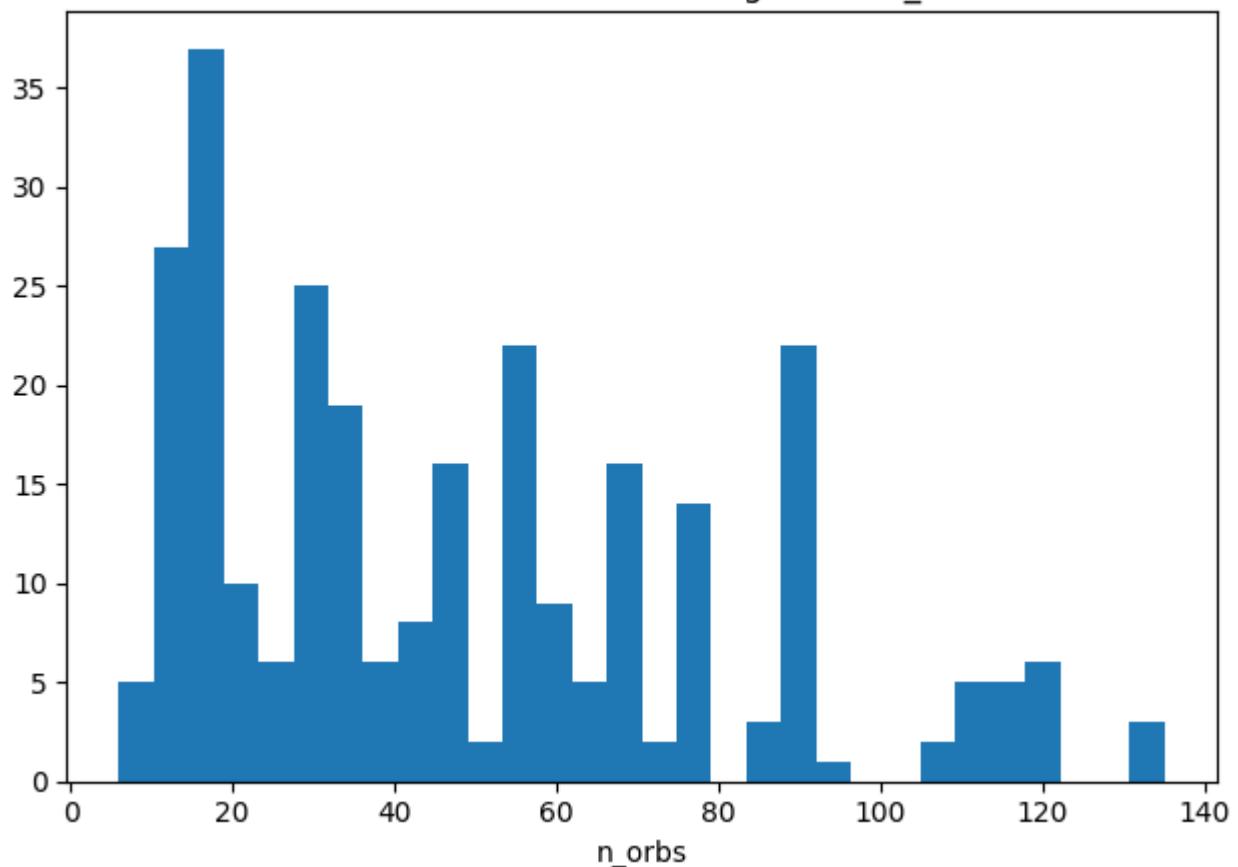
Hamiltonian features: histogram of log_fci_dim



Hamiltonian features: histogram of n_elec



Hamiltonian features: histogram of n_orbs



Hamiltonian features: histogram of df_gap

