GSEE Benchmark Standard Report

Report based on data from 2025-01-28T17:07:42.747013+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Tue Jan 28 11:45:36 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: Tue Jan 28 11:45:40 2025

Problem Instance Summary Statistics

number of `problem_instances`: 84.

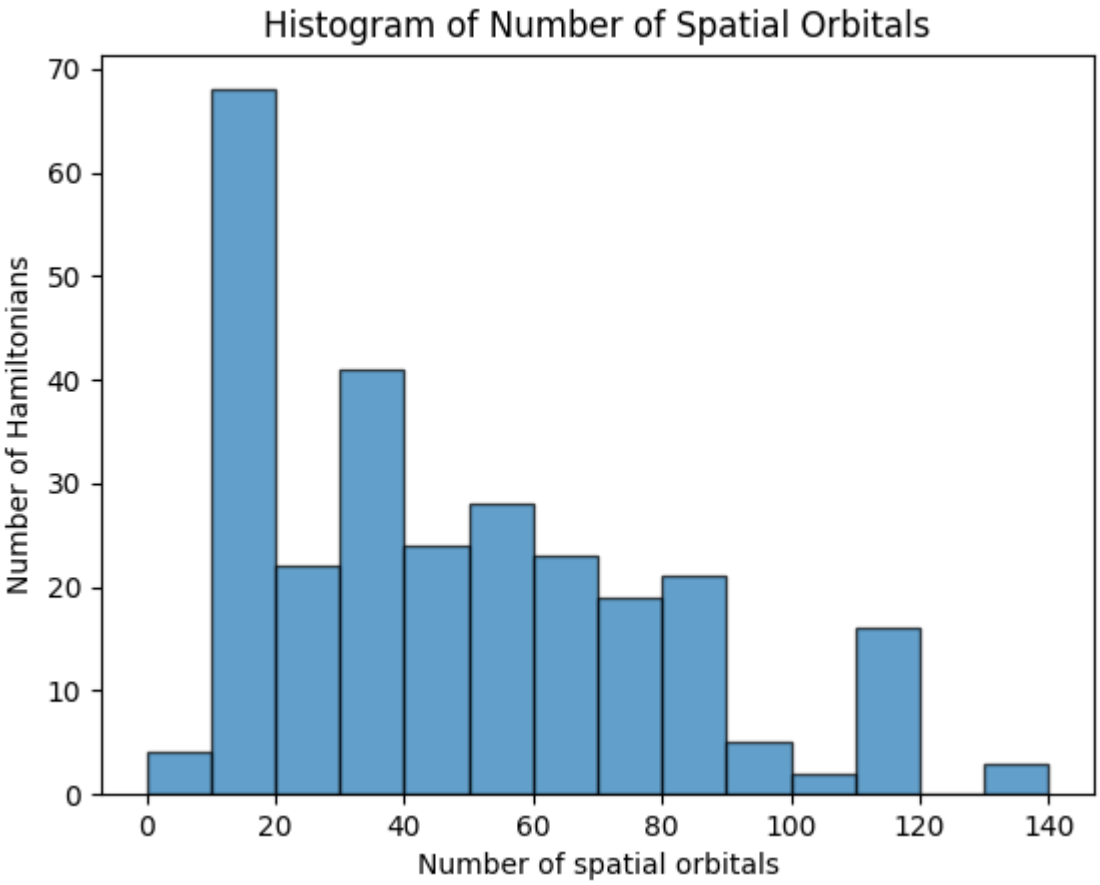
`problem_instance.json` with the most tasks: 30 (hubbard_square/614c4444-a31a-4348-b24d-01040208651c)

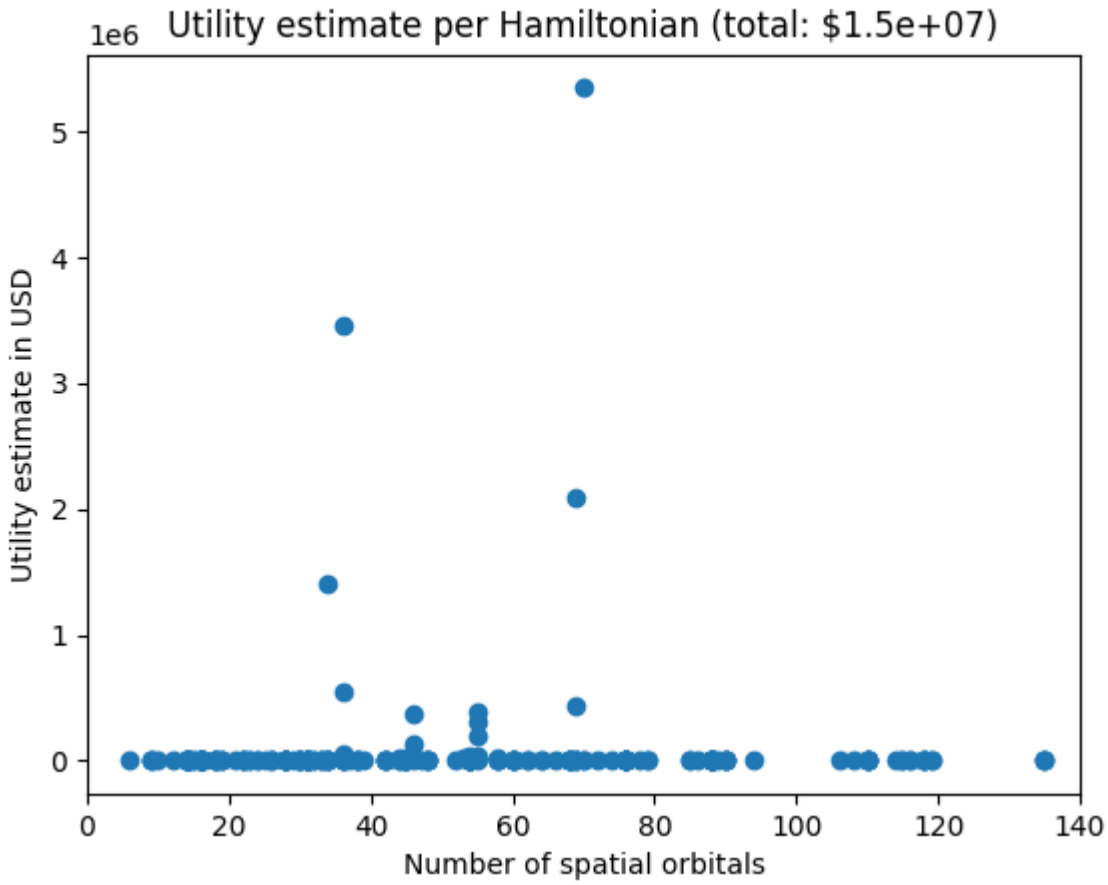
number of Hamiltonians (i.e., tasks) we have features calculated for: 276

minimum number of orbitals: 6

median number of orbitals: 42.0

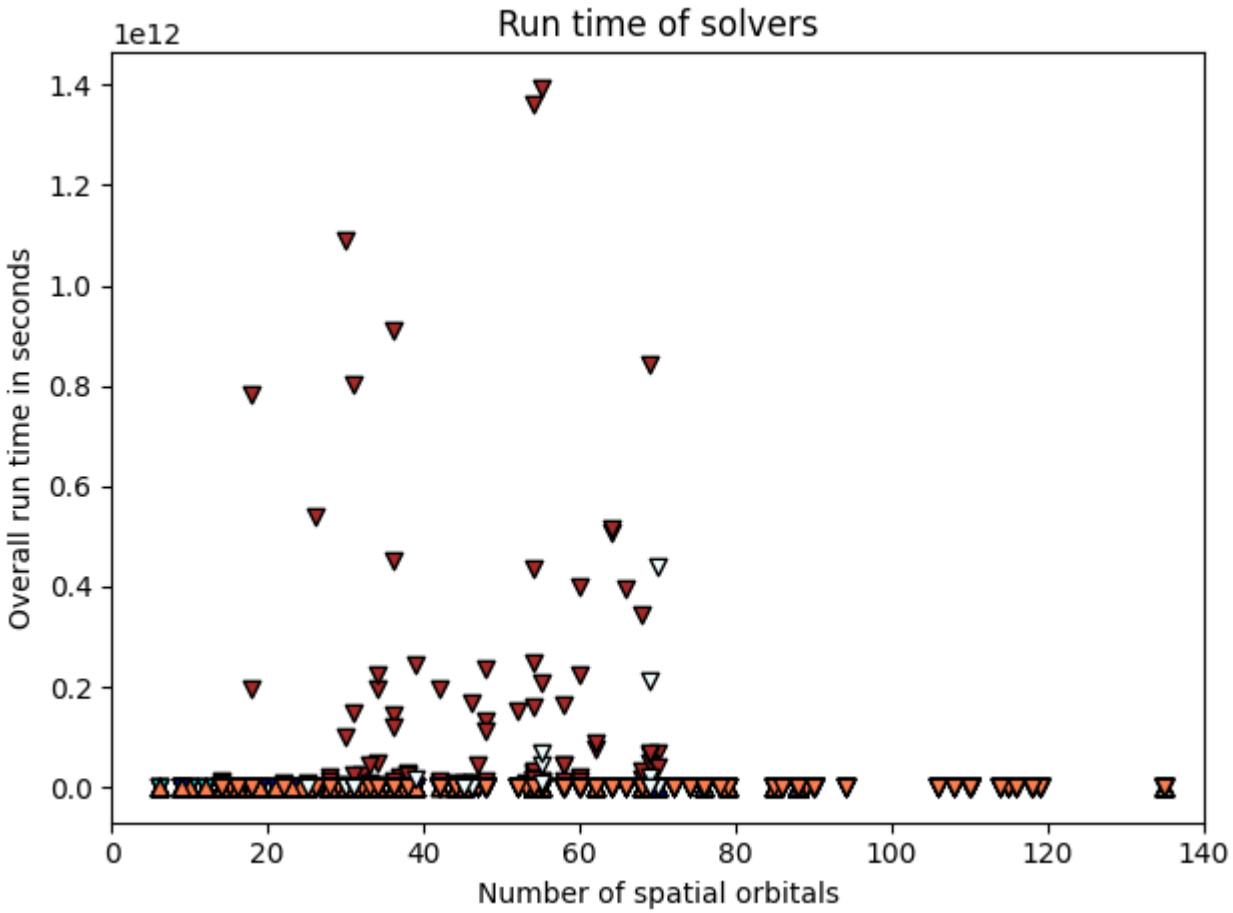
maximum number of orbitals: 135


Histogram of Number of Spatial Orbitals
Number of Hamiltonians
Number of spatial orbitals
0
10
20
30
40
50
60
70
0
20
40
60
80
100
120
140

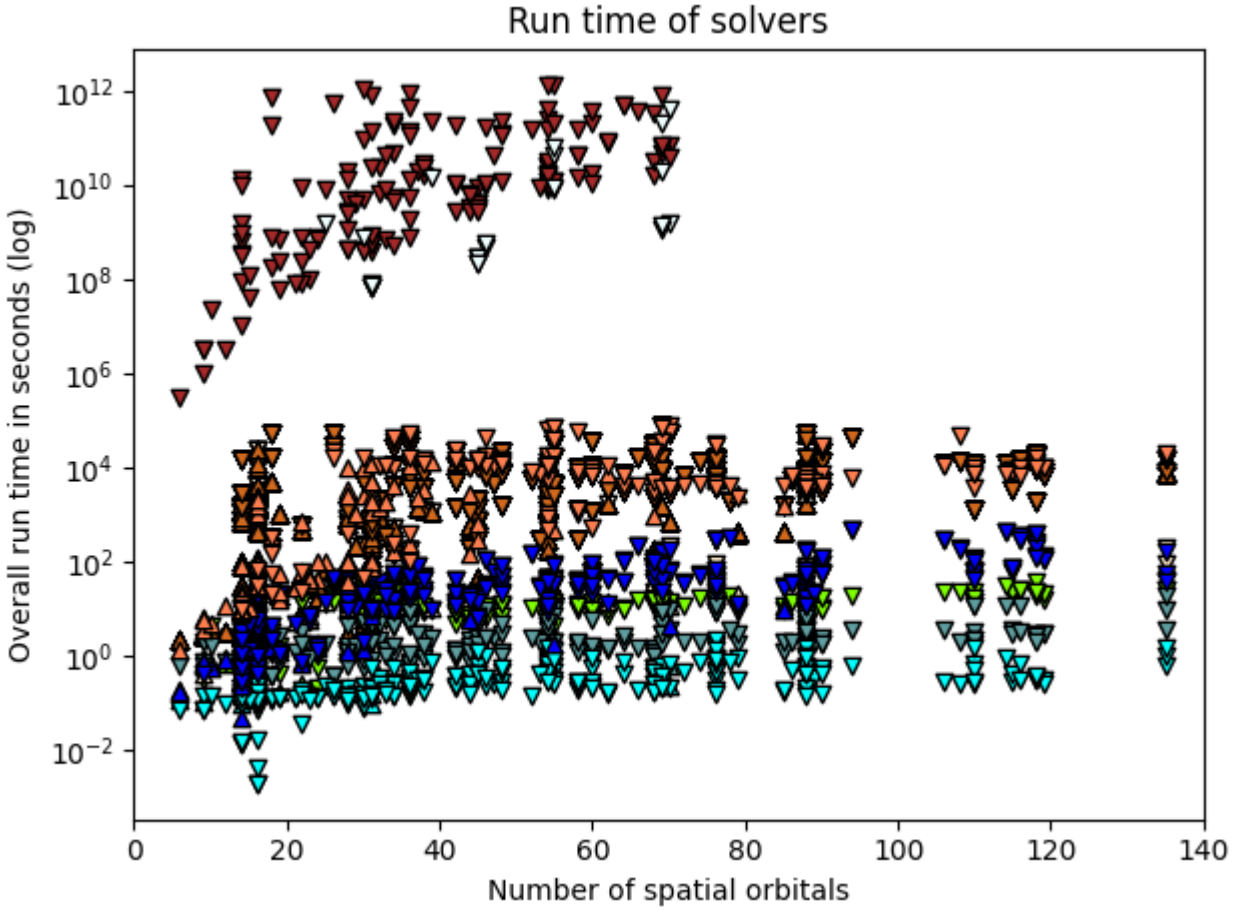


Solver Summary Statistics

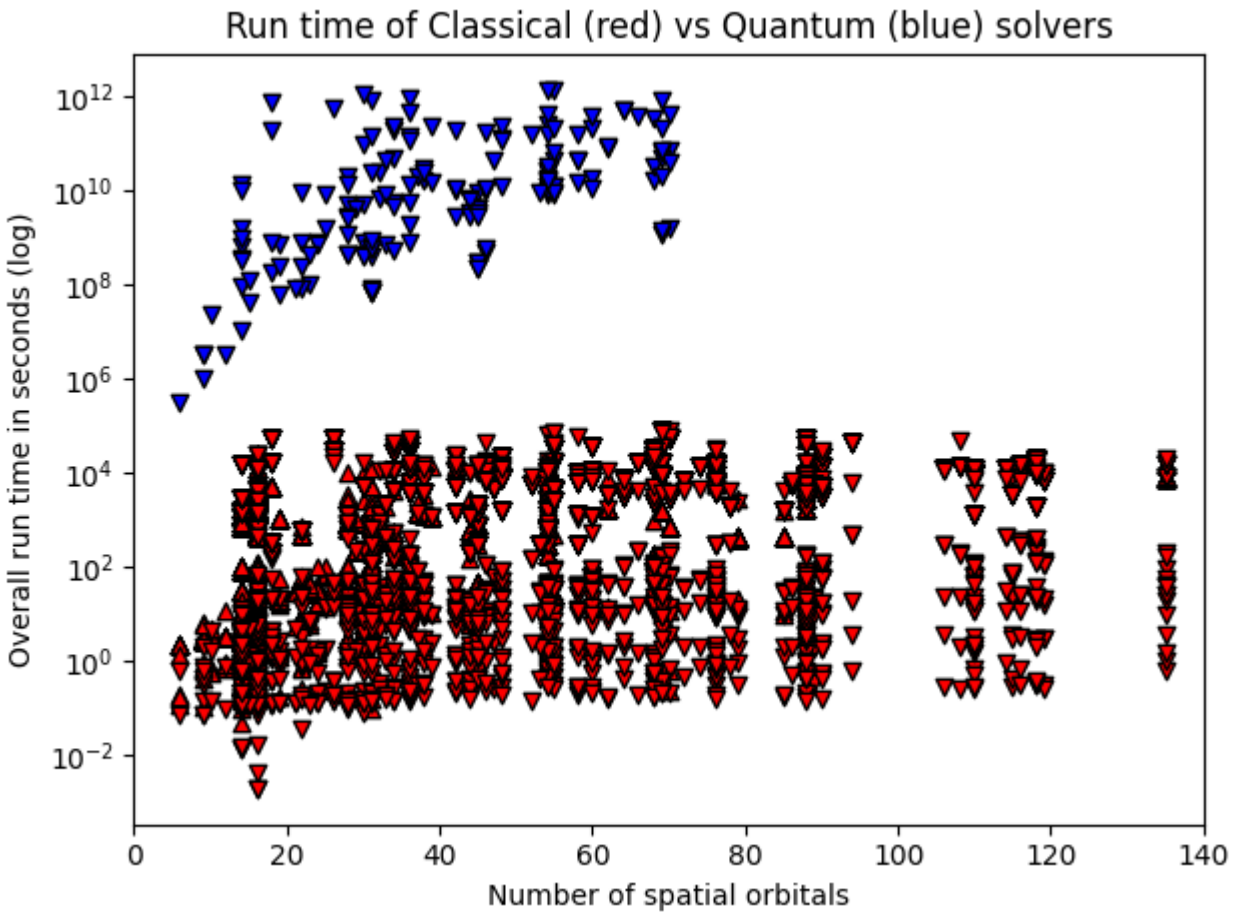
number of unique participating solvers: 17



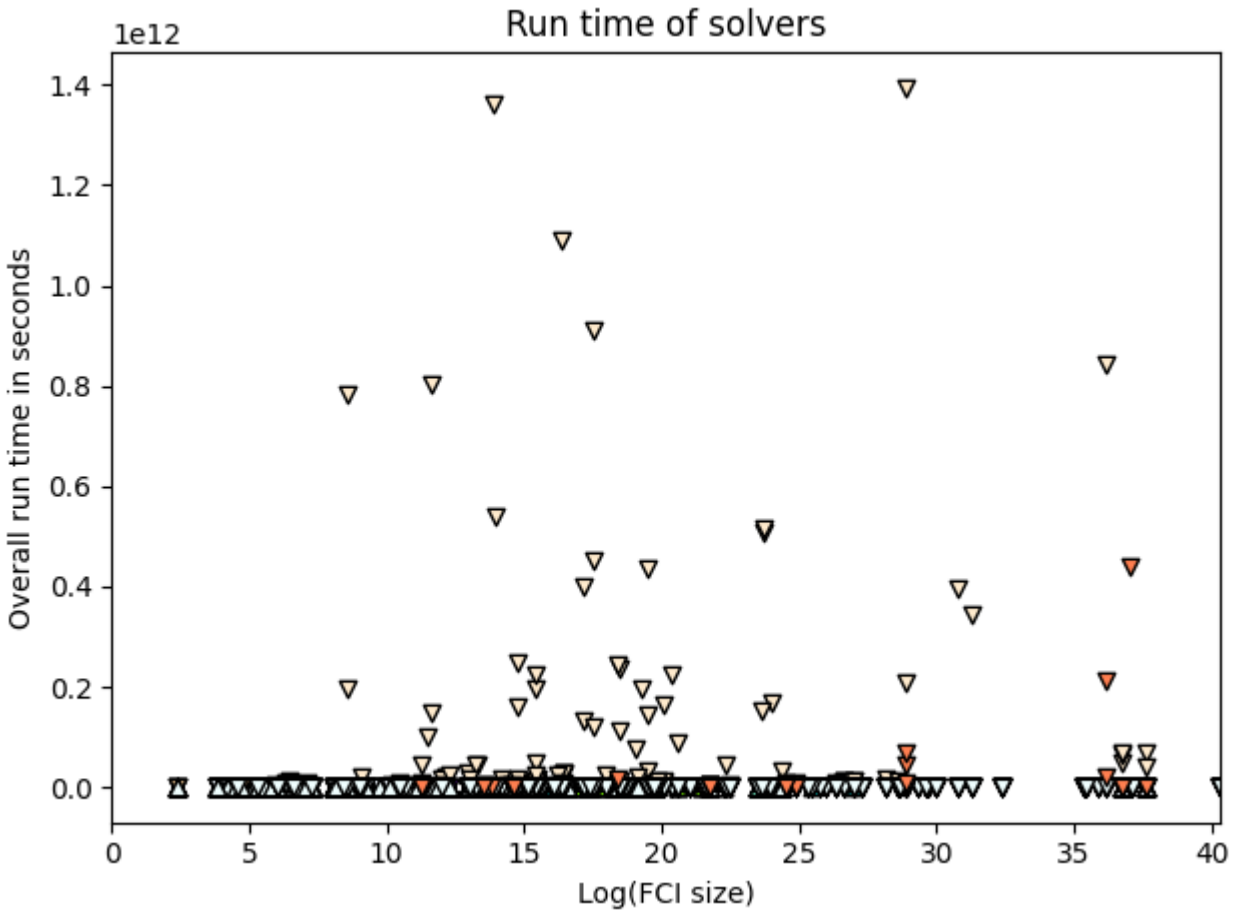
NOTE: only `attempted` tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.



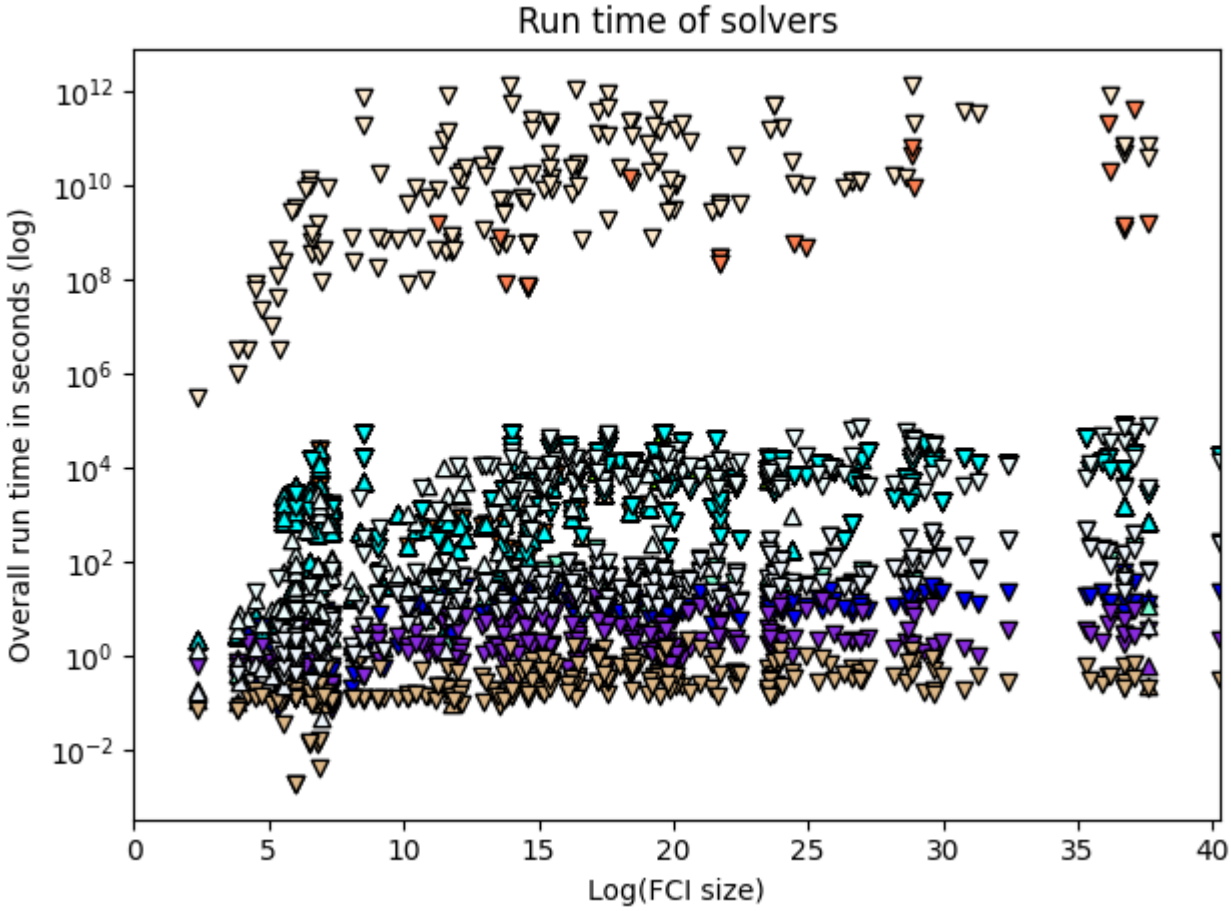
NOTE: only `attempted` tasks are plotted on the chart. Triangle up/down indicates solved/unsolved.



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



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 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: 7adbdf90-dbaa-467f-b454-29336d2a218b

creation_timestamp: 2025-01-28T17:07:42.747013+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

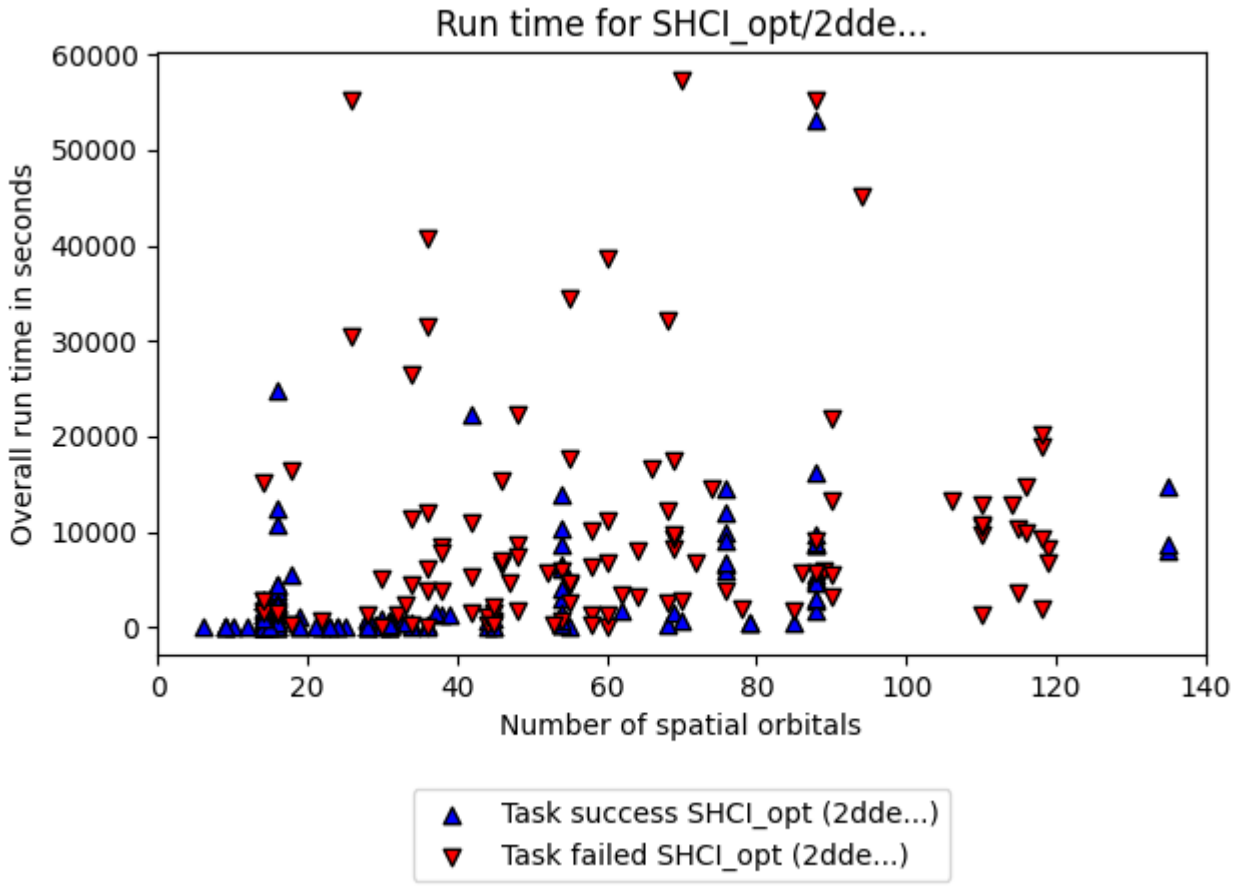
max_run_time_of_attempted_tasks: 57334.2

sum_of_run_time_of_attempted_tasks: 1553340.6179999998

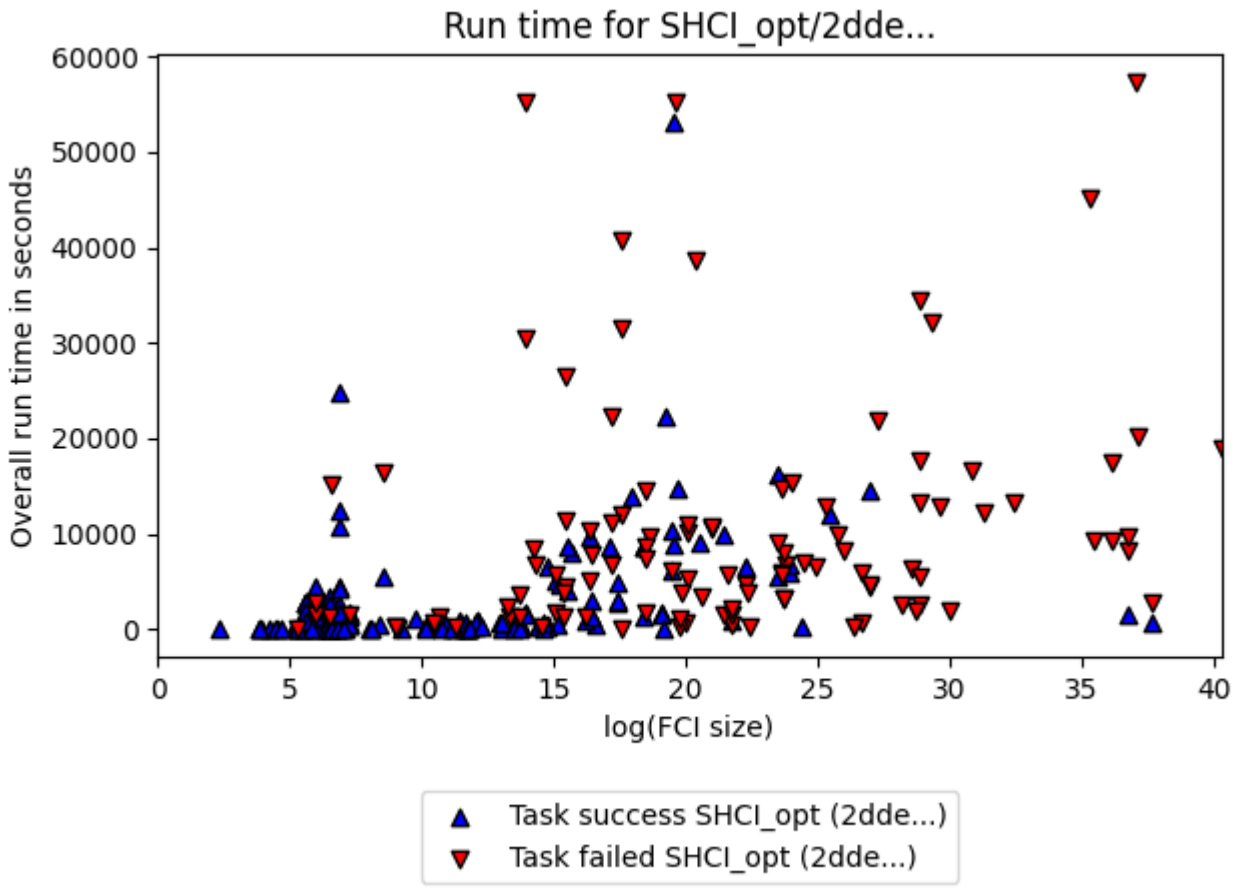
solvability_ratio: 1.0

f1_score: [0.8333333333333334, 0.993421052631579]

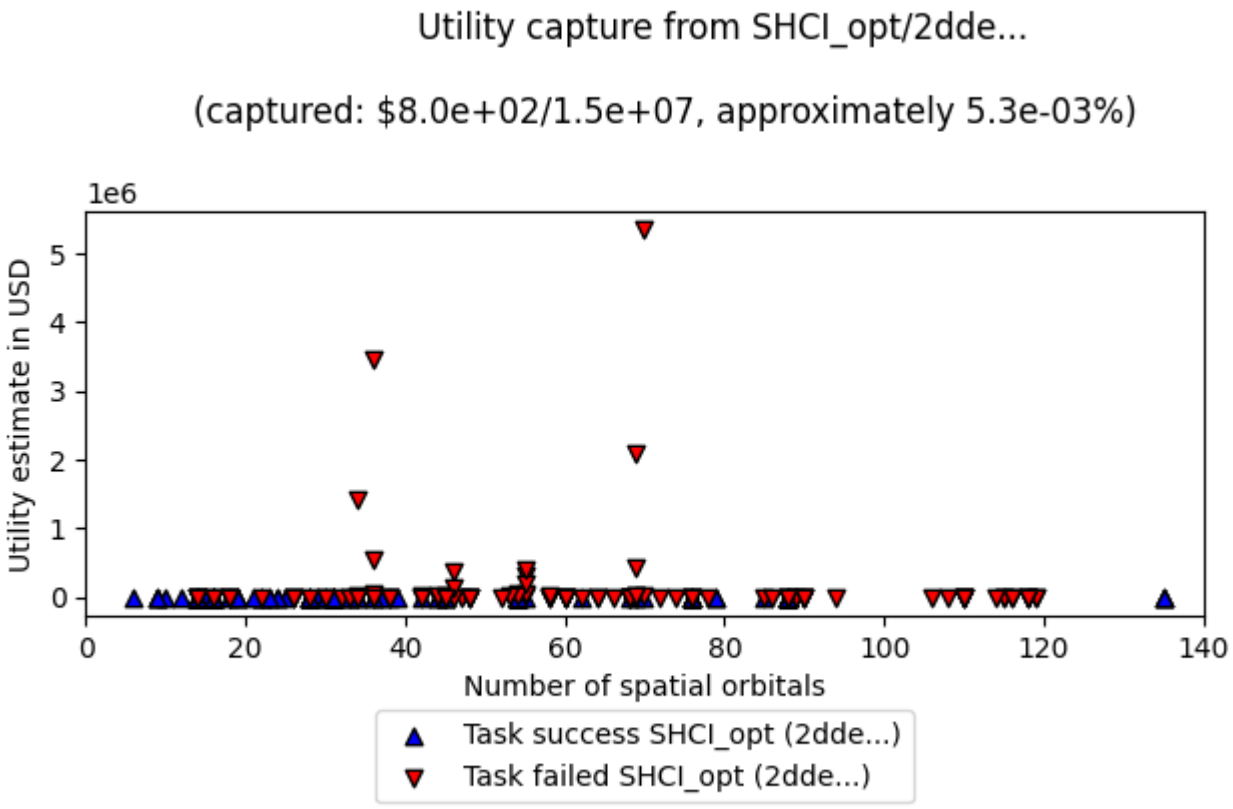
ml_metrics_calculator_version: 1

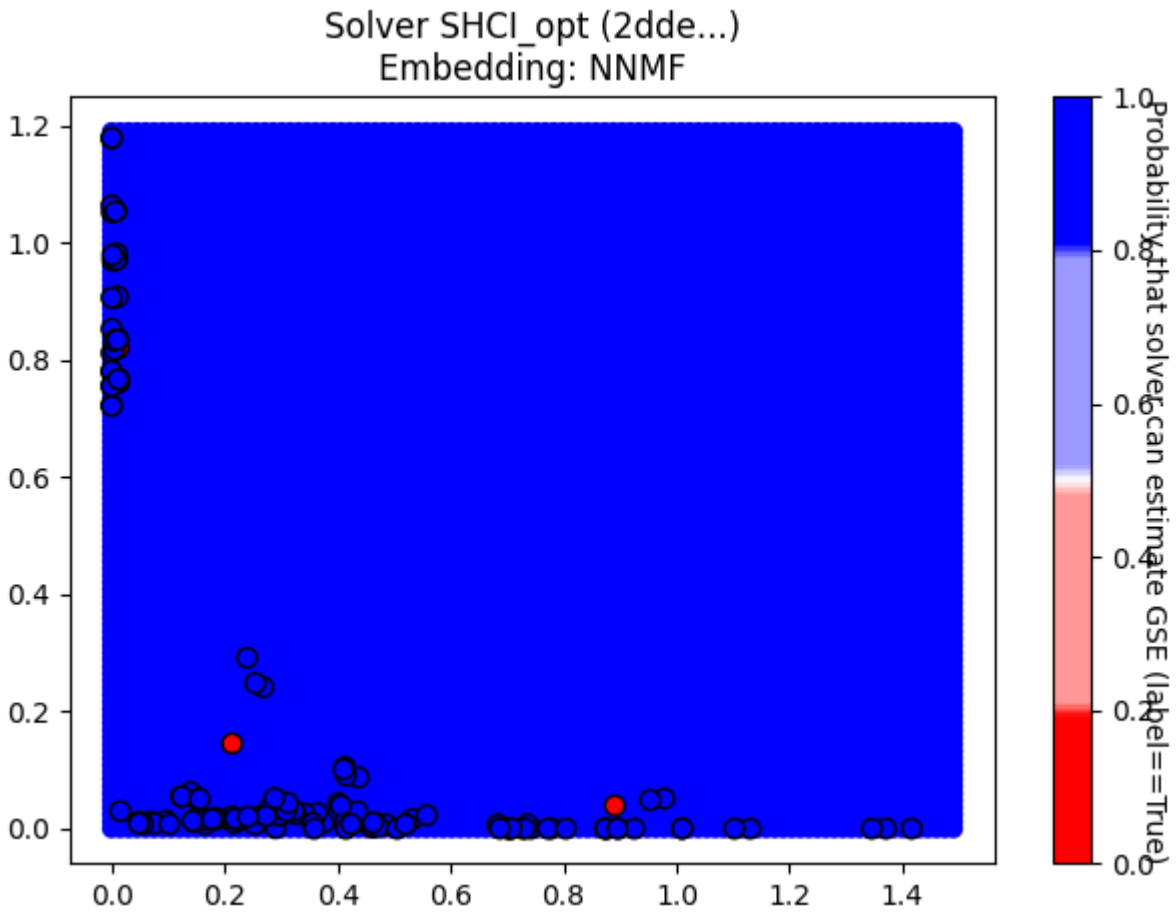


Note: plot only contains `attempted` tasks.

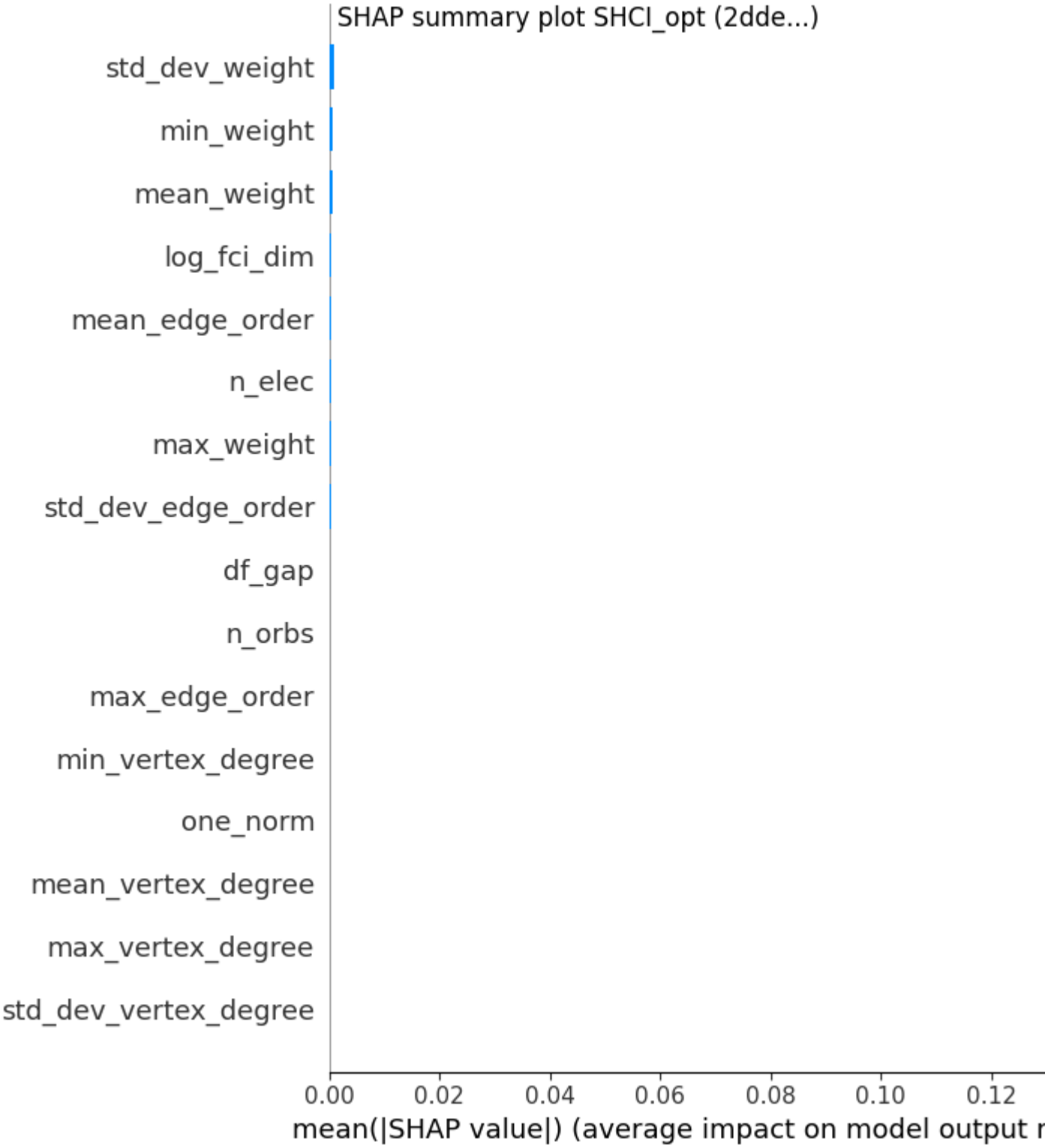


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_opt/2dde...
(captured: $8.0e+02/1.5e+07, approximately 5.3e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_opt (2dde...)
Task failed SHCI_opt (2dde...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: befcfa2d-16e8-4dbb-995f-9fc52809fec2

creation_timestamp: 2025-01-28T17:07:42.747013+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

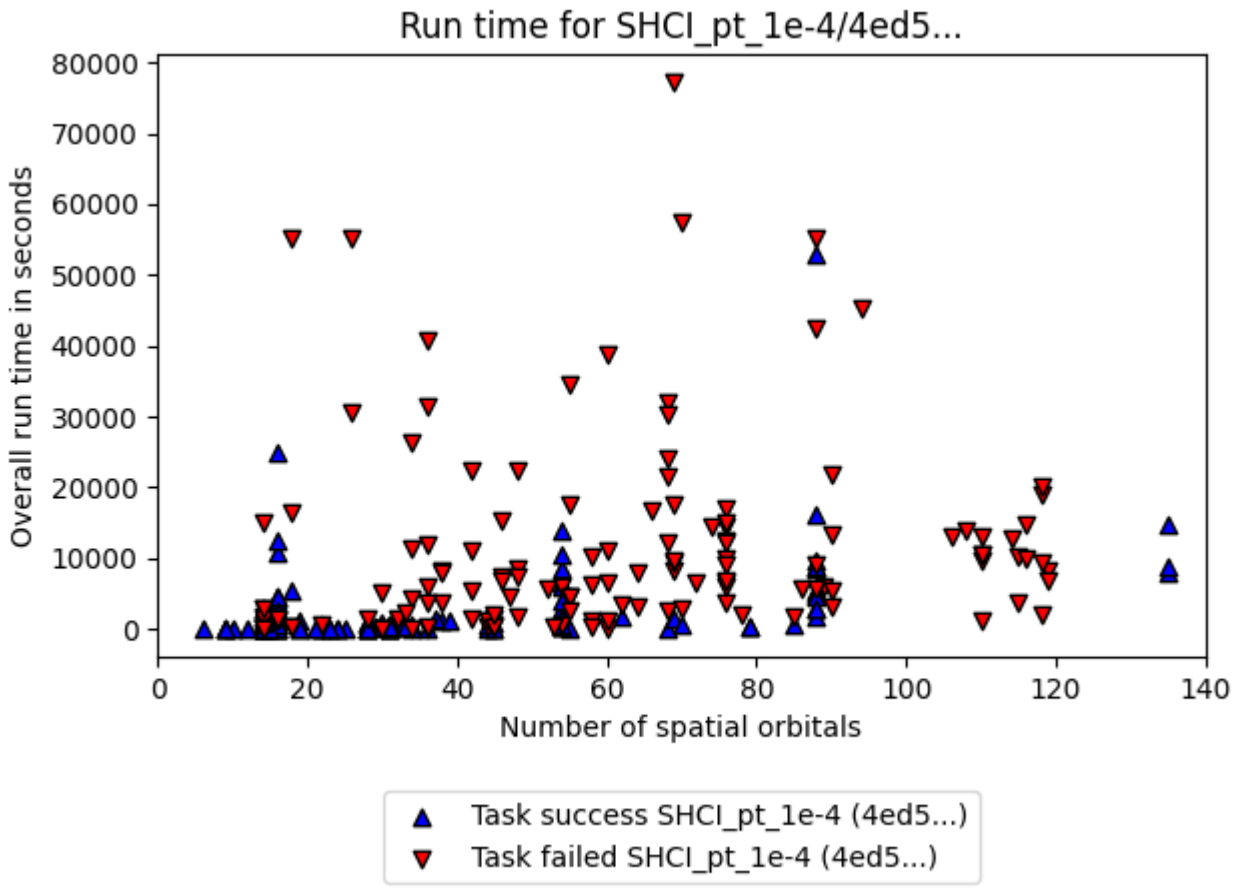
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

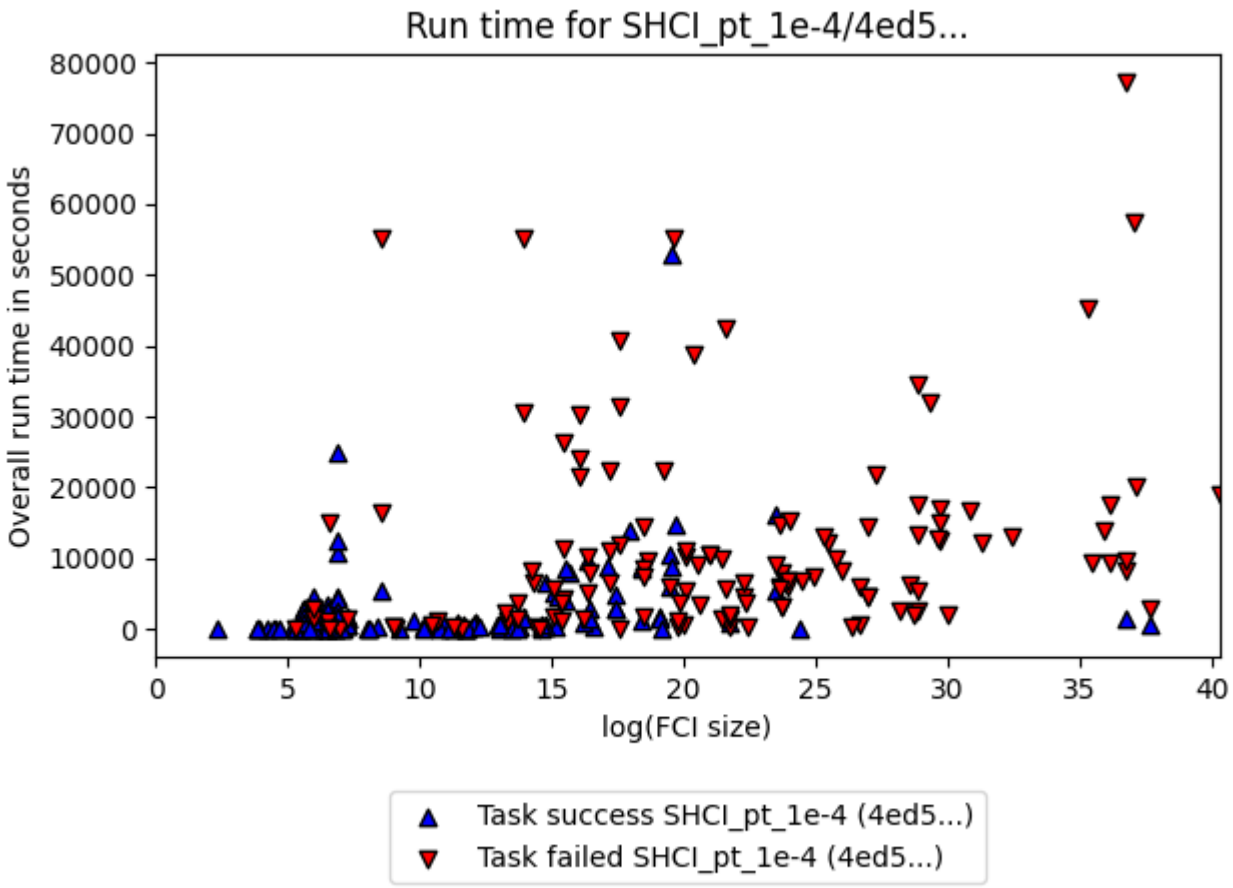
solvability_ratio: 0.547

f1_score: [0.8, 0.9750889679715302]

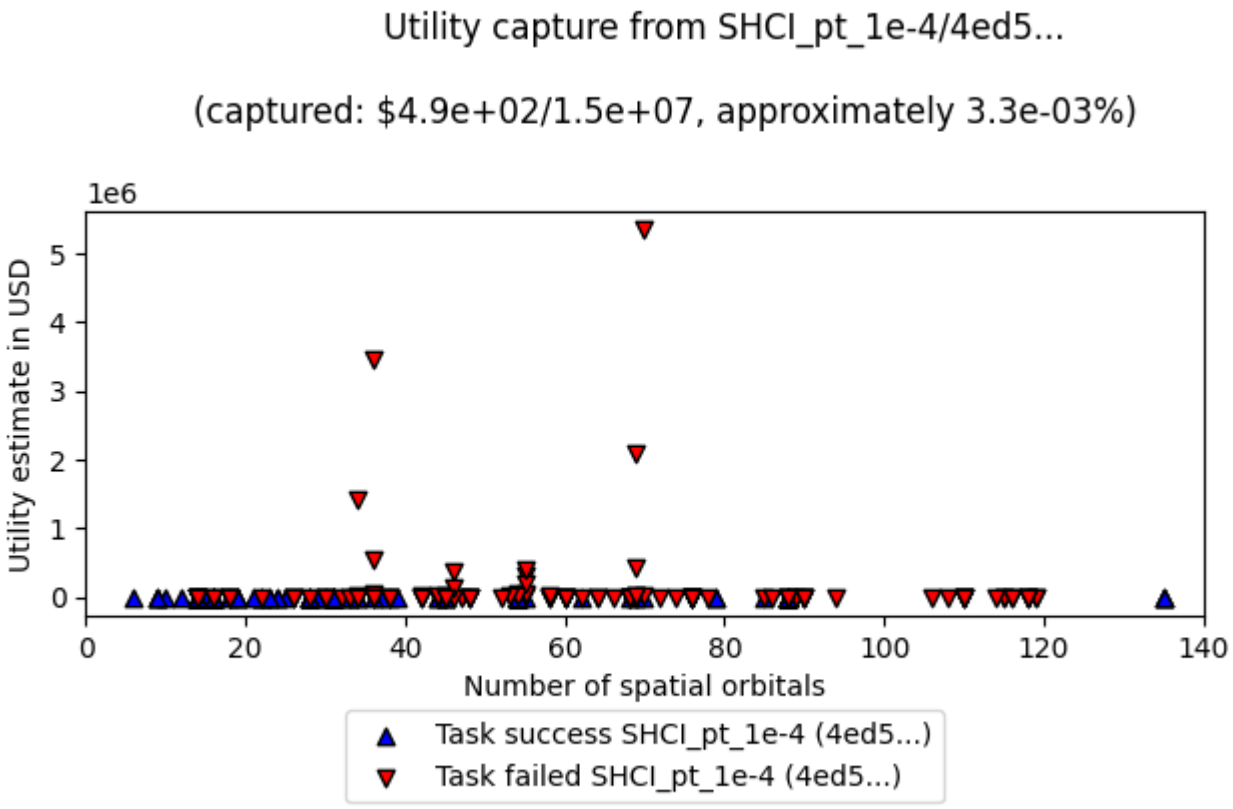
ml_metrics_calculator_version: 1

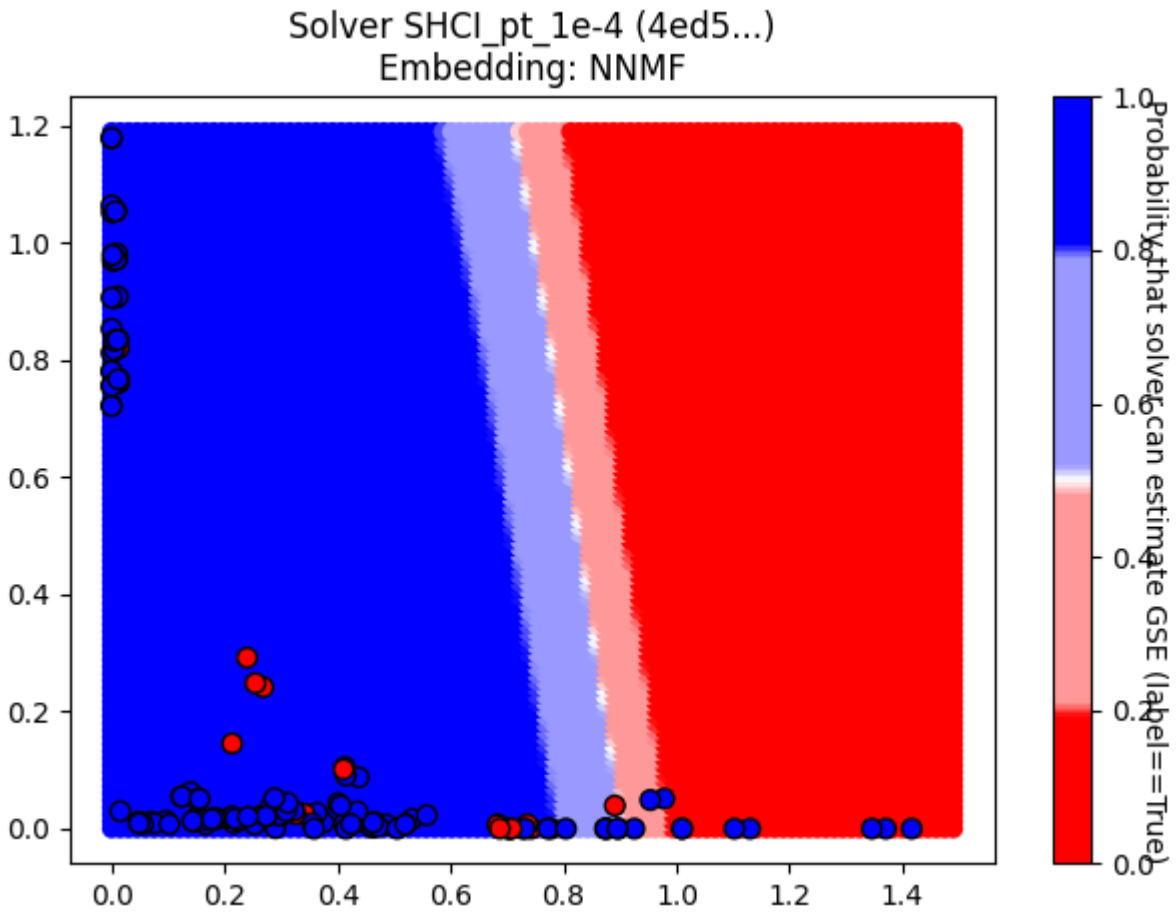


Note: plot only contains `attempted` tasks.

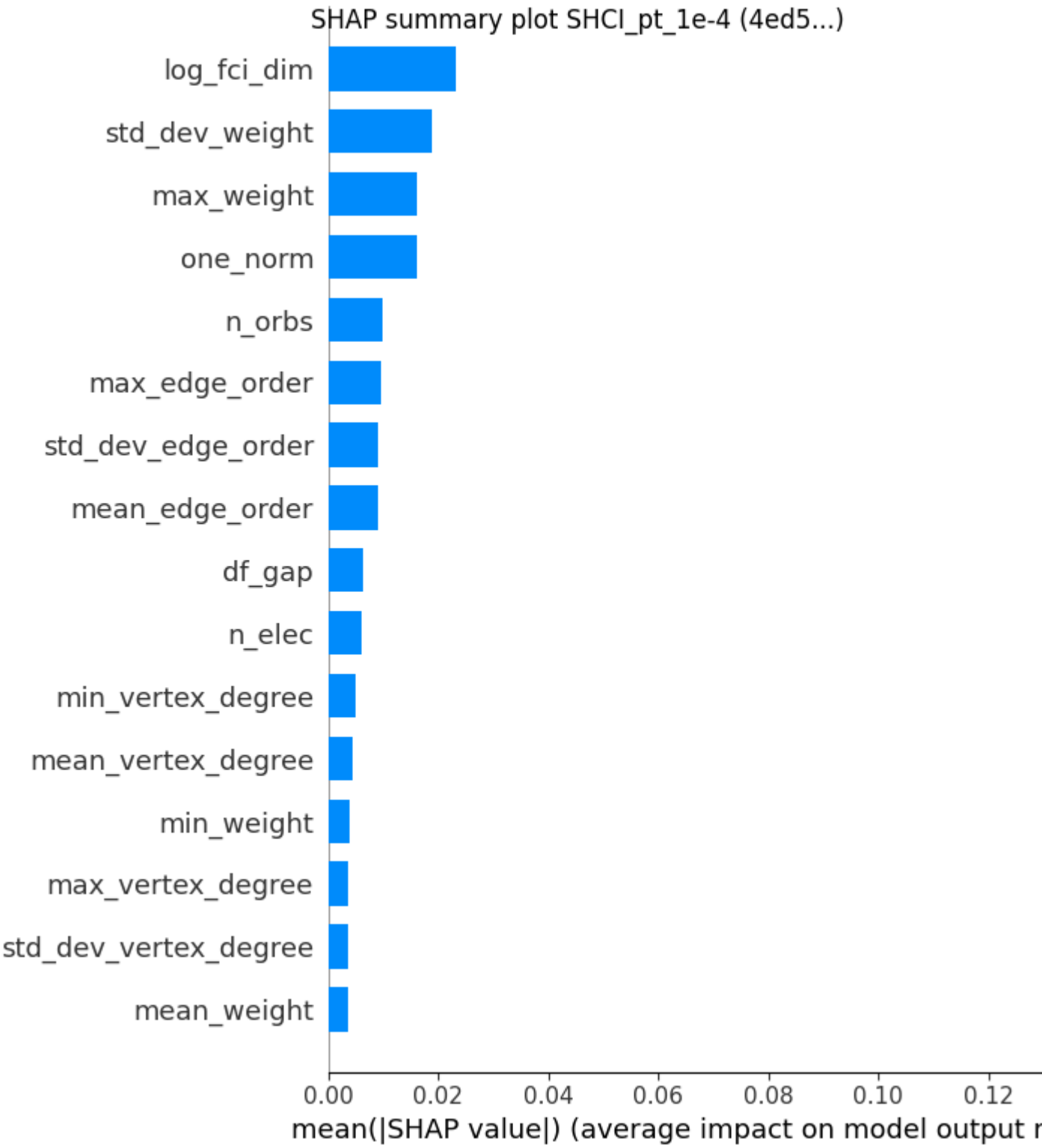


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_pt_1e-4/4ed5...
(captured: $4.9e+02/1.5e+07, approximately 3.3e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_pt_1e-4 (4ed5...)
Task failed SHCI_pt_1e-4 (4ed5...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: 67964365-6d54-49eb-a188-c11a778a50ec

creation_timestamp: 2025-01-28T17:07:42.747013+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

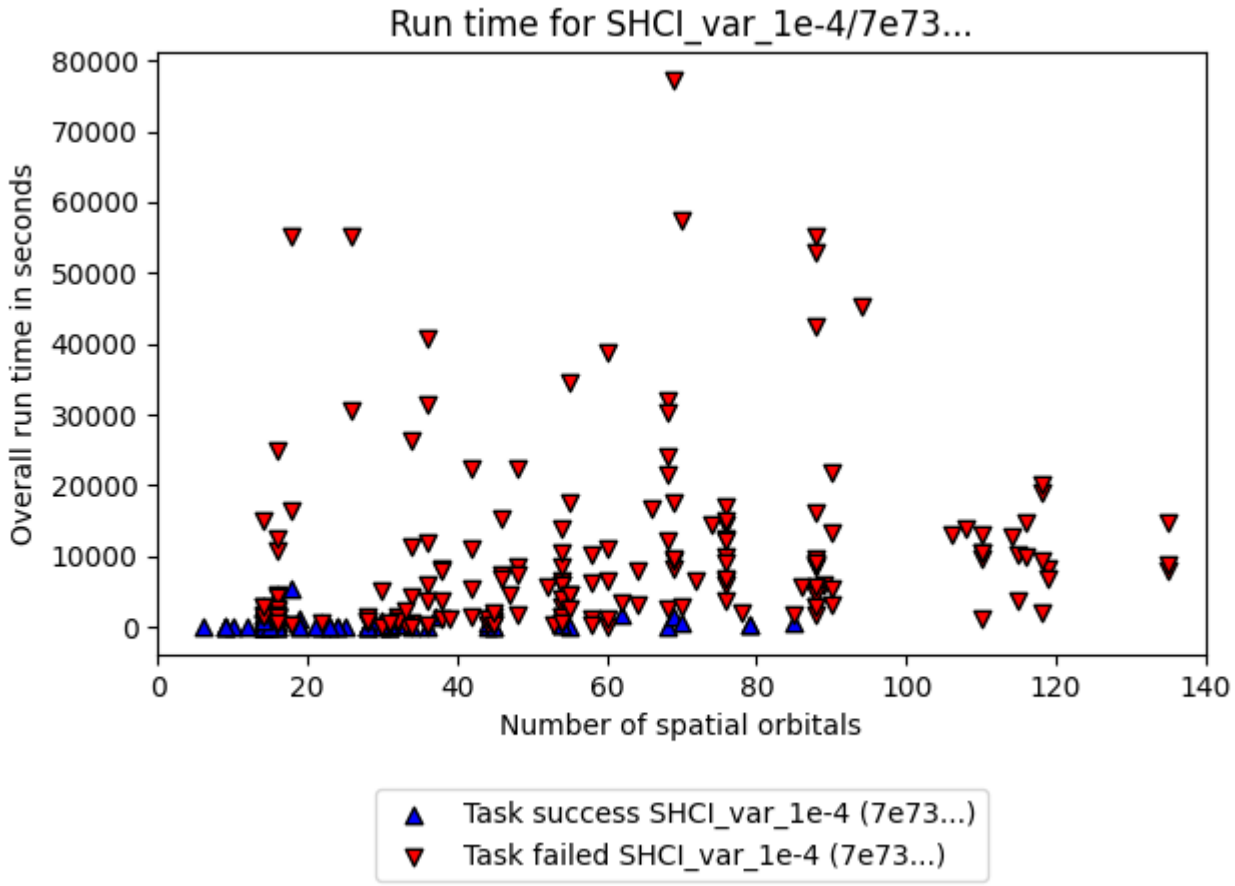
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

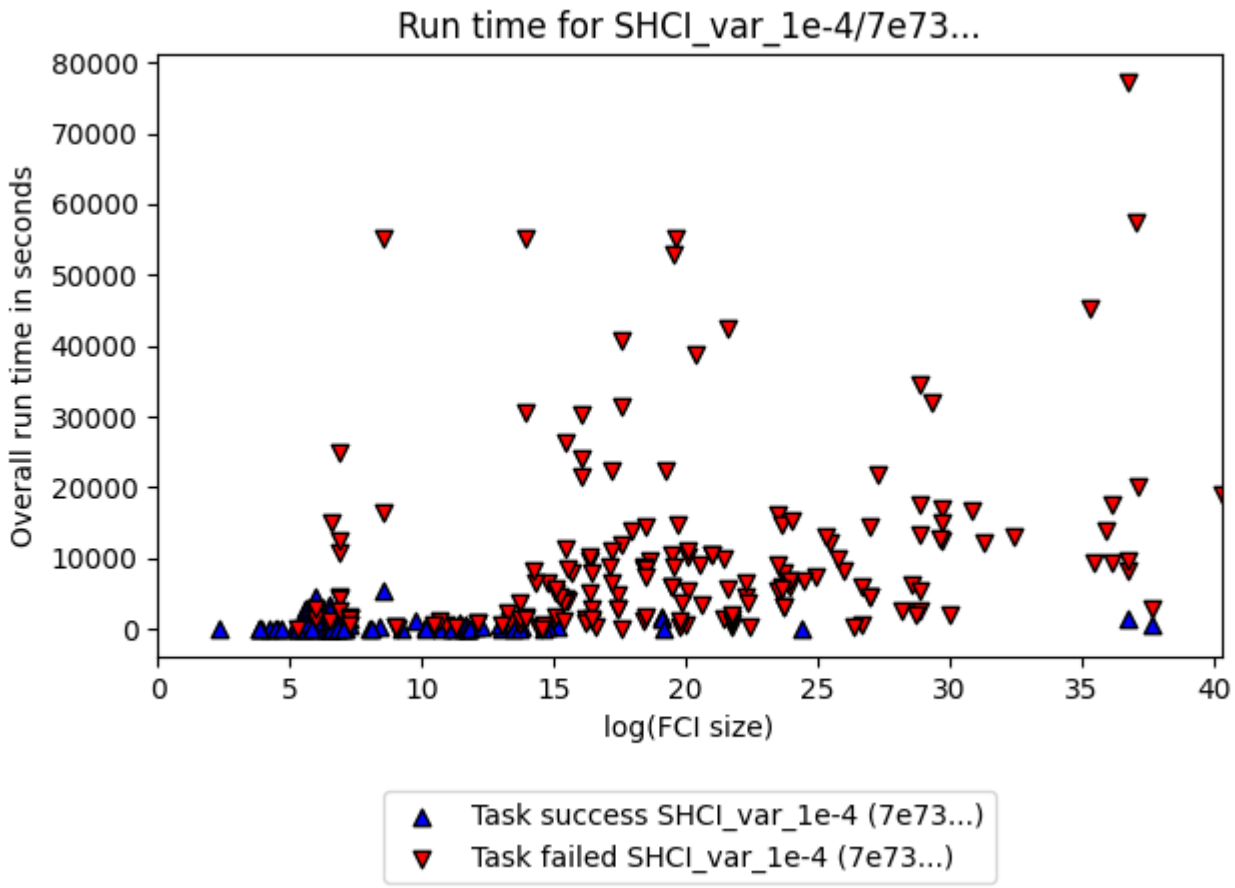
solvability_ratio: 0.9262

f1_score: [0.9841269841269841, 0.9894736842105263]

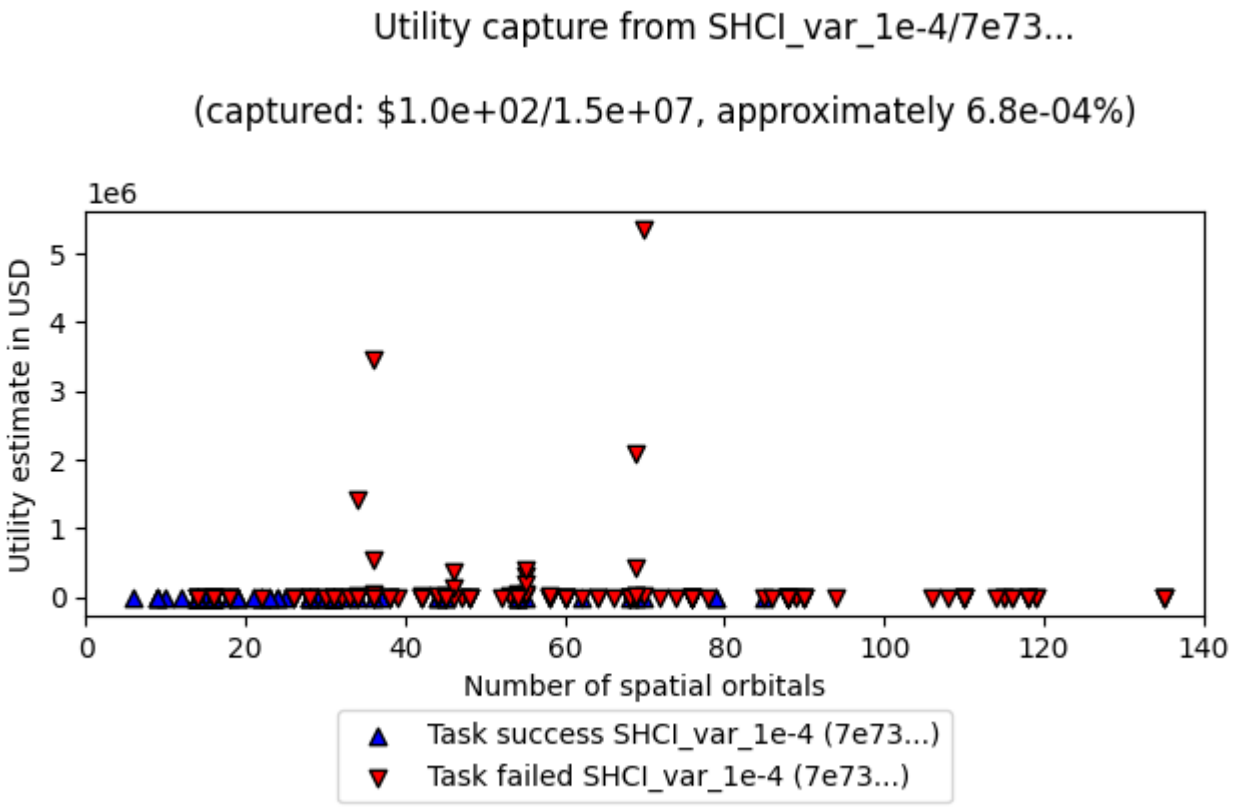
ml_metrics_calculator_version: 1

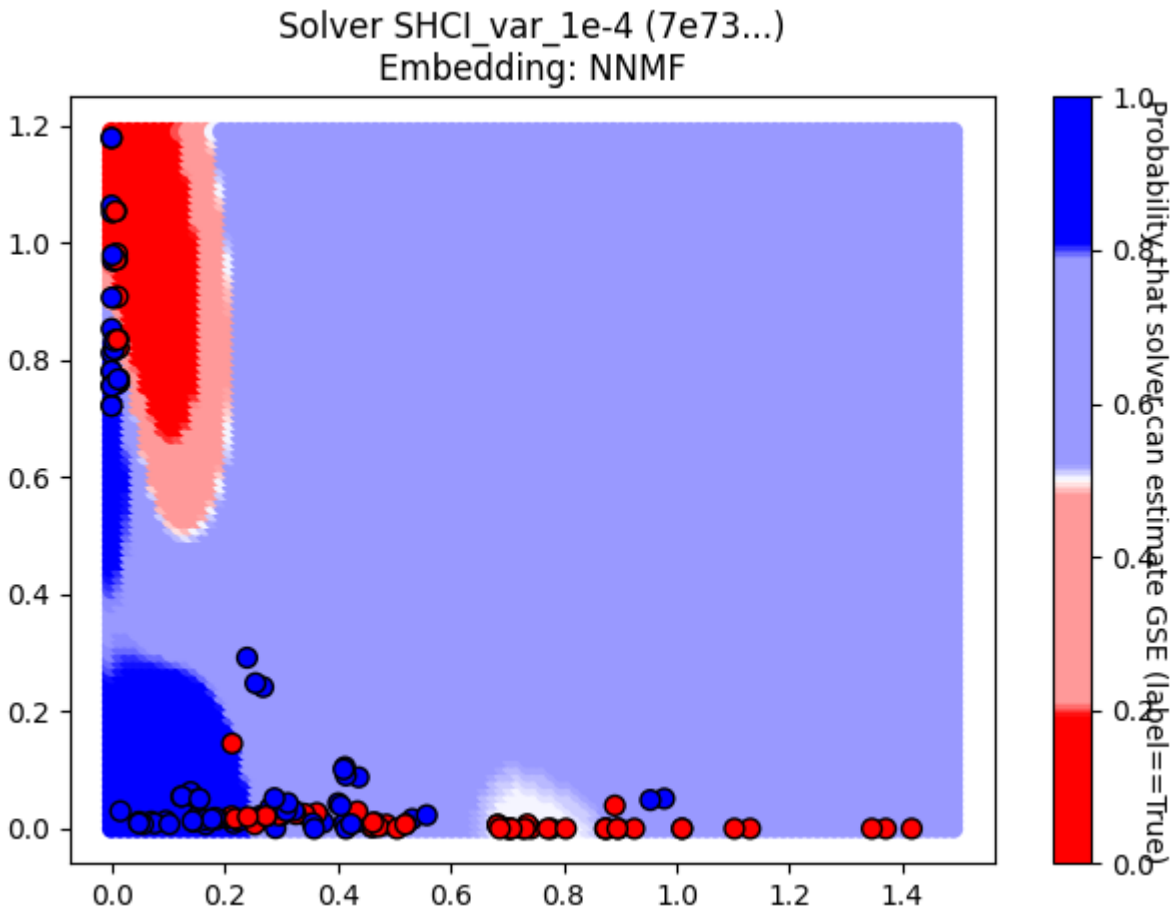


Note: plot only contains `attempted` tasks.

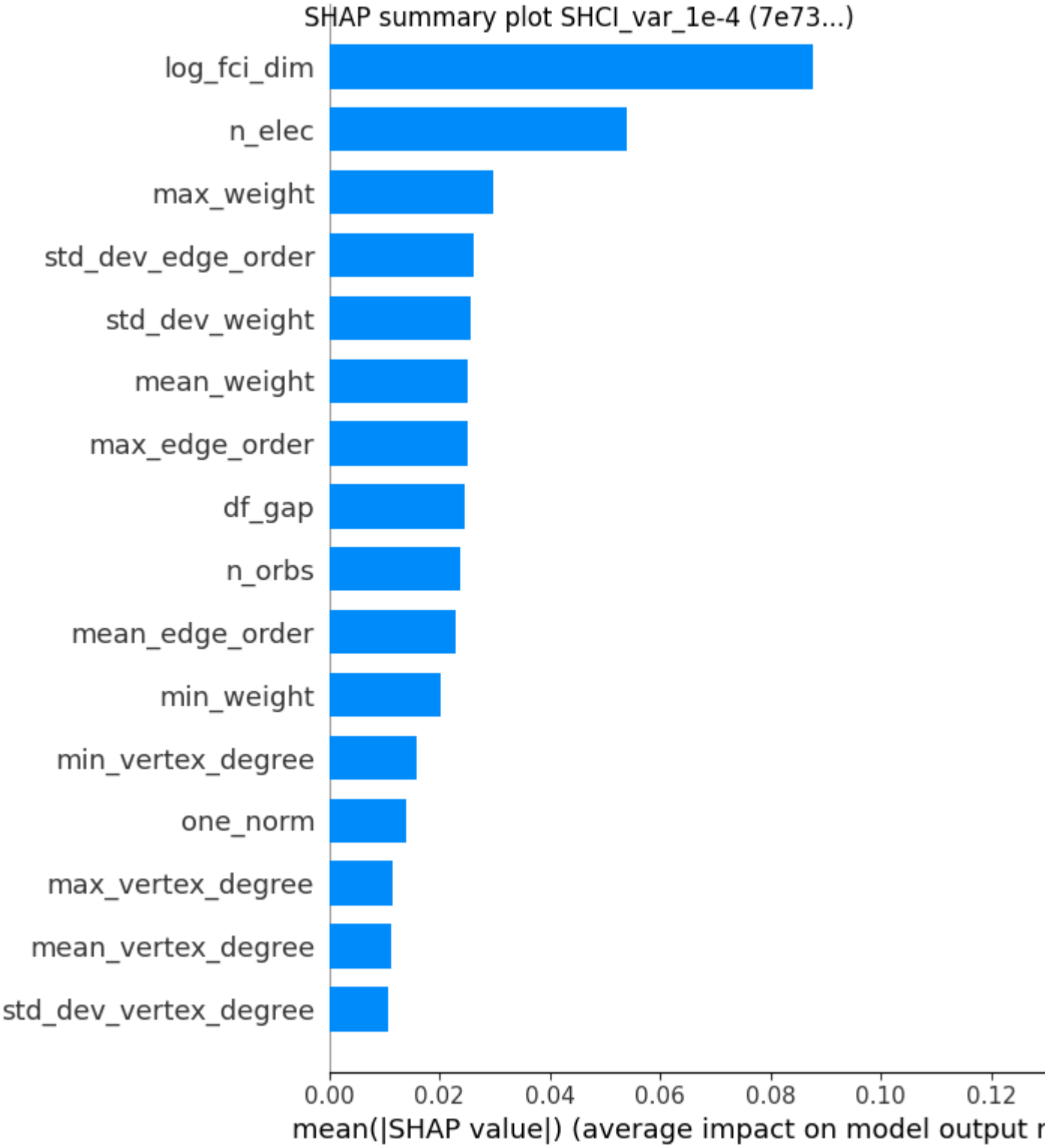


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_var_1e-4/7e73...
(captured: $1.0e+02/1.5e+07, approximately 6.8e-04%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_var_1e-4 (7e73...)
Task failed SHCI_var_1e-4 (7e73...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: 2657eba4-a179-4d81-a1af-9fc71ec31d0c

creation_timestamp: 2025-01-28T17:07:42.747013+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

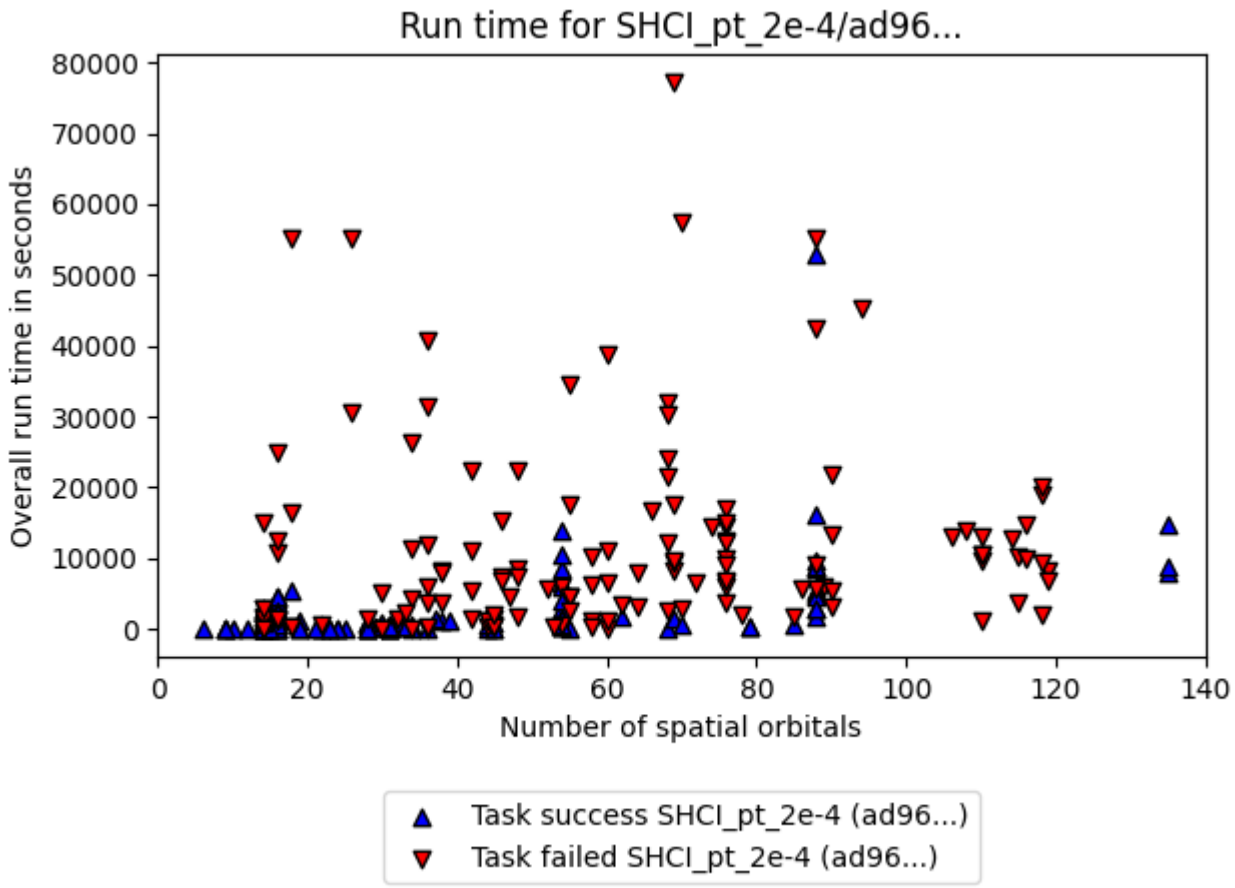
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

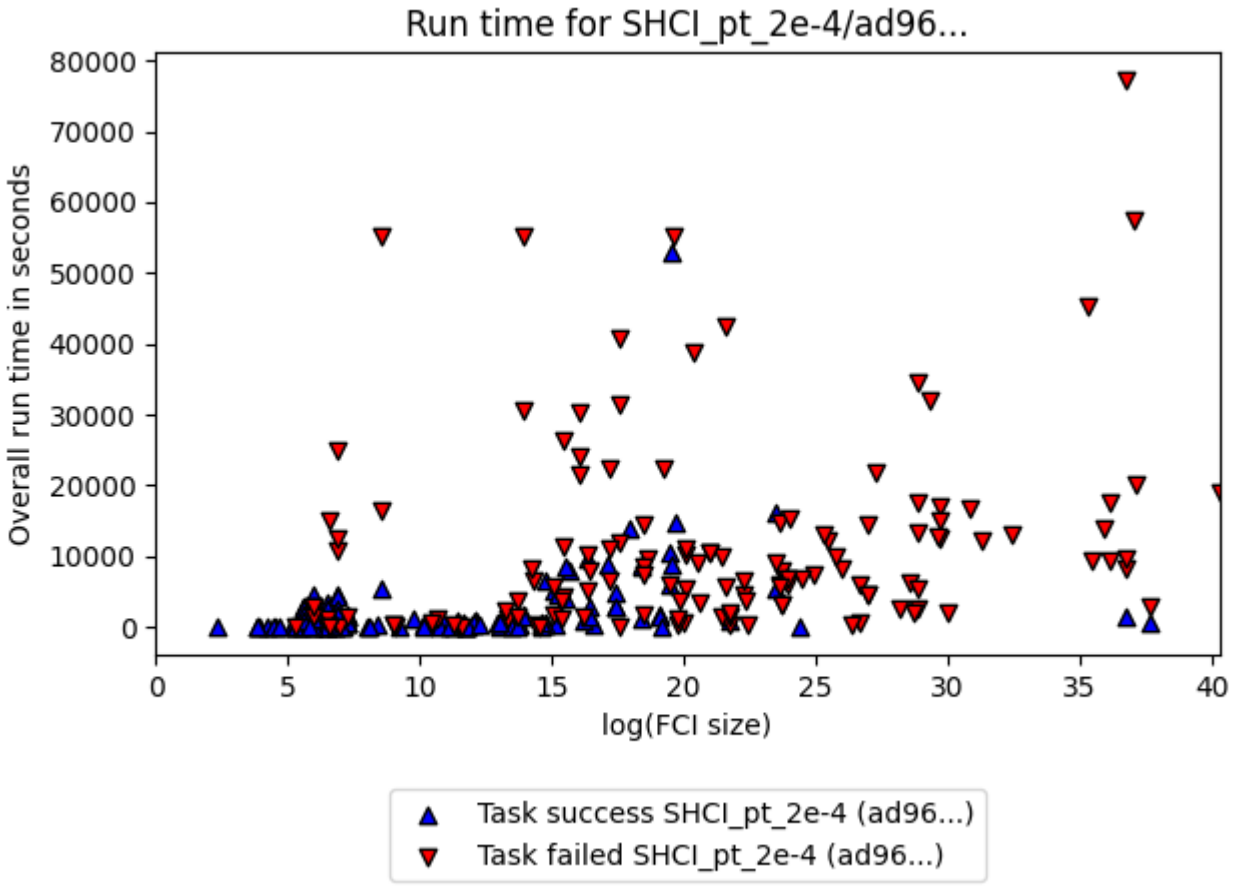
solvability_ratio: 0.5184

f1_score: [0.6486486486486487, 0.953405017921147]

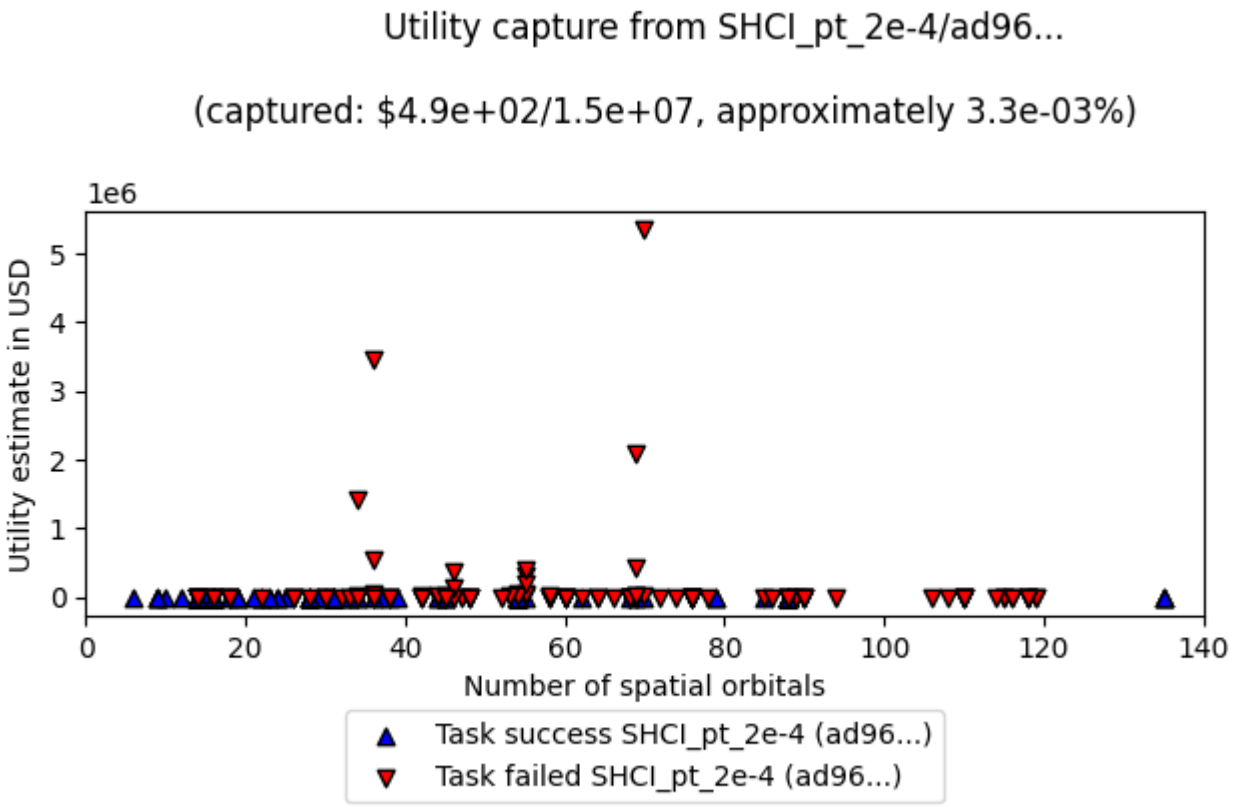
ml_metrics_calculator_version: 1

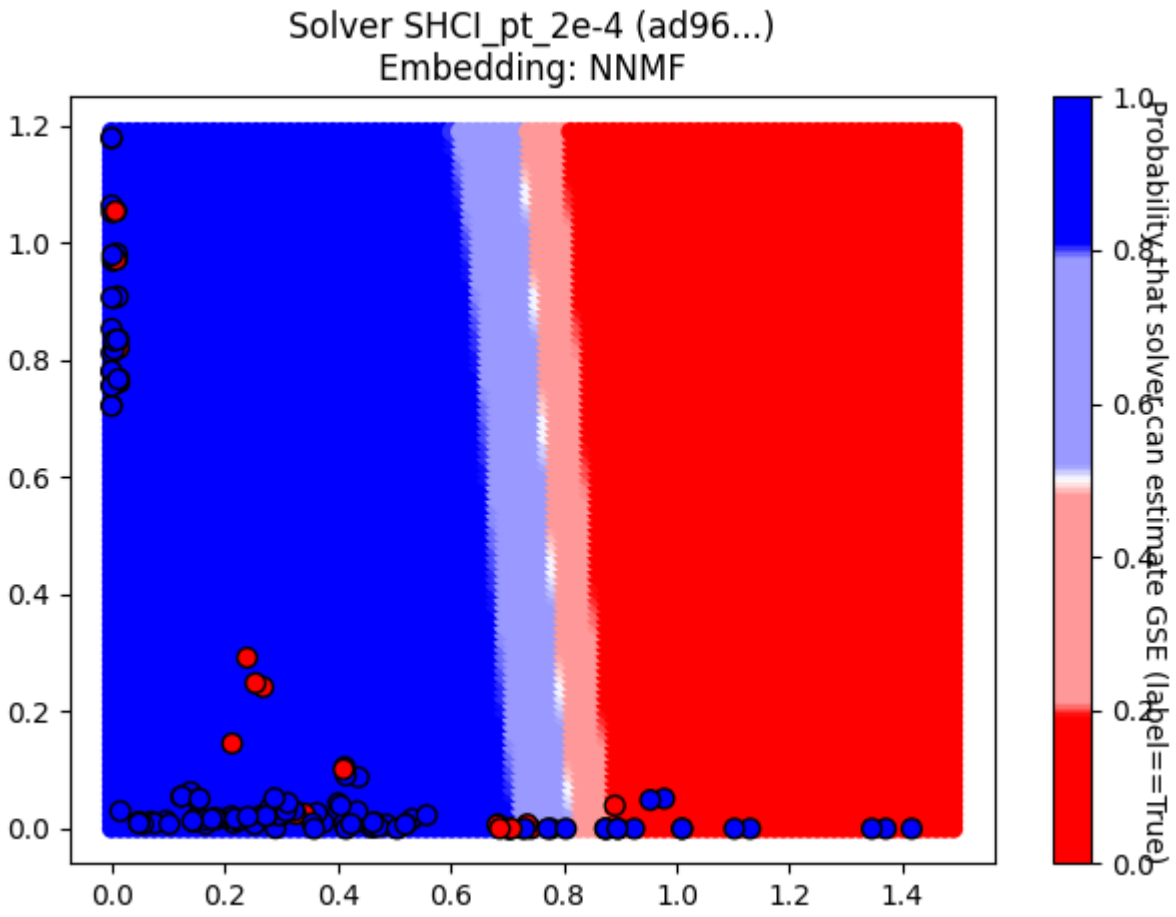


Note: plot only contains `attempted` tasks.

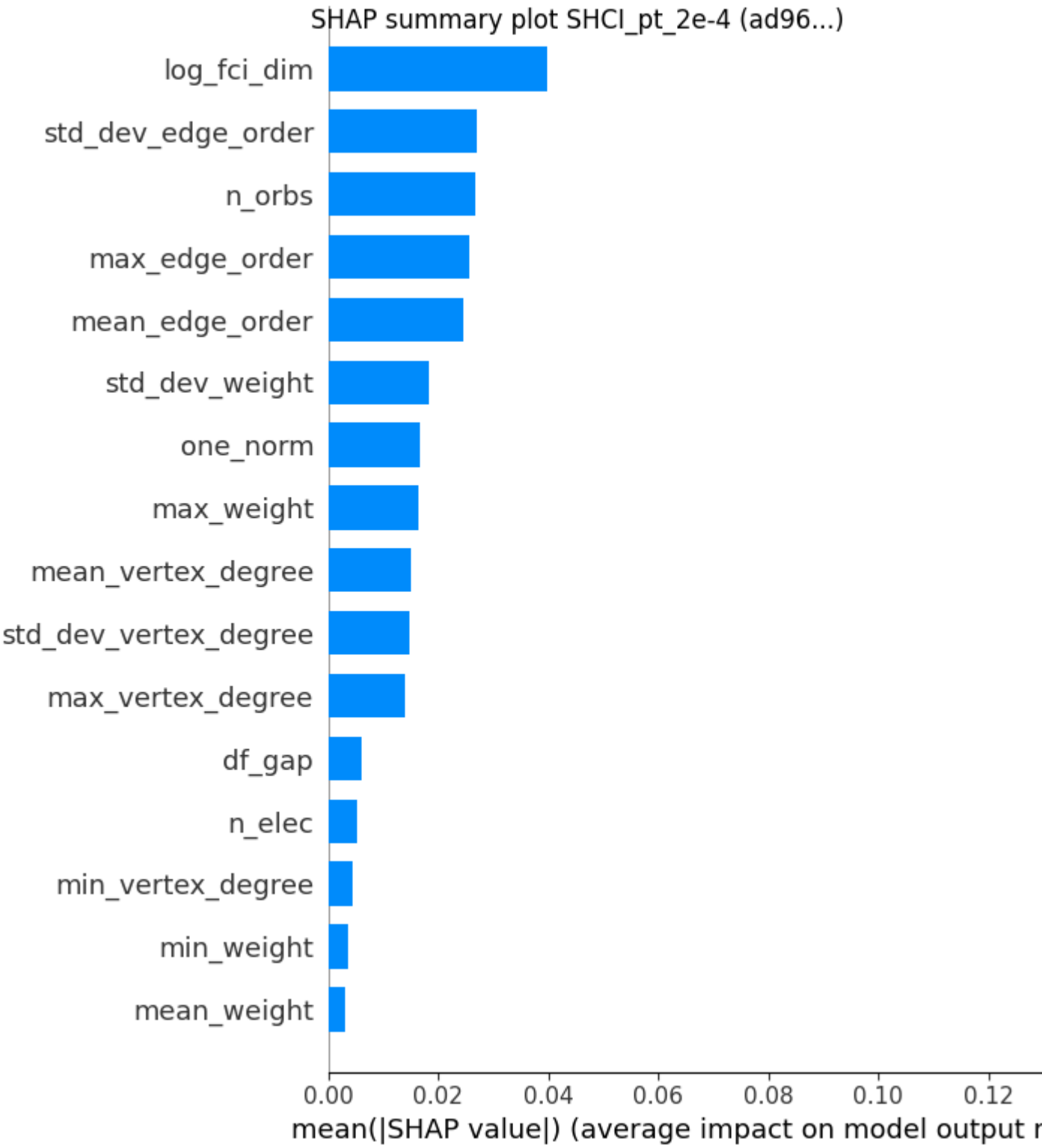


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_pt_2e-4/ad96...
(captured: $4.9e+02/1.5e+07, approximately 3.3e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_pt_2e-4 (ad96...)
Task failed SHCI_pt_2e-4 (ad96...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: cb2a5002-0658-4d82-be07-24f3bf003941

creation_timestamp: 2025-01-28T17:07:42.747013+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

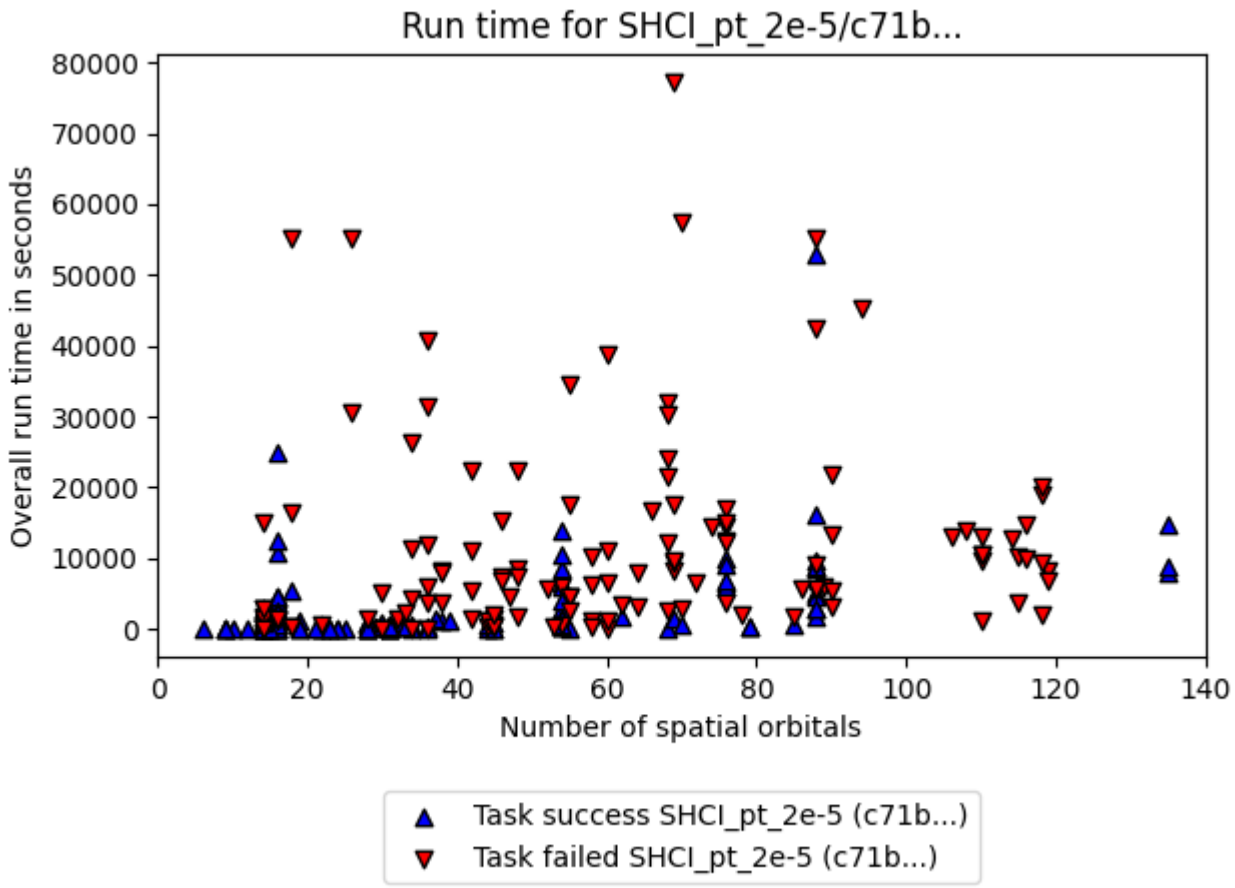
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

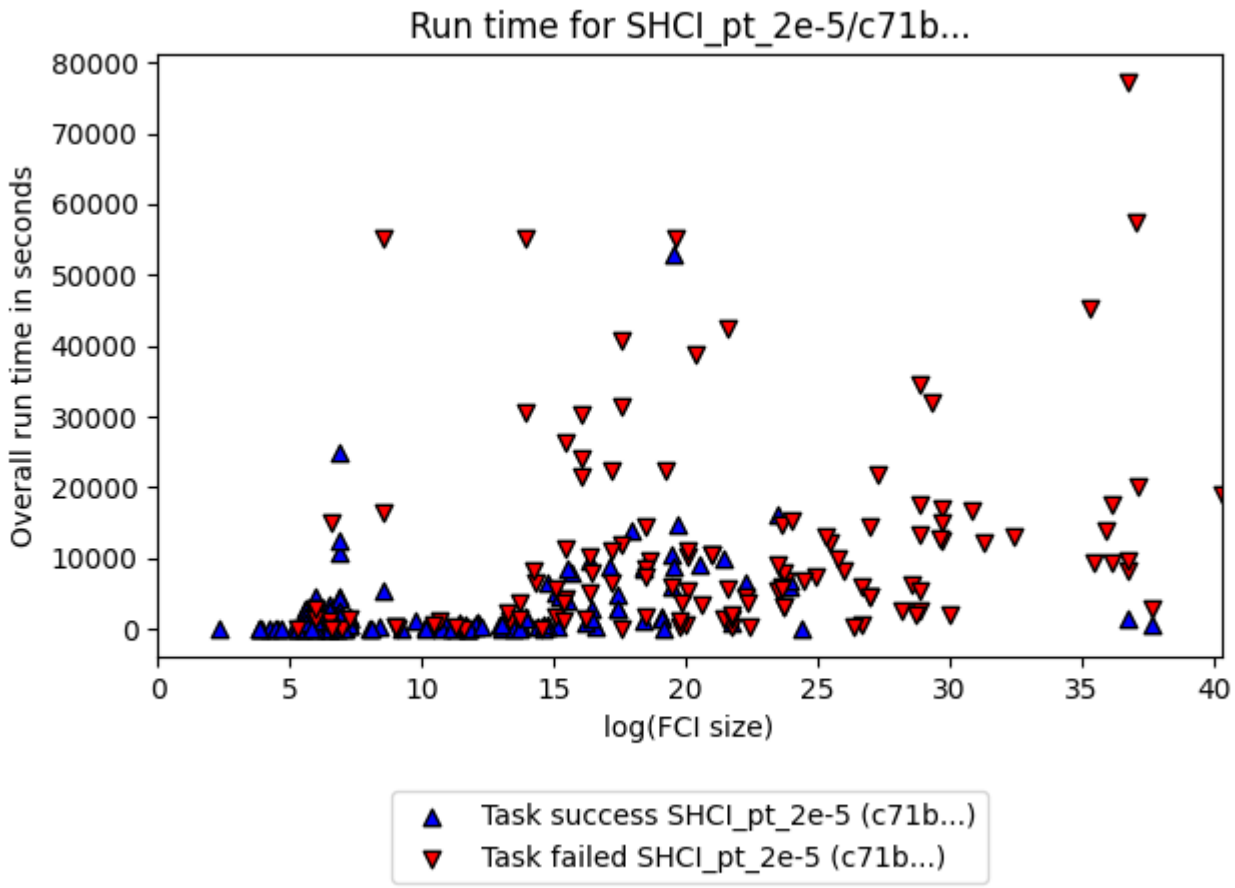
solvability_ratio: 0.8922

f1_score: [1.0, 1.0]

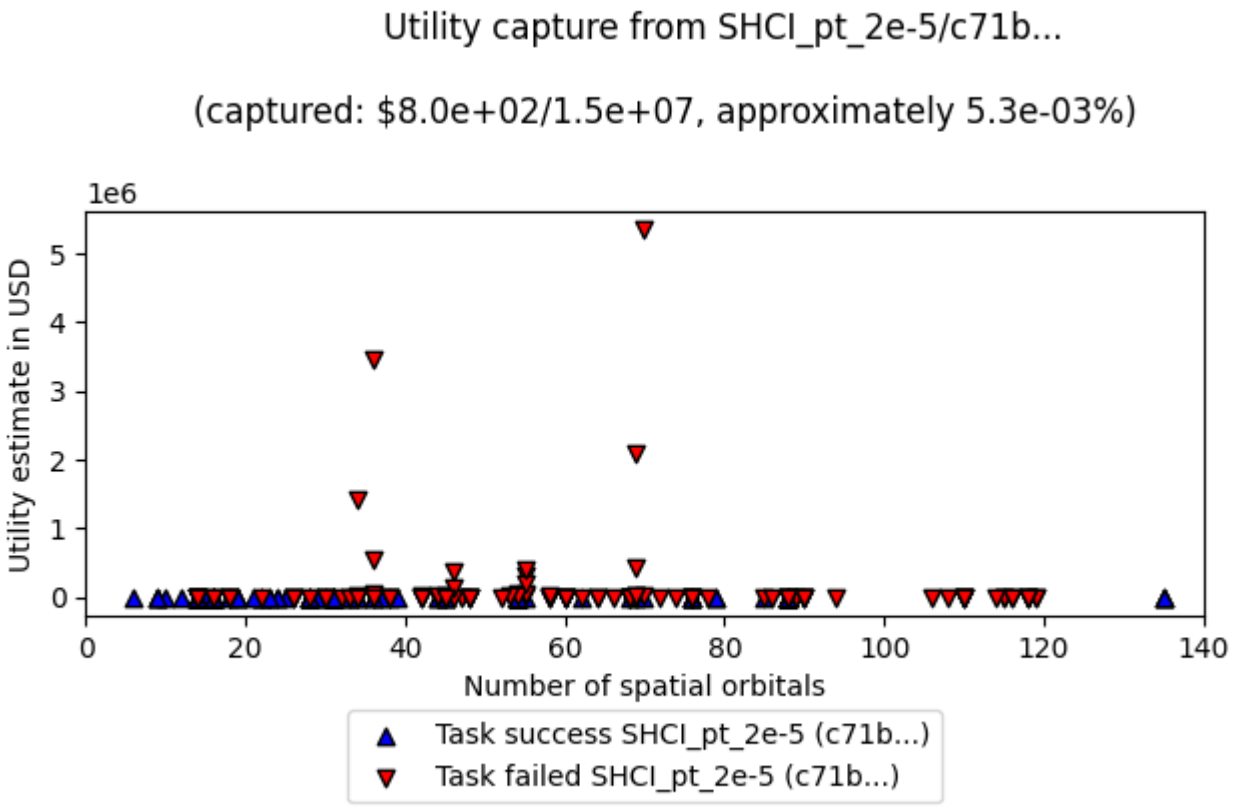
ml_metrics_calculator_version: 1

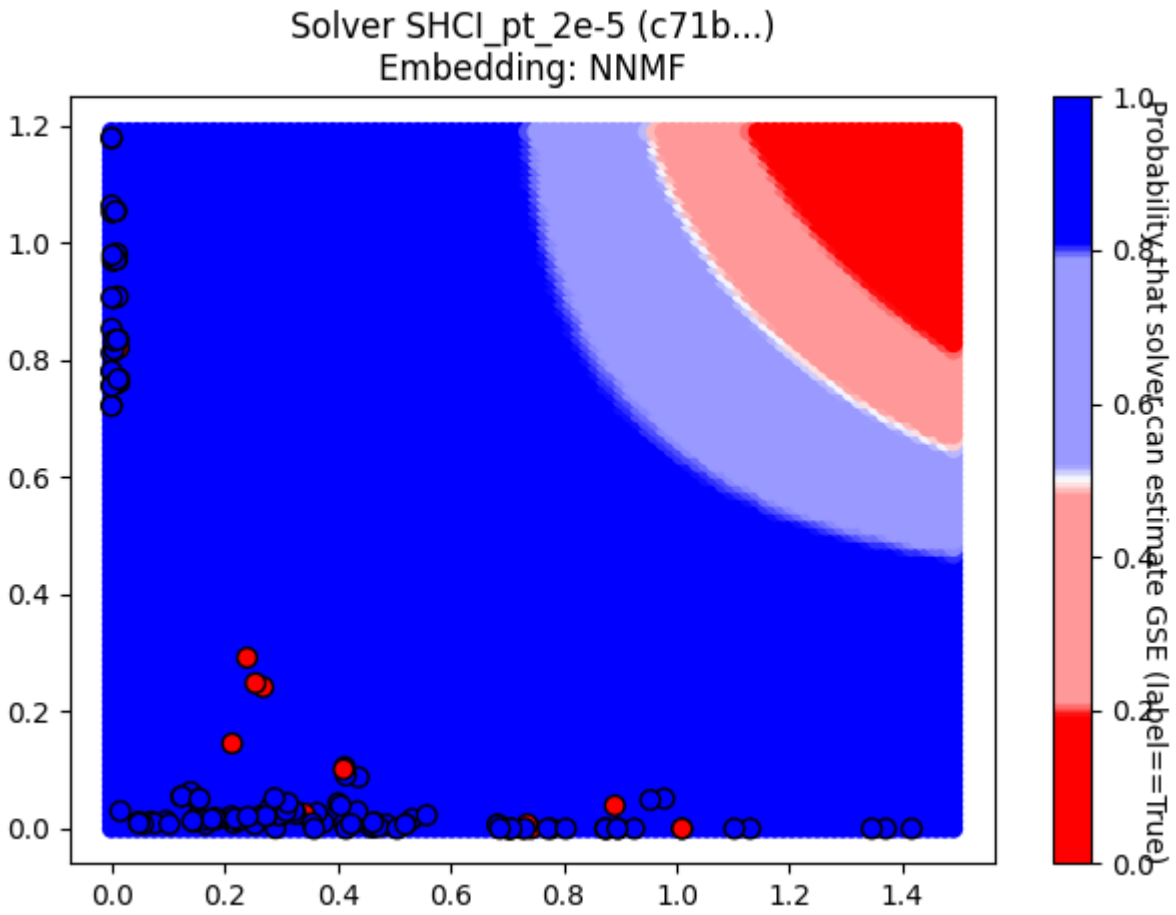


Note: plot only contains `attempted` tasks.

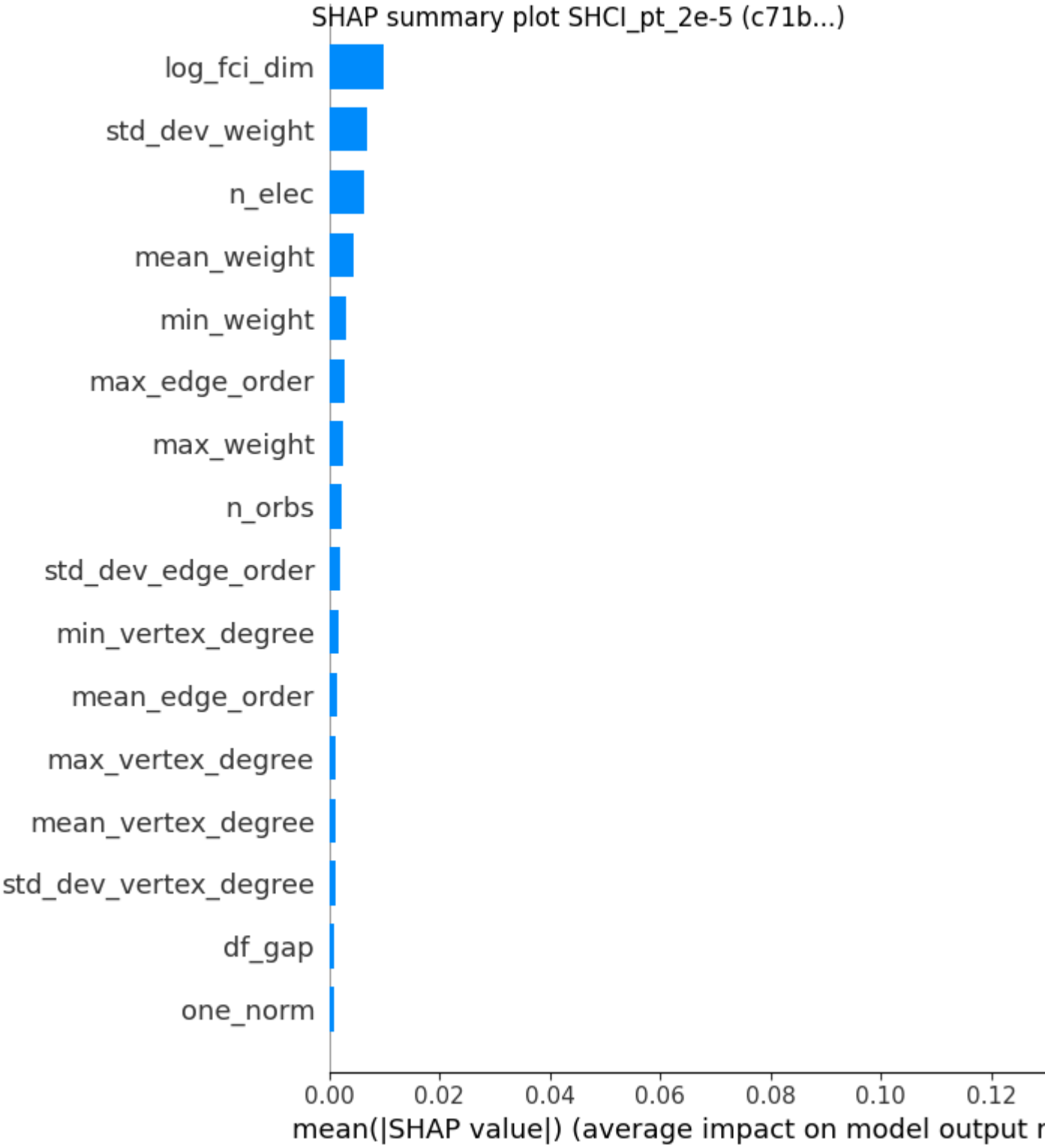


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_pt_2e-5/c71b...
(captured: $8.0e+02/1.5e+07, approximately 5.3e-03%)
1e6
Utility estimate in USD
0
1
2
3
4
5
0
20
40
60
80
100
120
140
Number of spatial orbitals
Task success SHCI_pt_2e-5 (c71b...)
Task failed SHCI_pt_2e-5 (c71b...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: 9a4c296f-2c56-4d43-8ca5-b0d7724f156f

creation_timestamp: 2025-01-28T17:07:42.747013+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

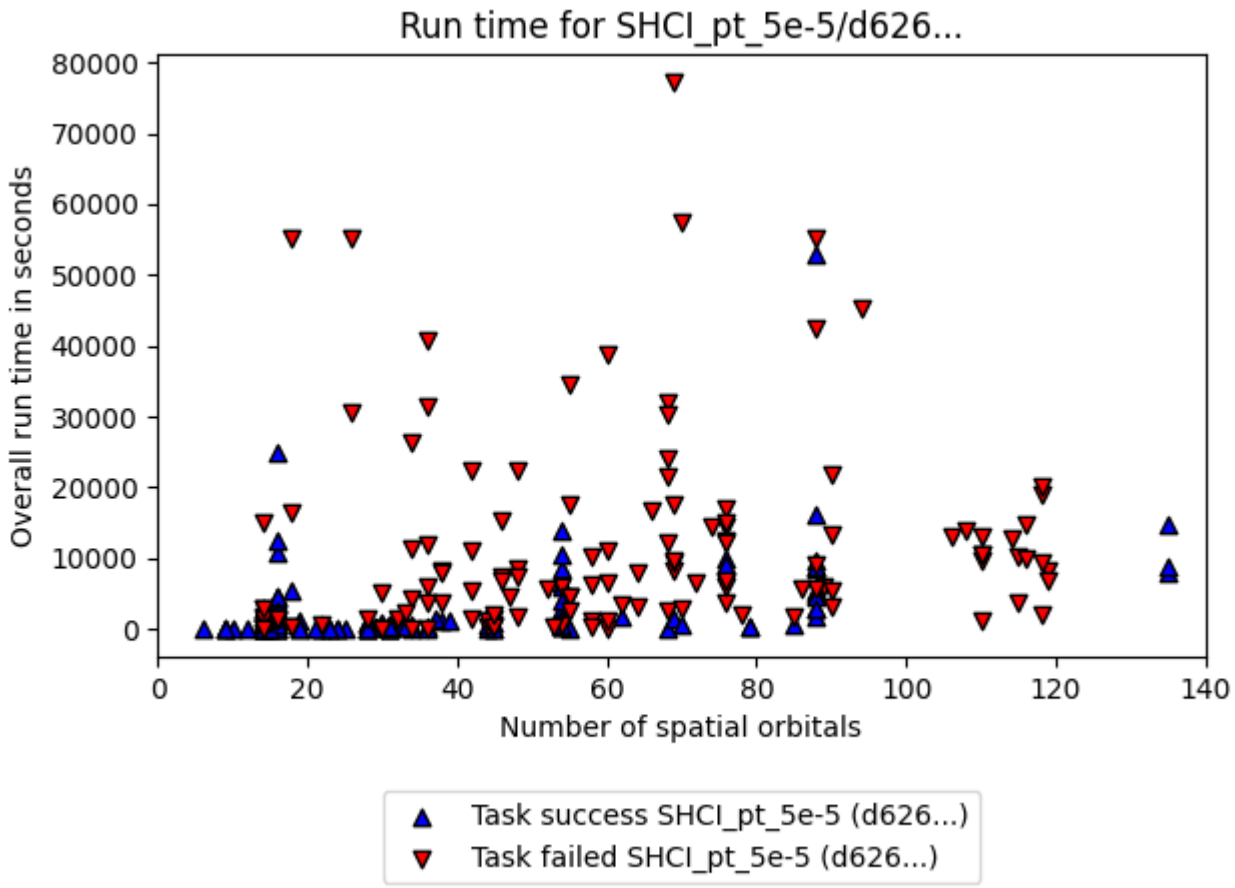
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

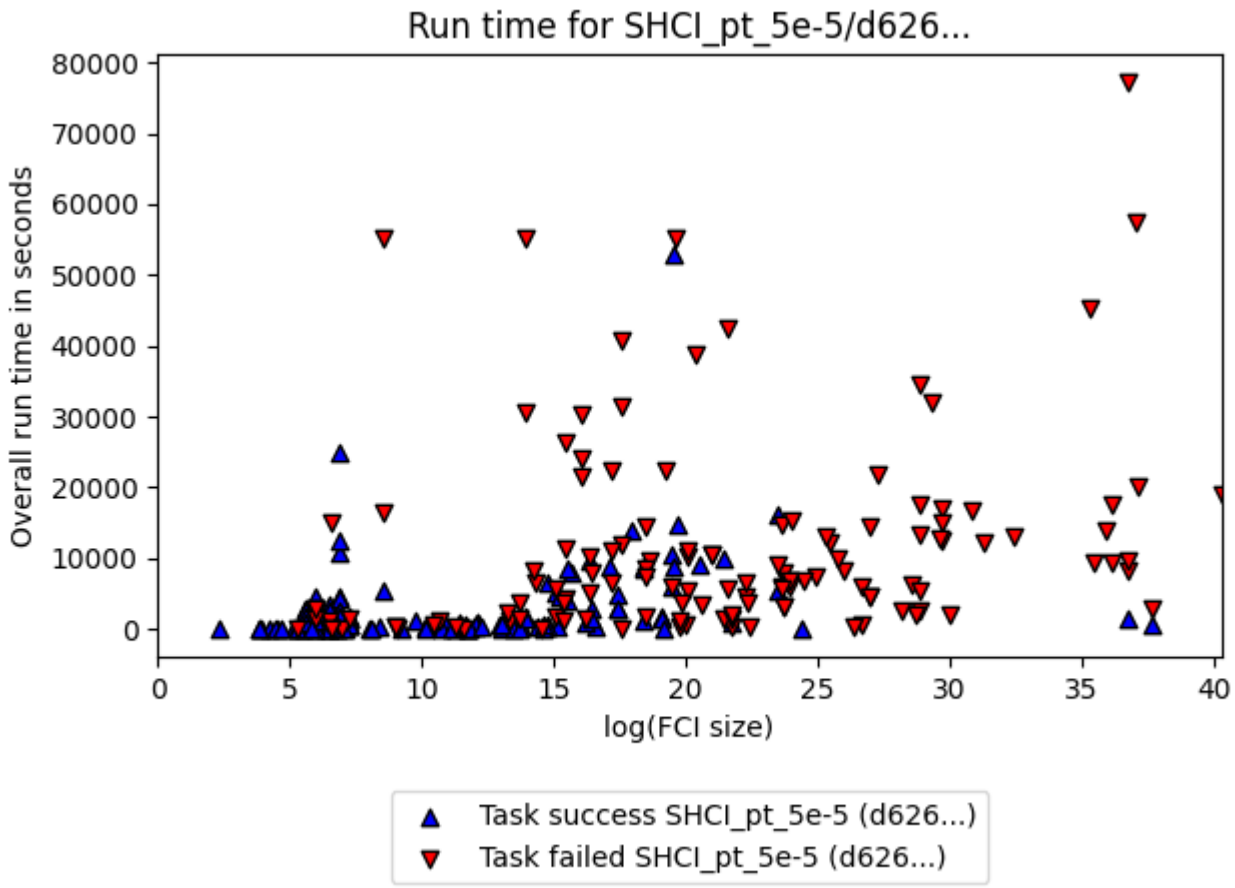
solvability_ratio: 0.482

f1_score: [0.75, 0.971830985915493]

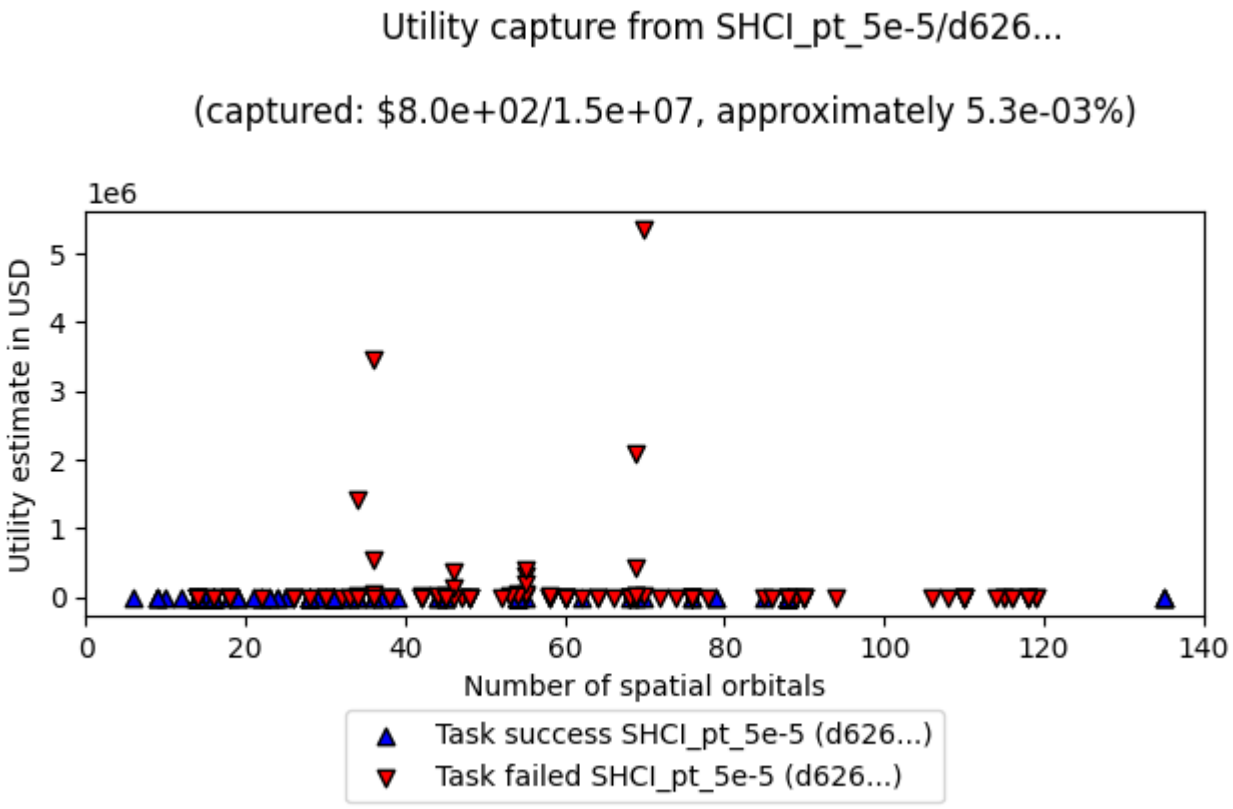
ml_metrics_calculator_version: 1

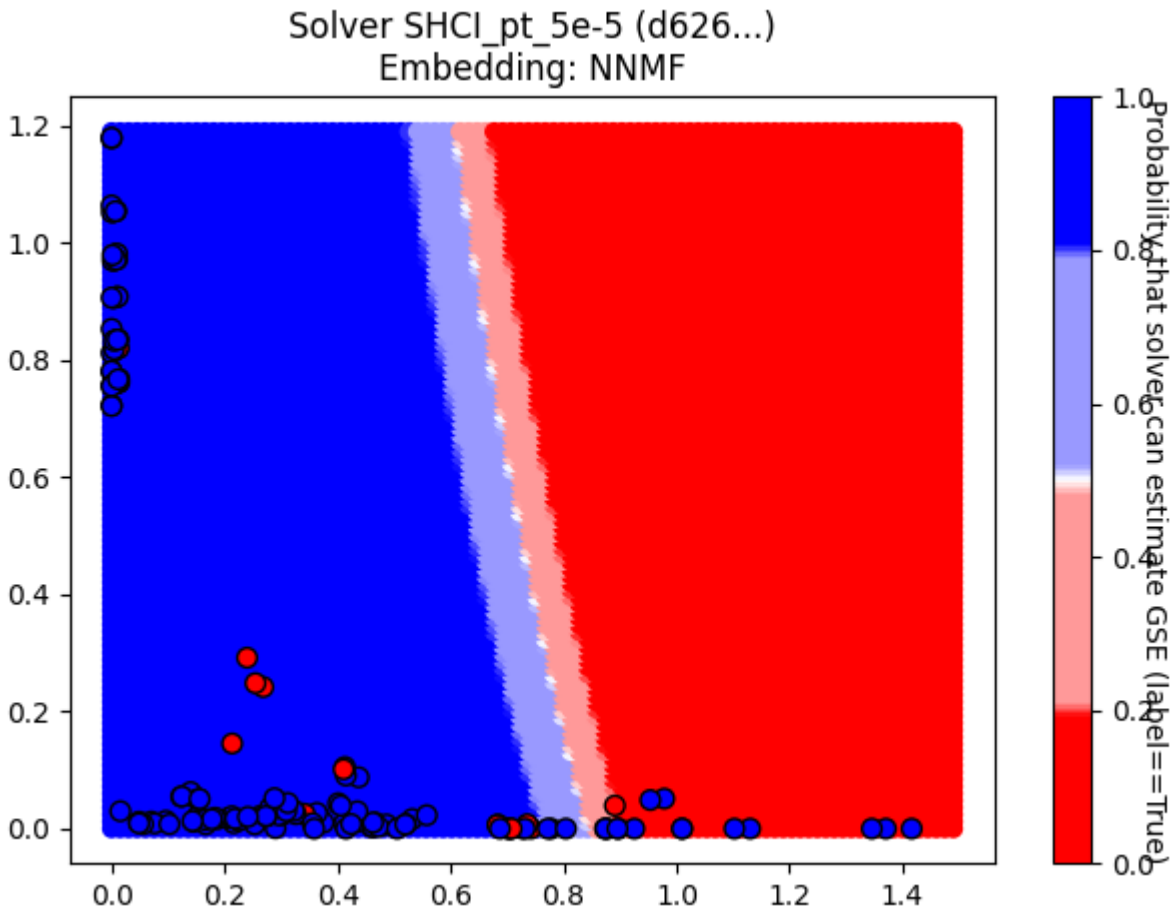


Note: plot only contains `attempted` tasks.

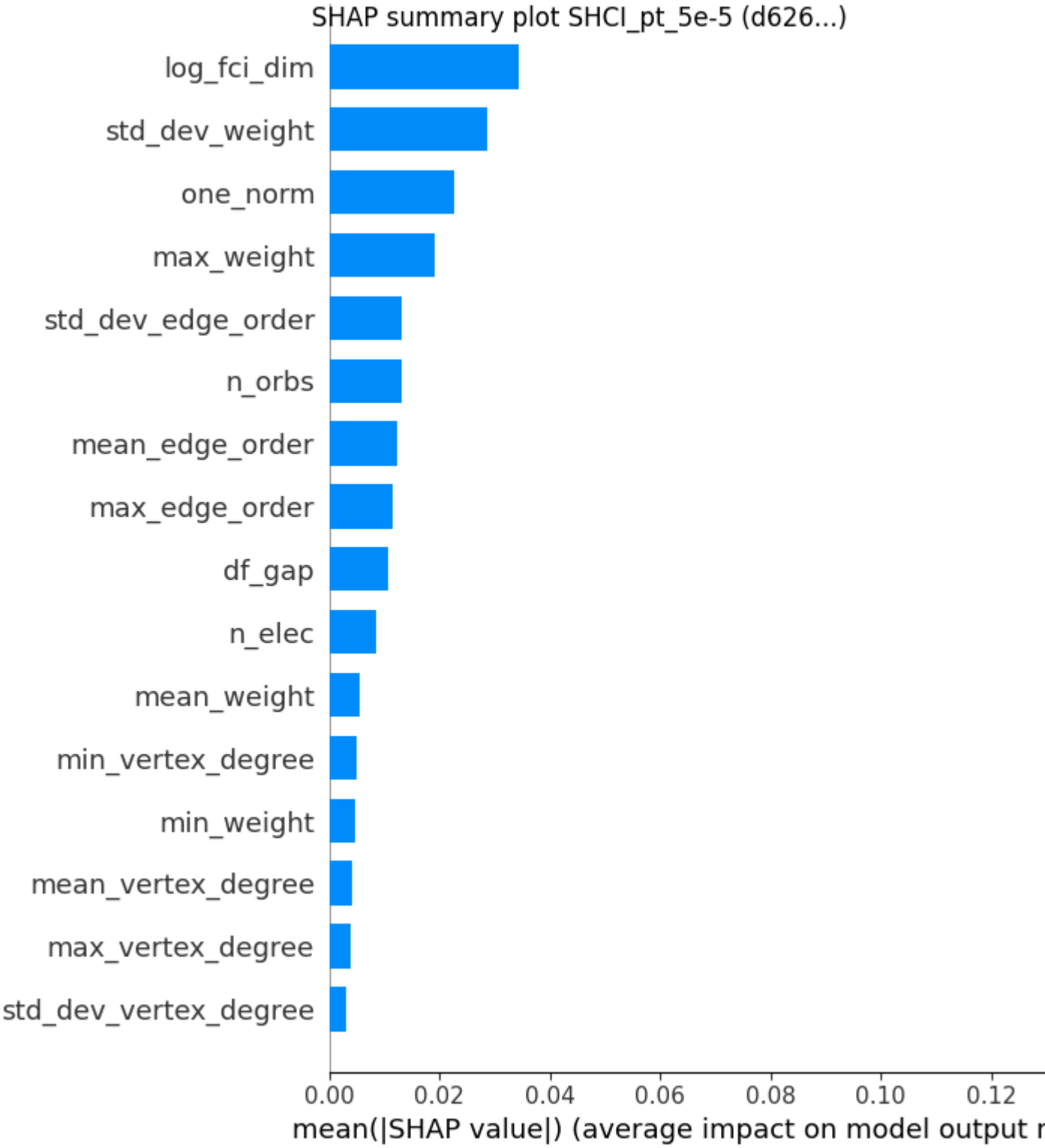


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_pt_5e-5/d626...
(captured: $8.0e+02/1.5e+07, approximately 5.3e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_pt_5e-5 (d626...)
Task failed SHCI_pt_5e-5 (d626...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: dd15fb24-e981-4464-81ac-fa60a71d2b2e

creation_timestamp: 2025-01-28T17:07:42.747013+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

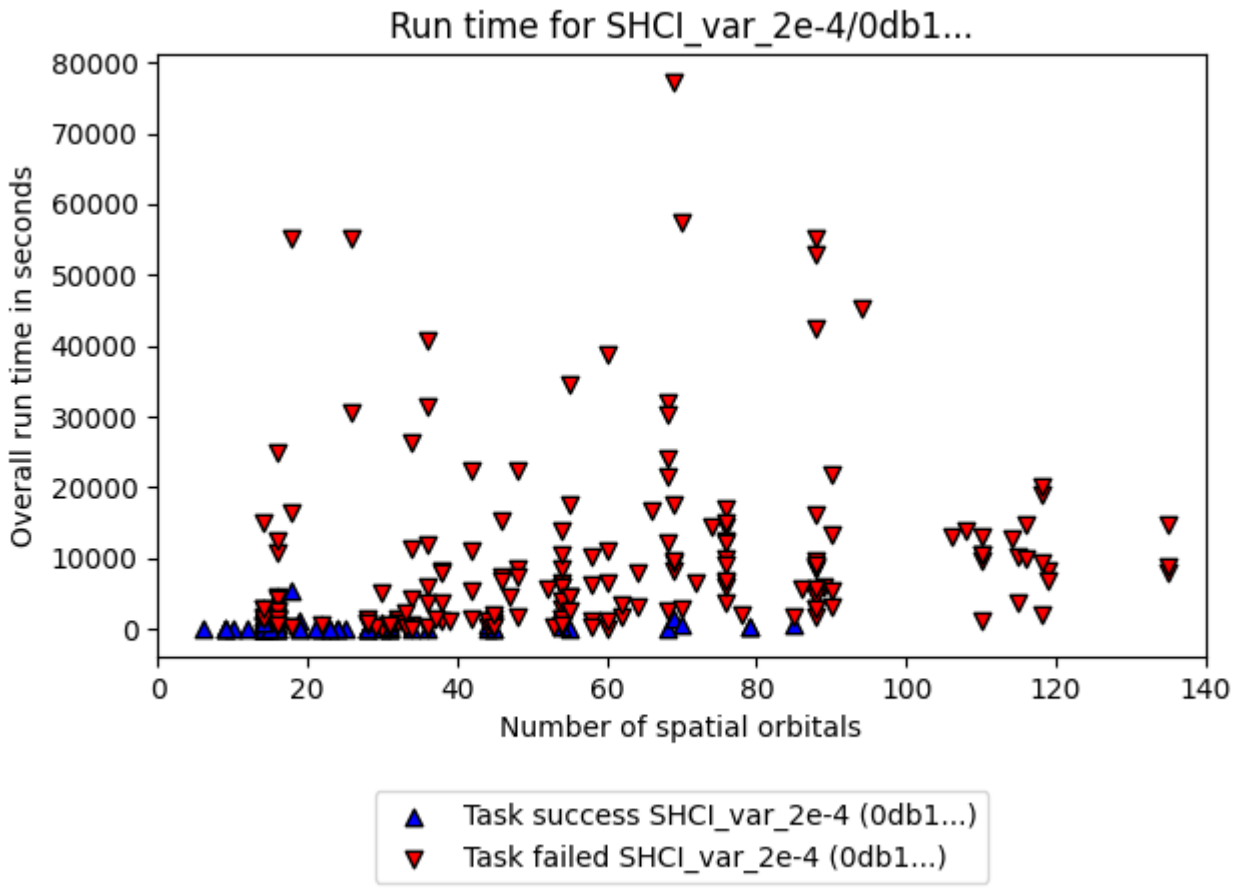
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

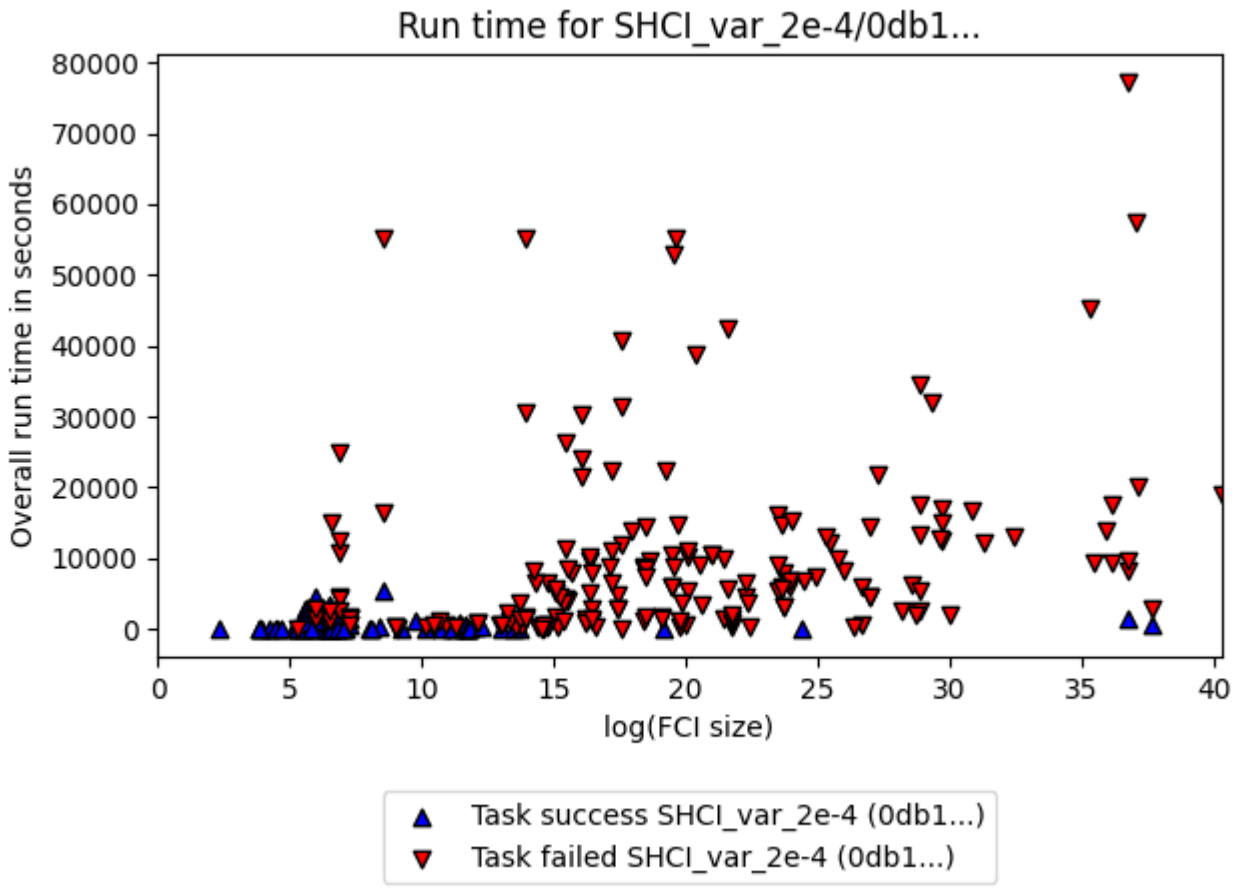
solvability_ratio: 0.3462

f1_score: [0.9864864864864865, 0.9880952380952381]

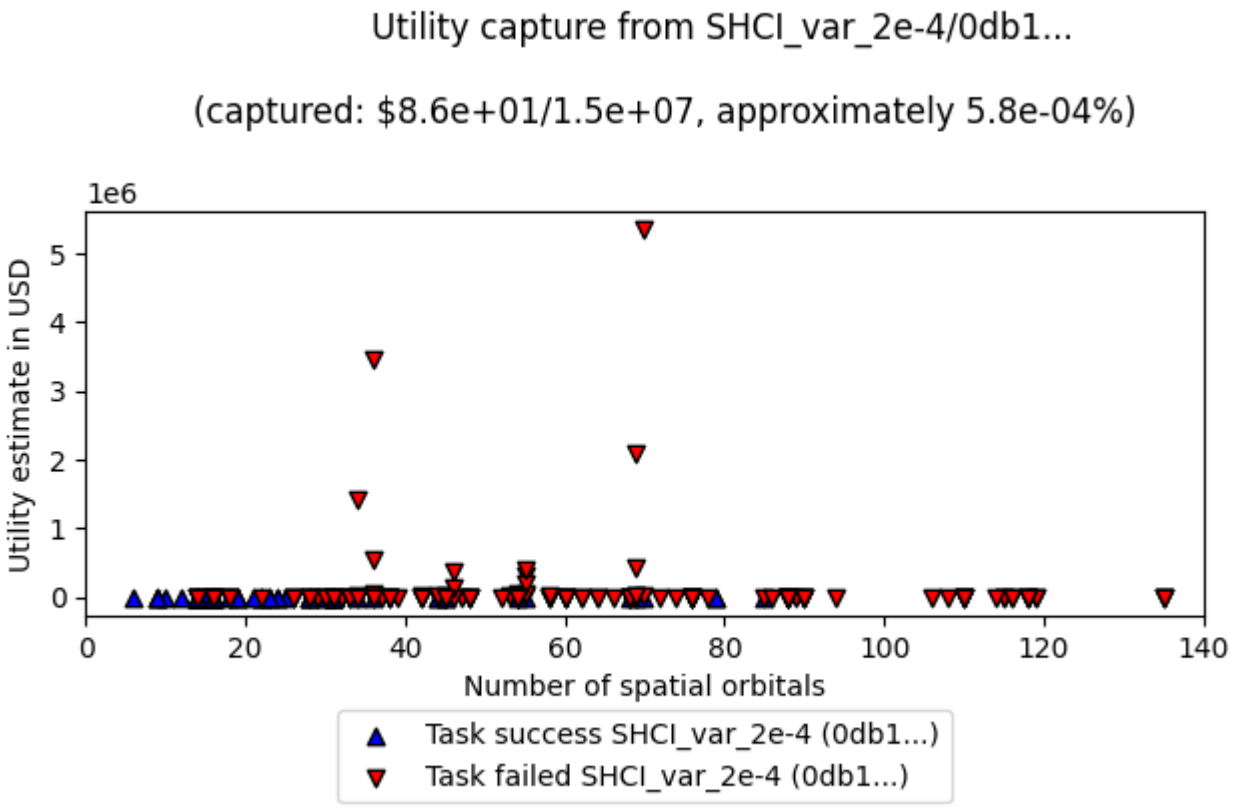
ml_metrics_calculator_version: 1

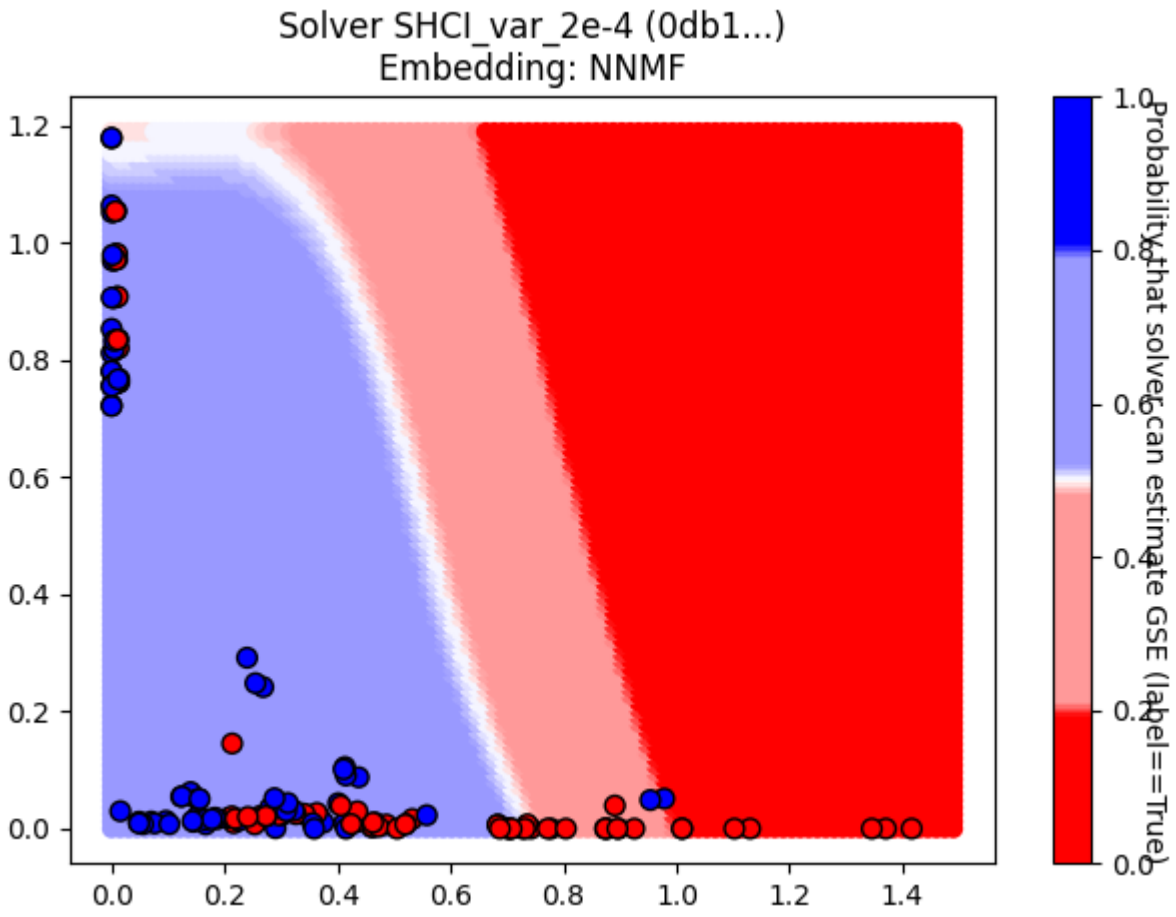


Note: plot only contains `attempted` tasks.

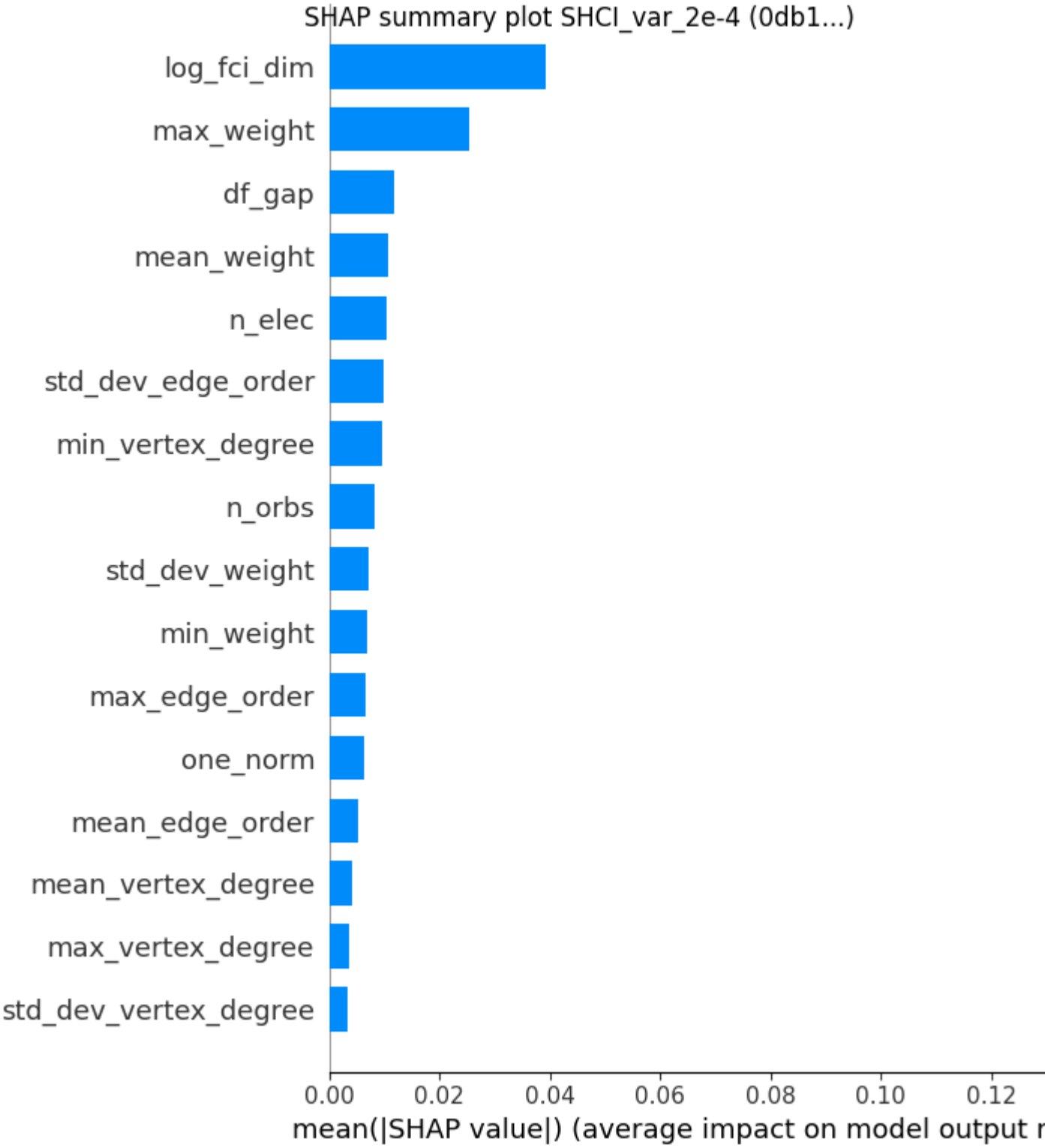


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_var_2e-4/0db1...
(captured: $8.6e+01/1.5e+07, approximately 5.8e-04%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_var_2e-4 (0db1...)
Task failed SHCI_var_2e-4 (0db1...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: a94c949a-a859-4d07-b25c-28094afea9db

creation_timestamp: 2025-01-28T17:07:42.747013+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

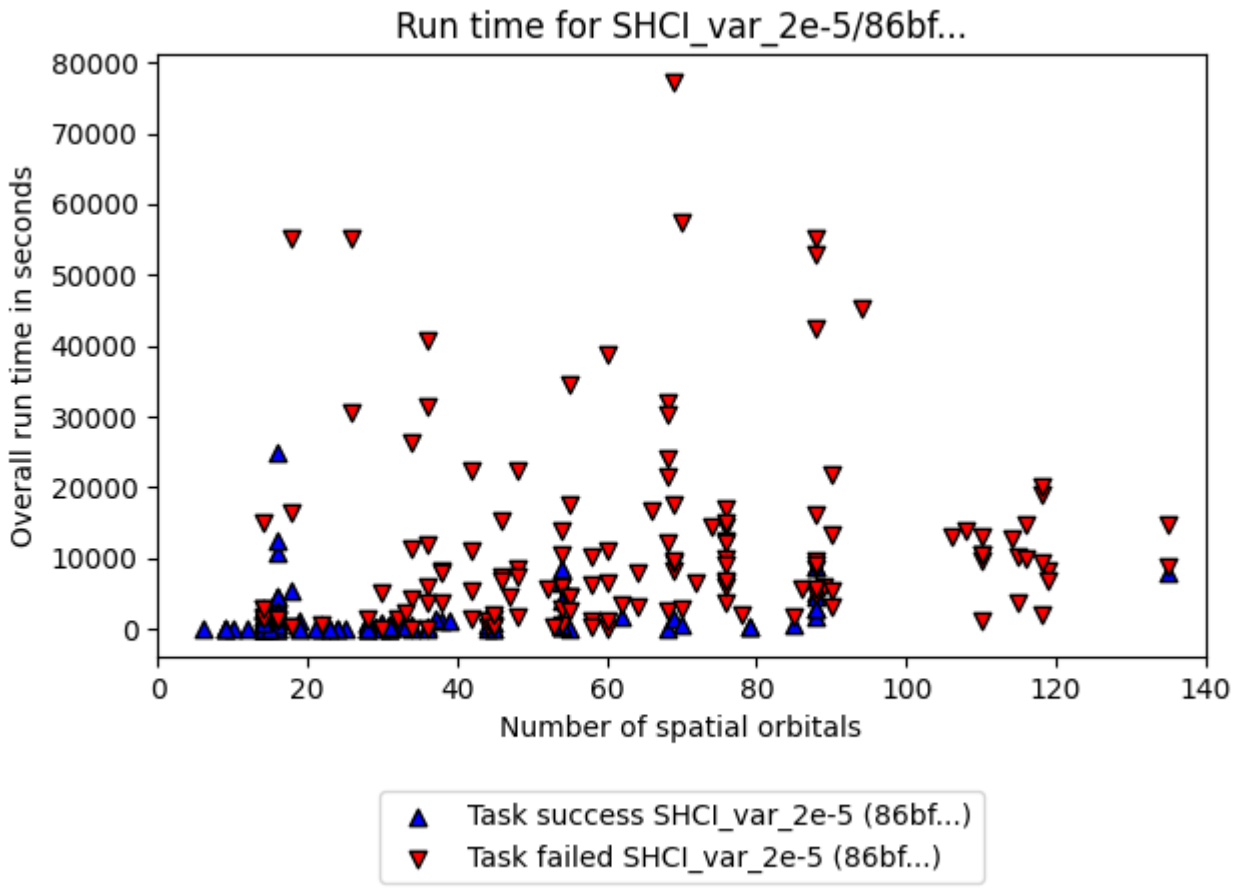
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

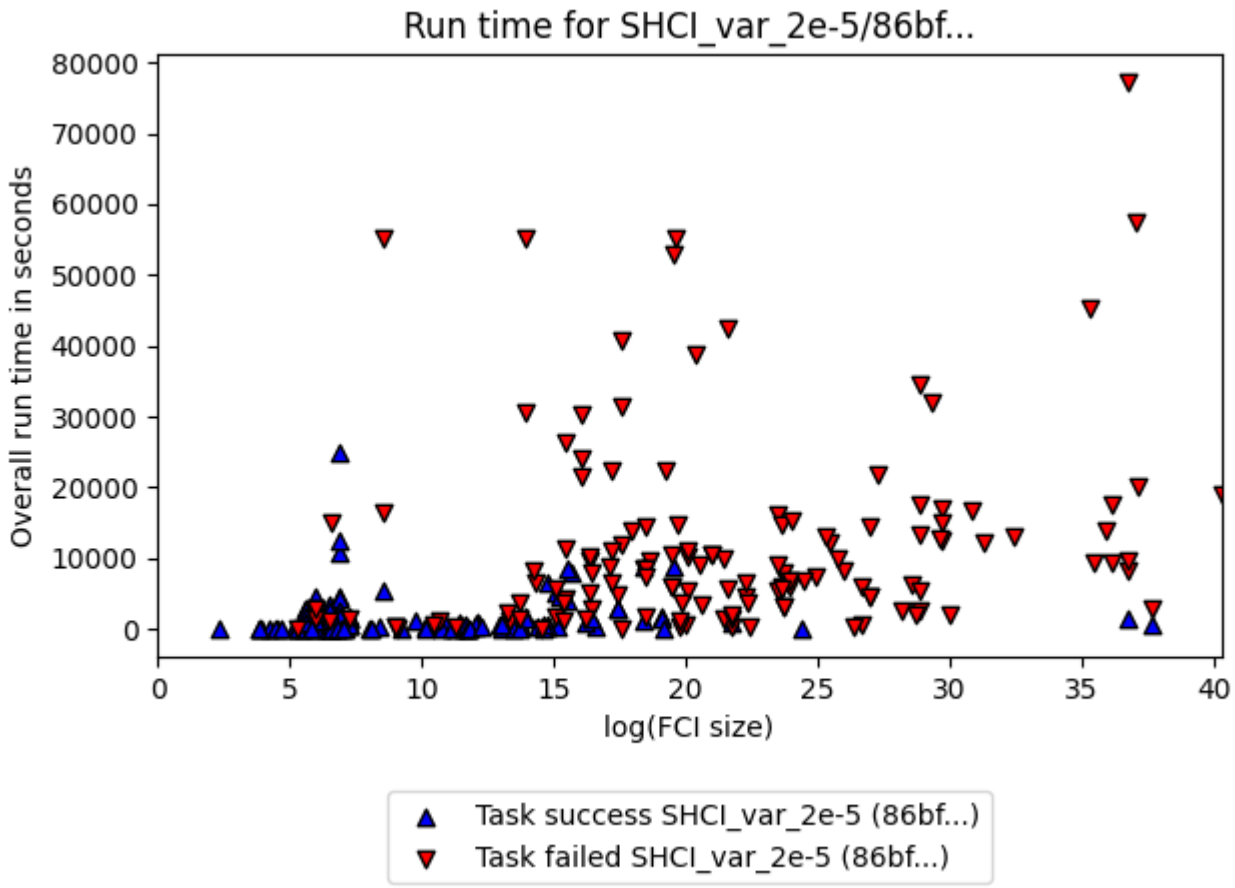
solvability_ratio: 0.592

f1_score: [0.8846153846153846, 0.9772727272727273]

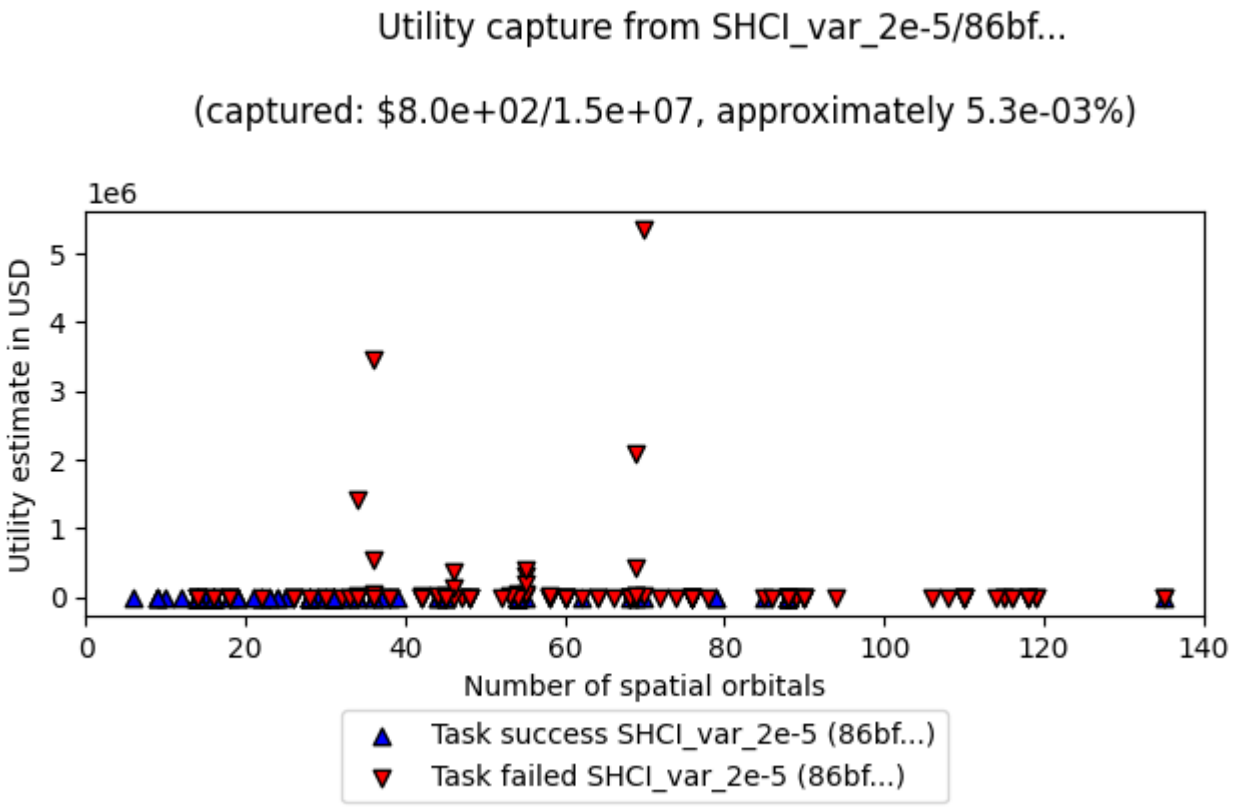
ml_metrics_calculator_version: 1

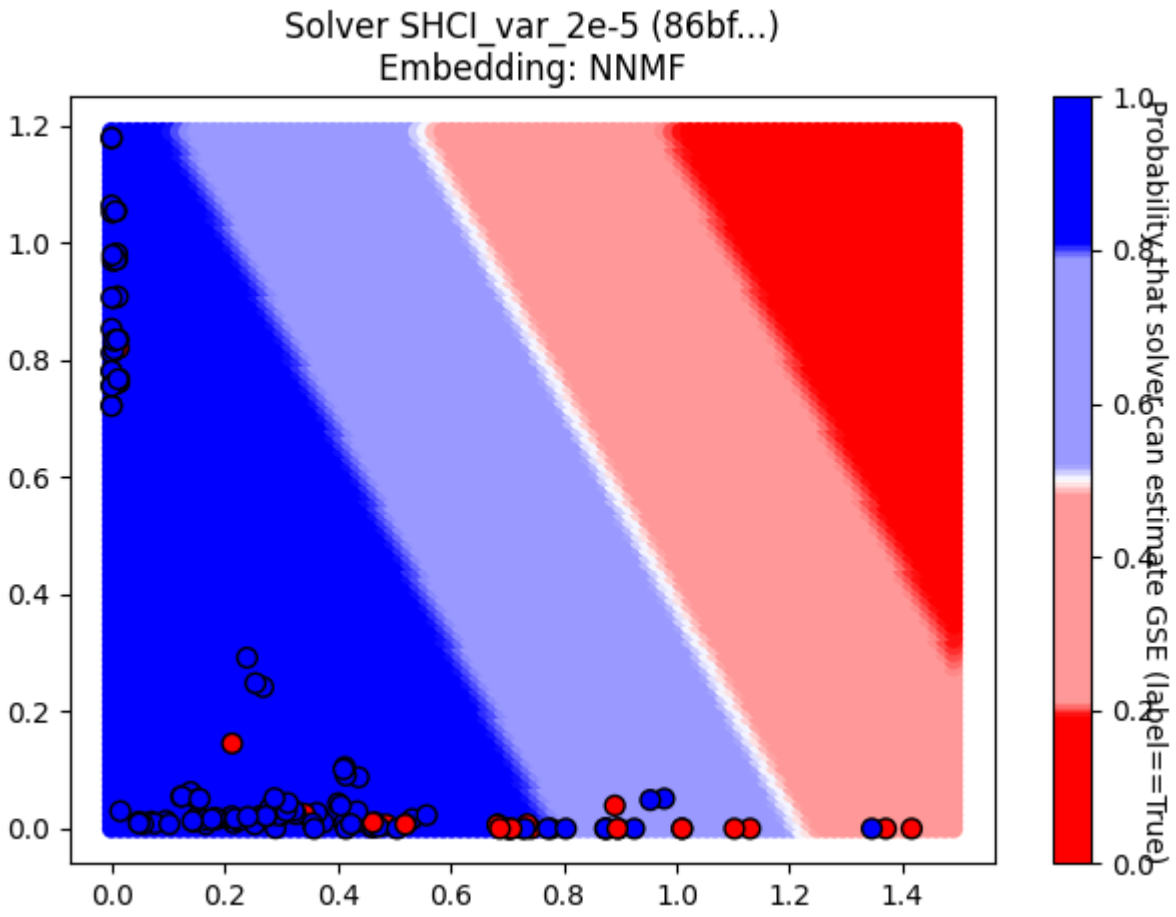


Note: plot only contains `attempted` tasks.

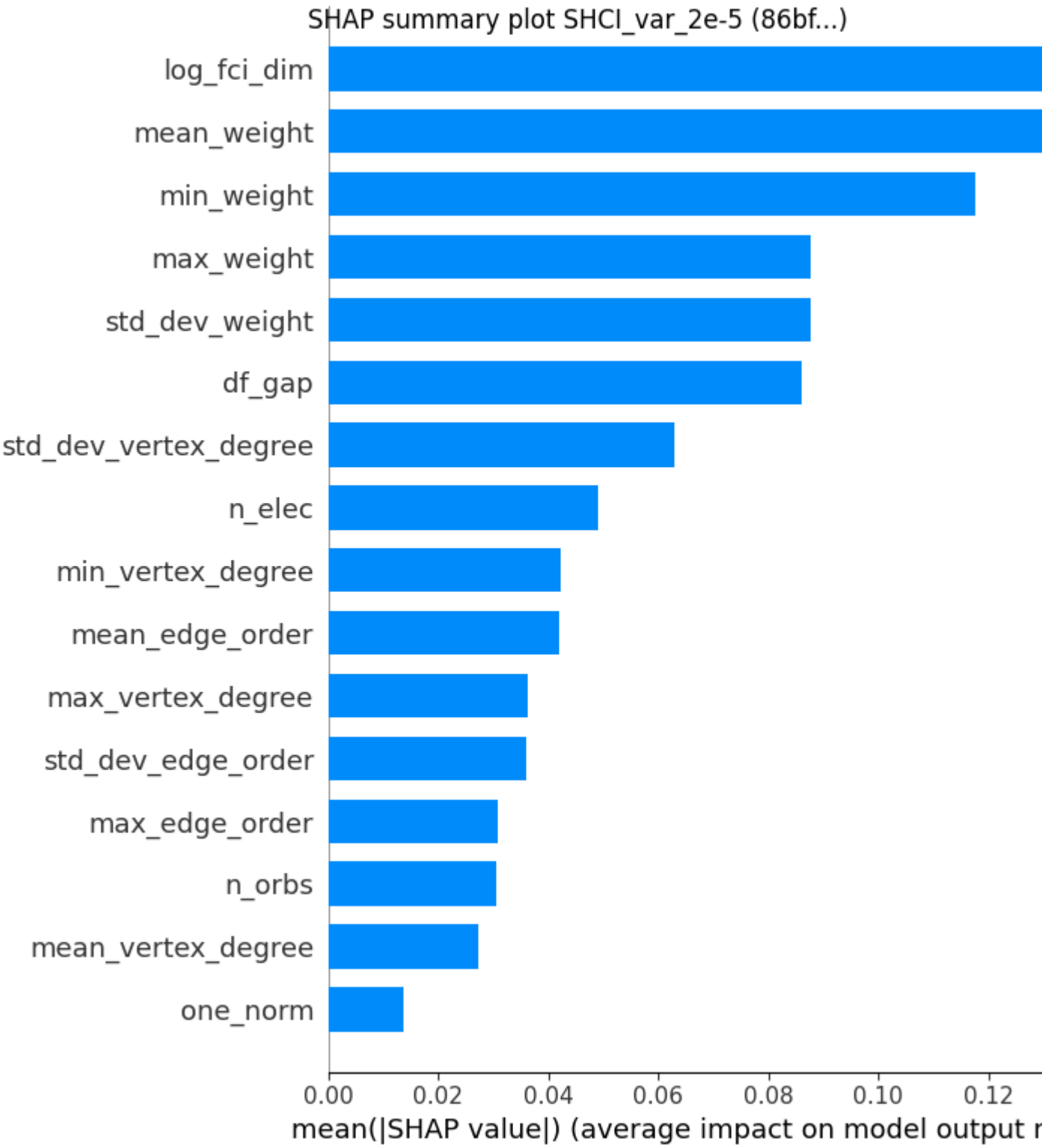


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_var_2e-5/86bf...
(captured: $8.0e+02/1.5e+07, approximately 5.3e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_var_2e-5 (86bf...)
Task failed SHCI_var_2e-5 (86bf...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: 48fc7a3a-bf8a-4fa4-b168-62de5ab1f49b

creation_timestamp: 2025-01-28T17:07:42.747013+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

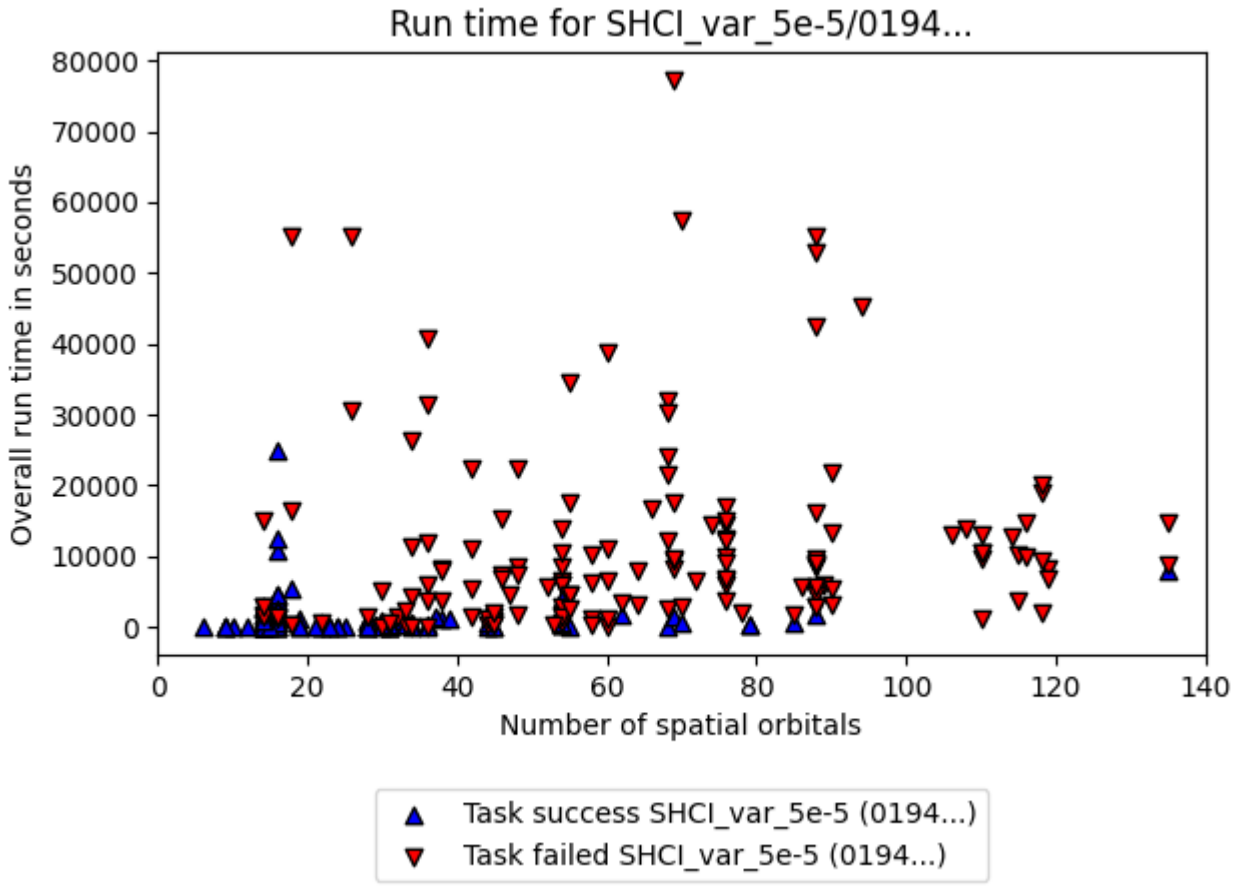
max_run_time_of_attempted_tasks: 77244.15200000002

sum_of_run_time_of_attempted_tasks: 1863349.633000001

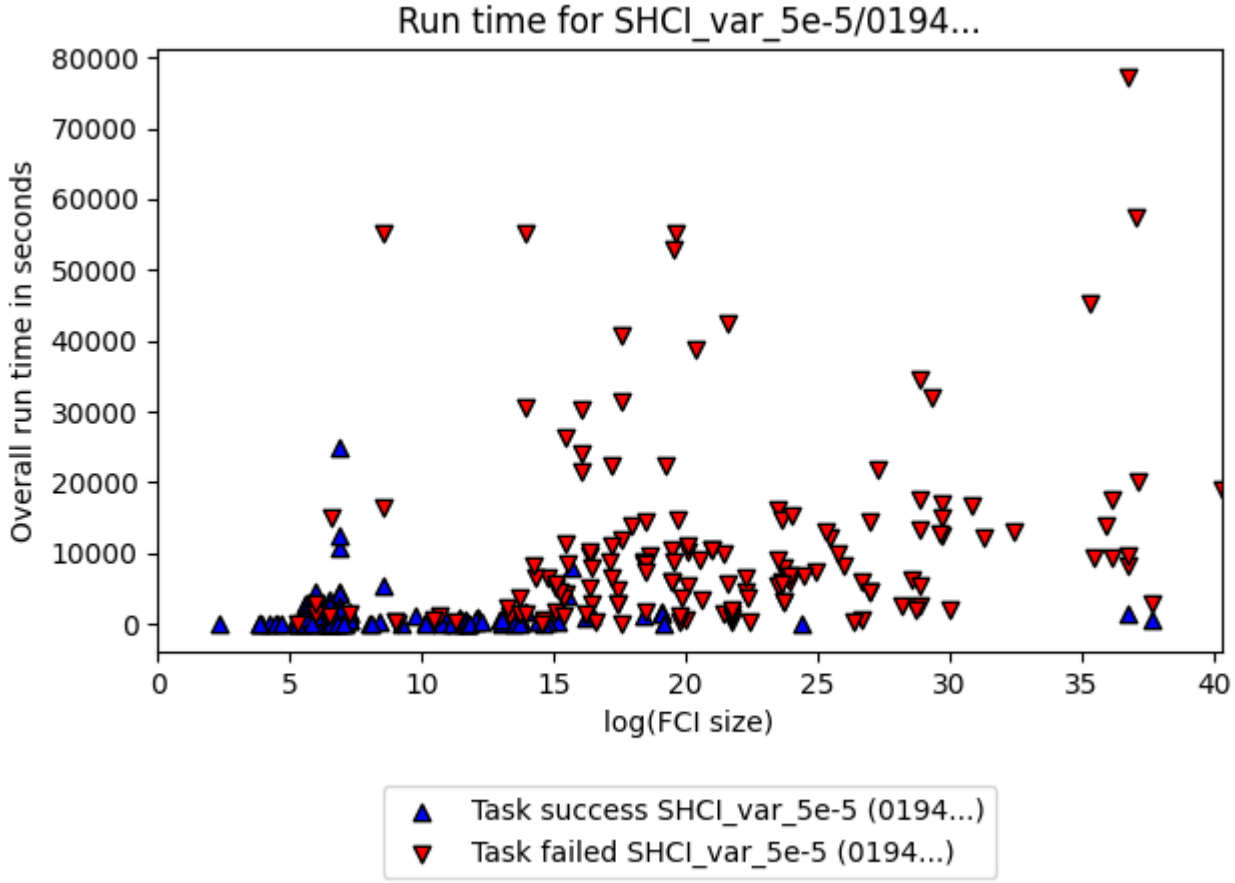
solvability_ratio: 0.3443

f1_score: [0.85, 0.9491525423728814]

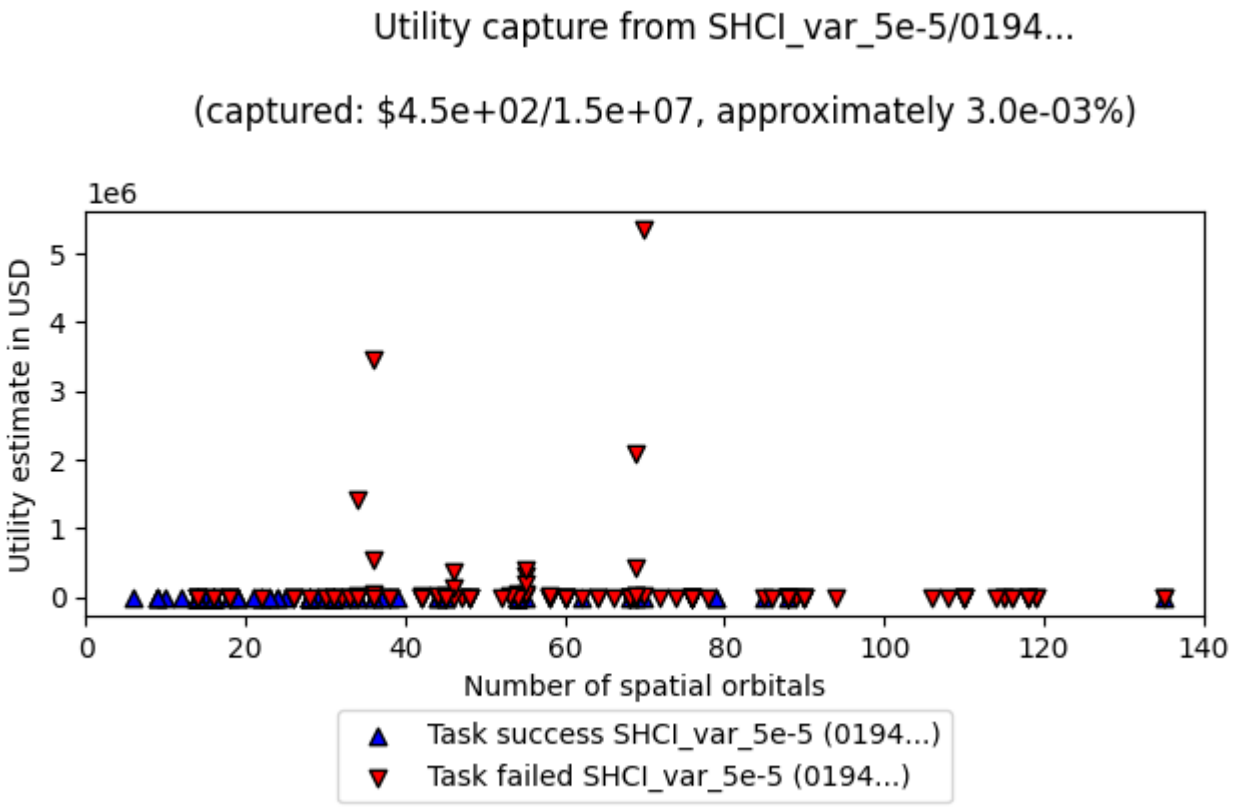
ml_metrics_calculator_version: 1

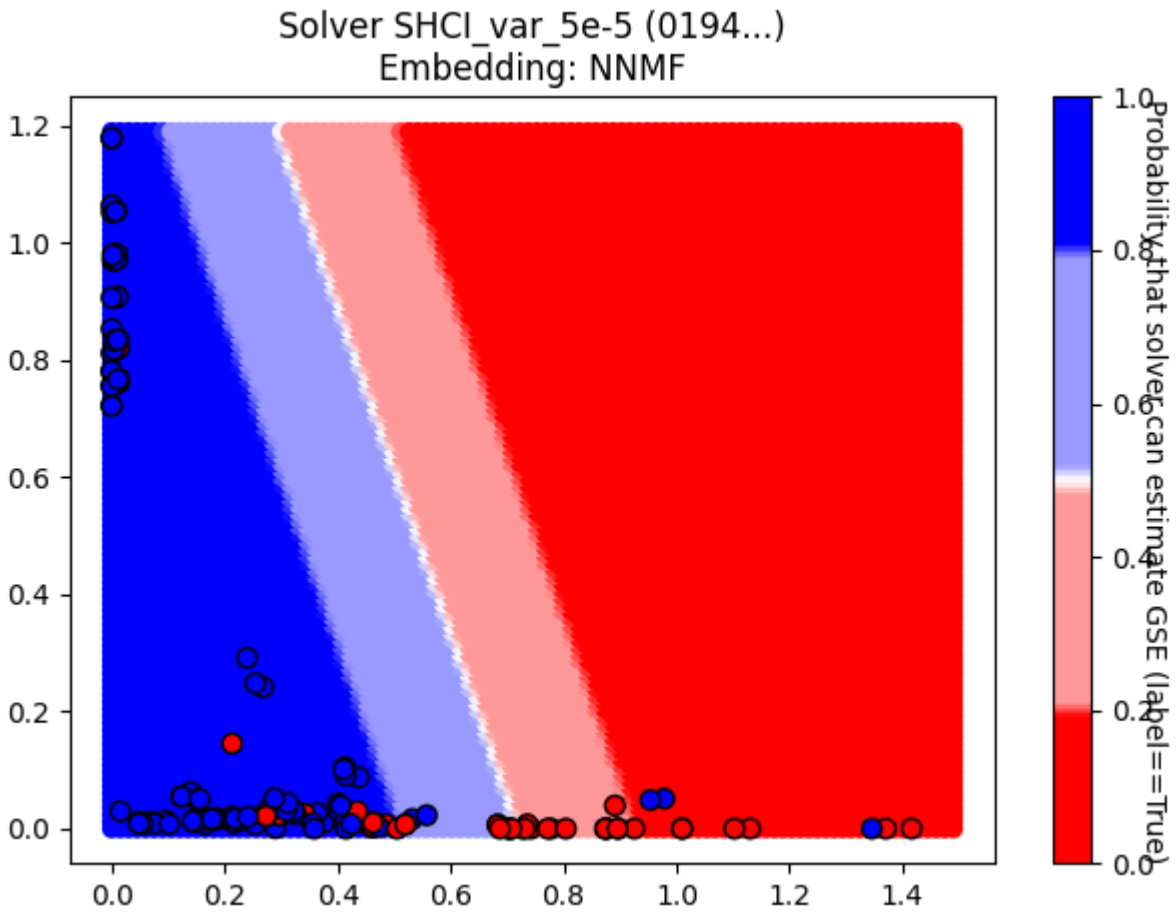


Note: plot only contains `attempted` tasks.

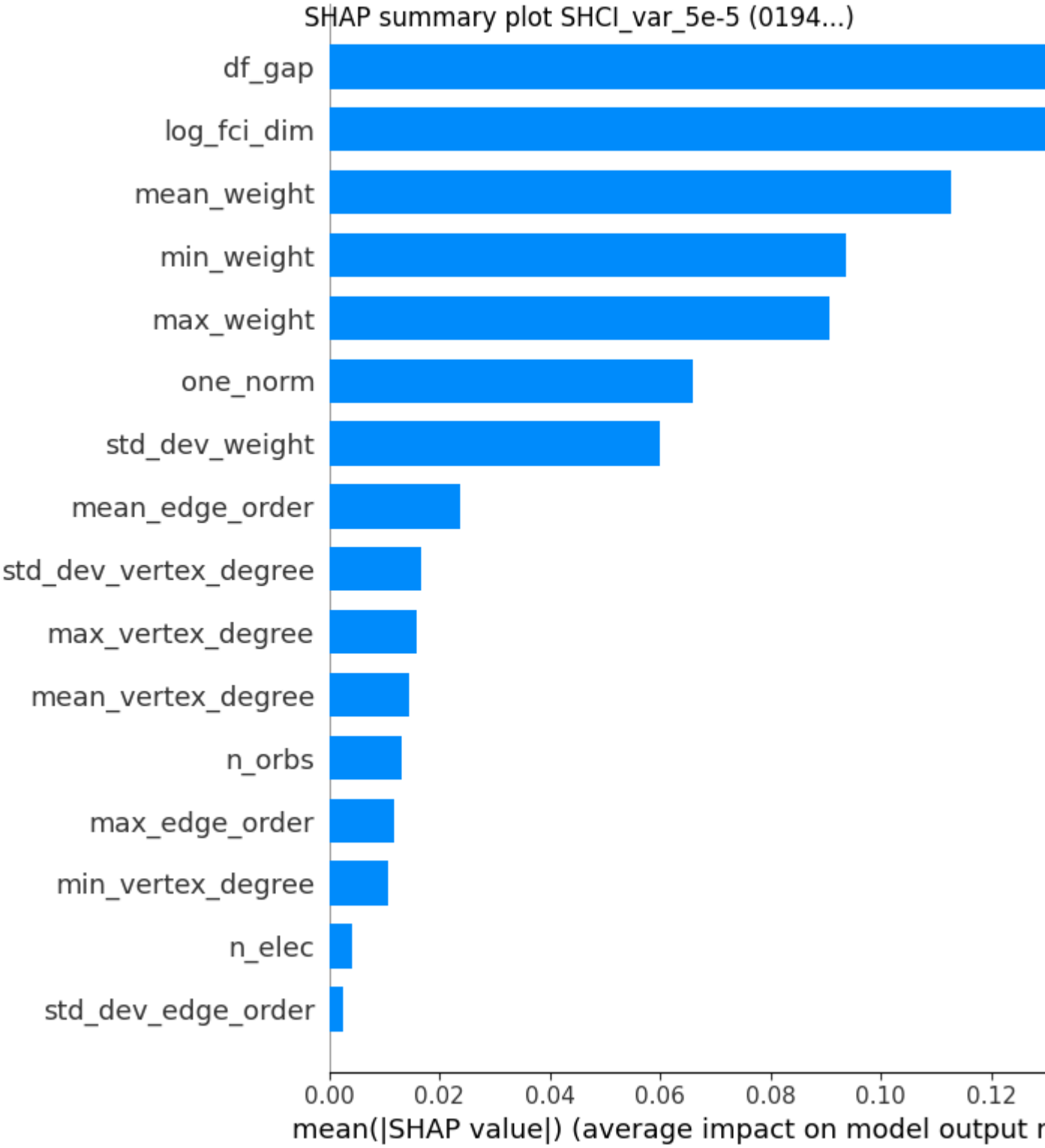


Note: plot only contains `attempted` tasks.


Utility capture from SHCI_var_5e-5/0194...
(captured: $4.5e+02/1.5e+07, approximately 3.0e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_var_5e-5 (0194...)
Task failed SHCI_var_5e-5 (0194...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: ff0f05ef-a965-43d1-8960-c8b0e3ca996d

creation_timestamp: 2025-01-28T17:07:42.747013+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

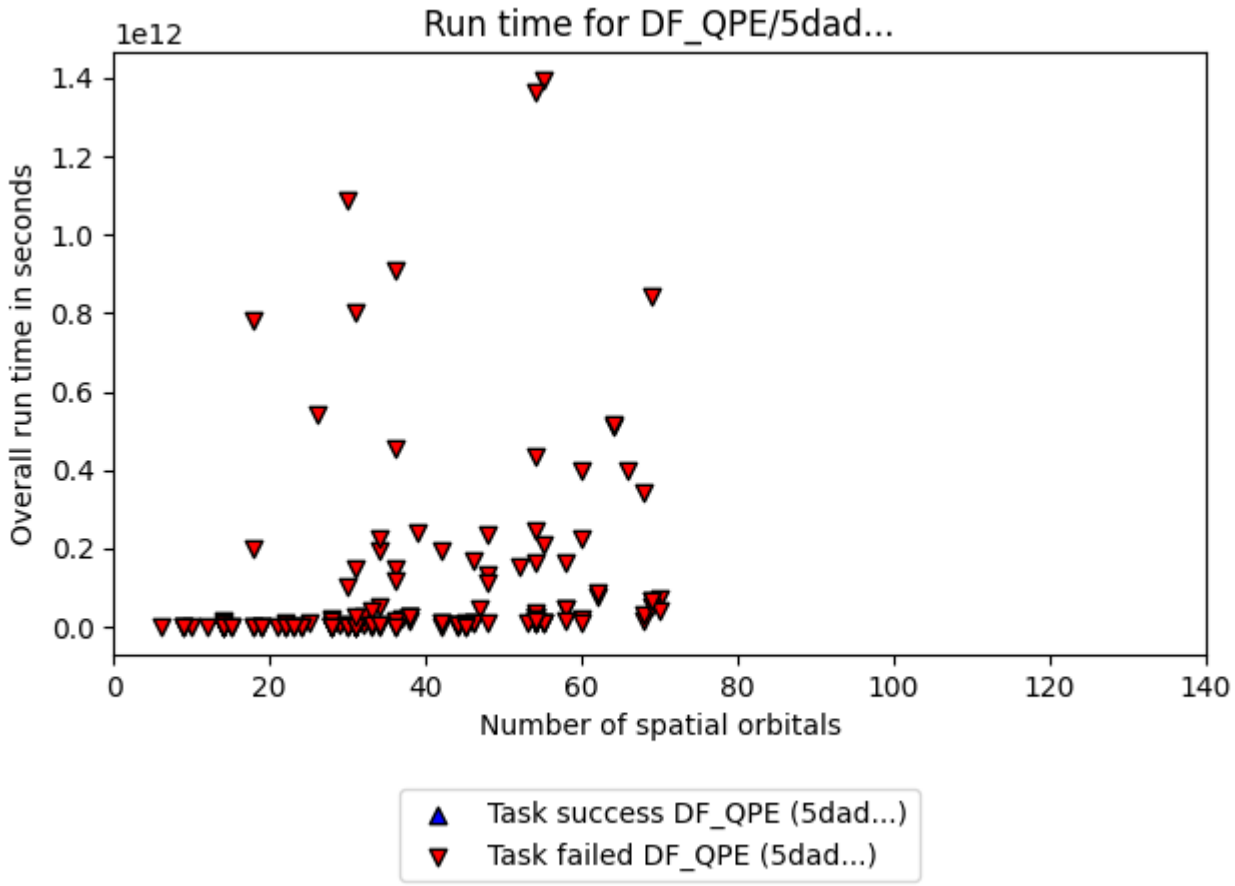
sum_of_run_time_of_attempted_tasks: 15652541022388.93

solvability_ratio: None

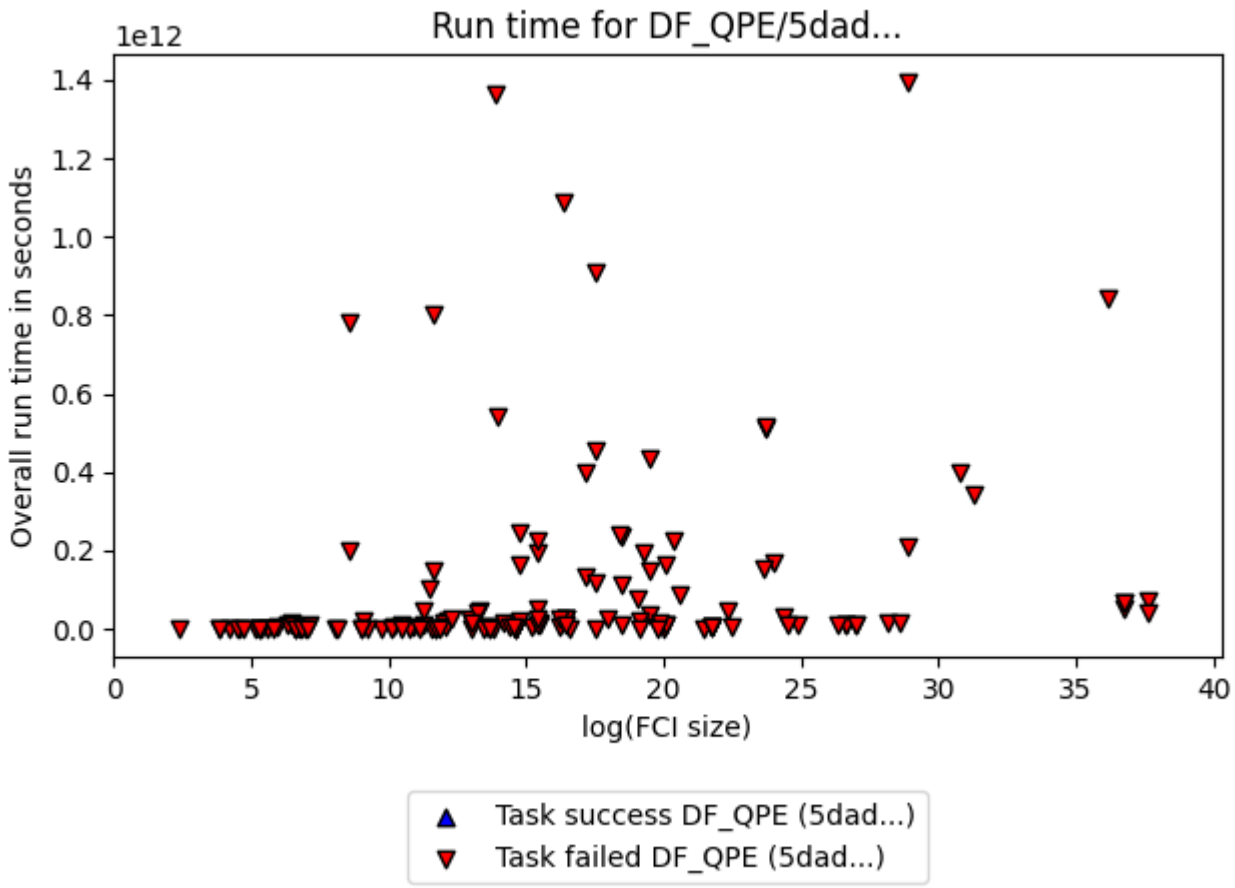
f1_score: None

ml_metrics_calculator_version: 1

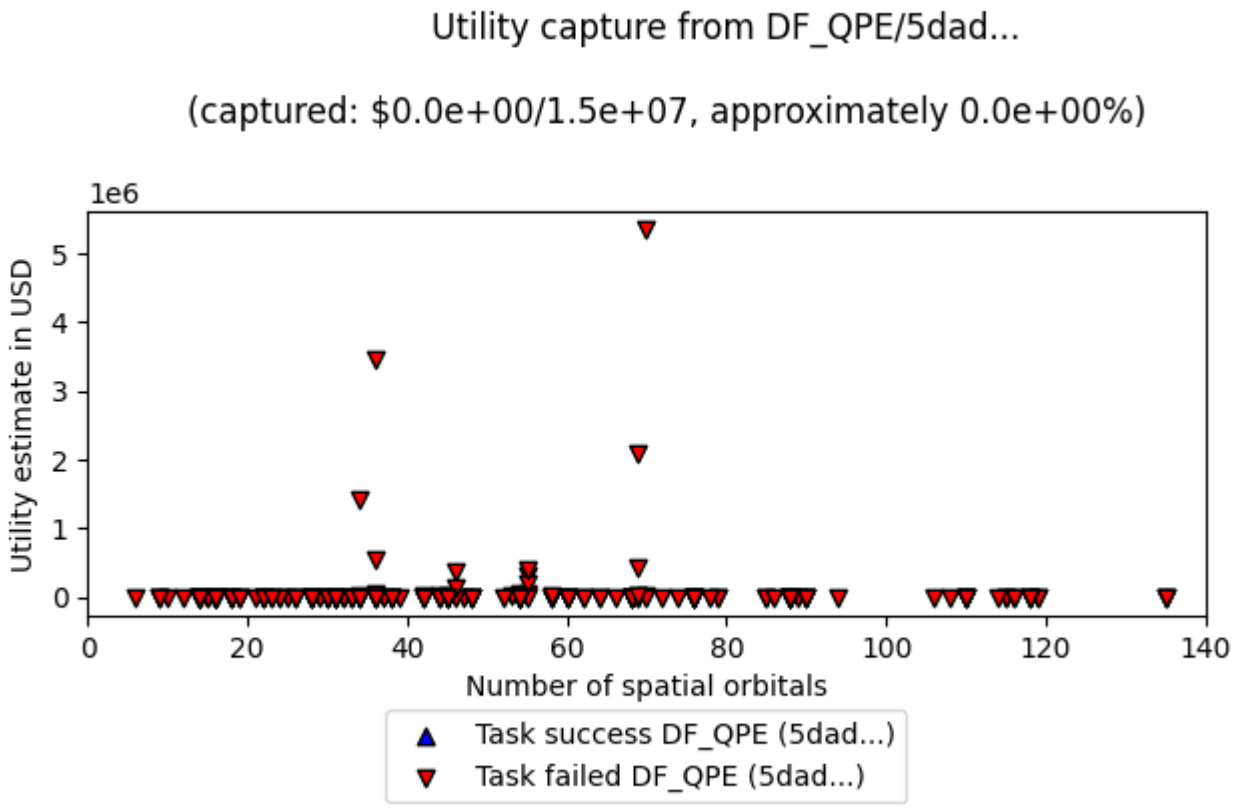
comment: All labels were either all `True` or all `False` and we cannot create an ML model with only one class.



Note: plot only contains `attempted` tasks.



Note: plot only contains `attempted` tasks.



Solver miniML plot

Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)

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: f977a25c-b18a-47f4-b8e0-81979949b19f

creation_timestamp: 2025-01-28T17:07:42.747013+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

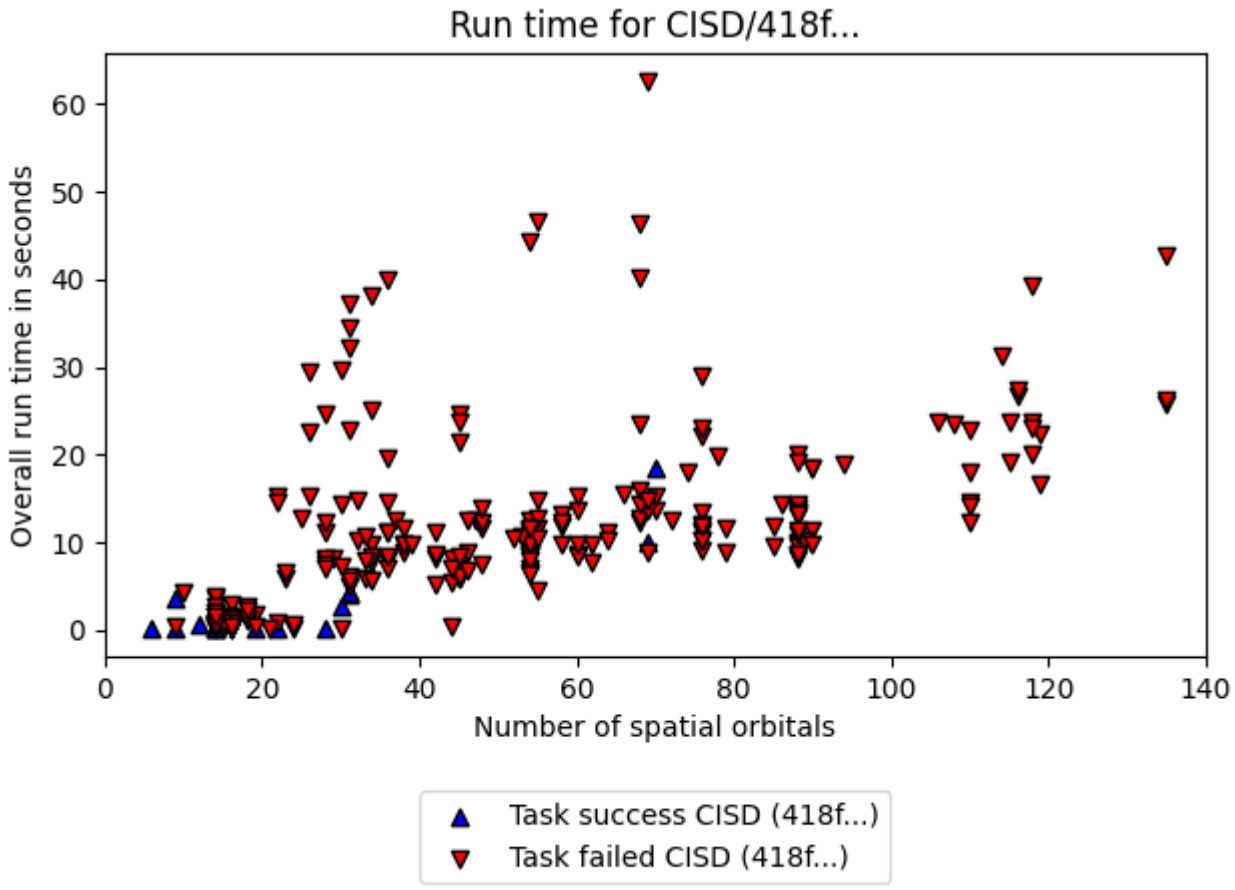
max_run_time_of_attempted_tasks: 62.58296537399292

sum_of_run_time_of_attempted_tasks: 2929.870177745819

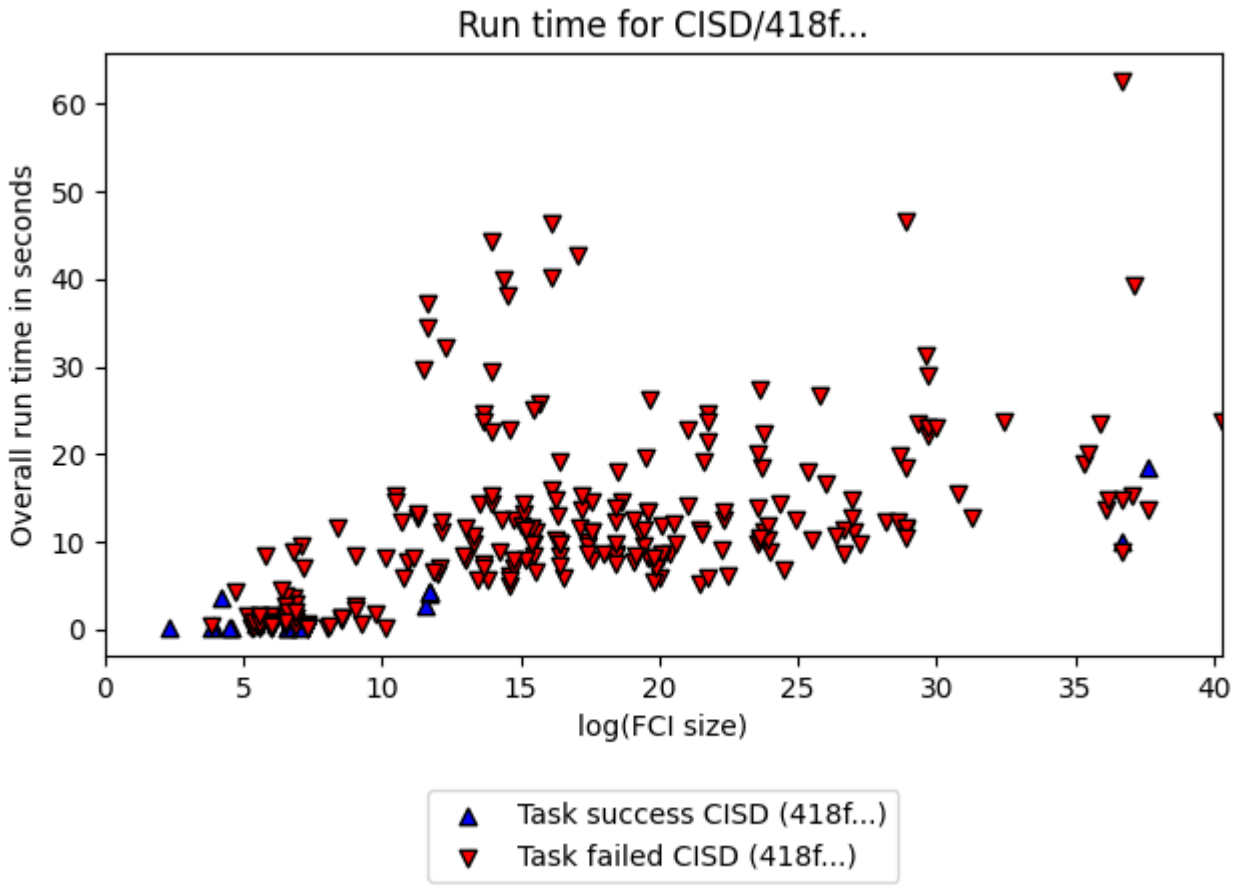
solvability_ratio: 0.2773

f1_score: [0.9819494584837545, 0.8717948717948718]

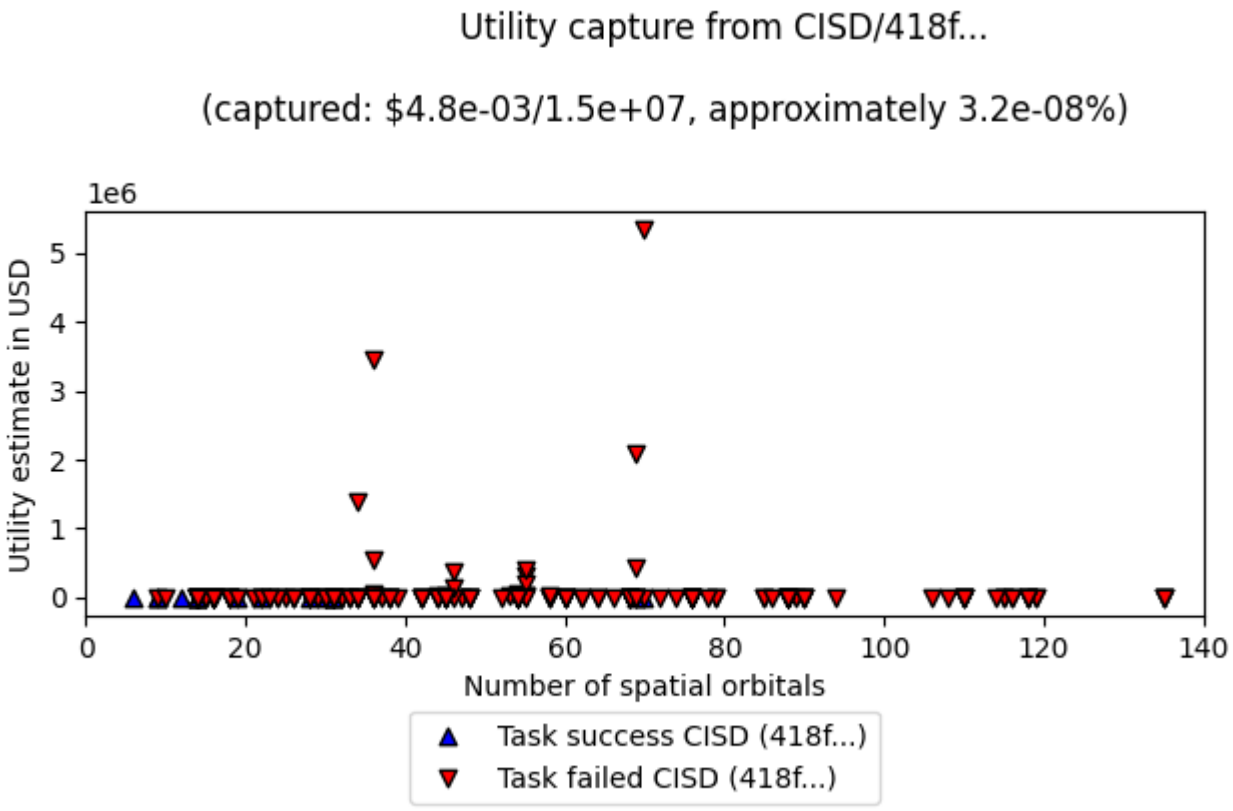
ml_metrics_calculator_version: 1

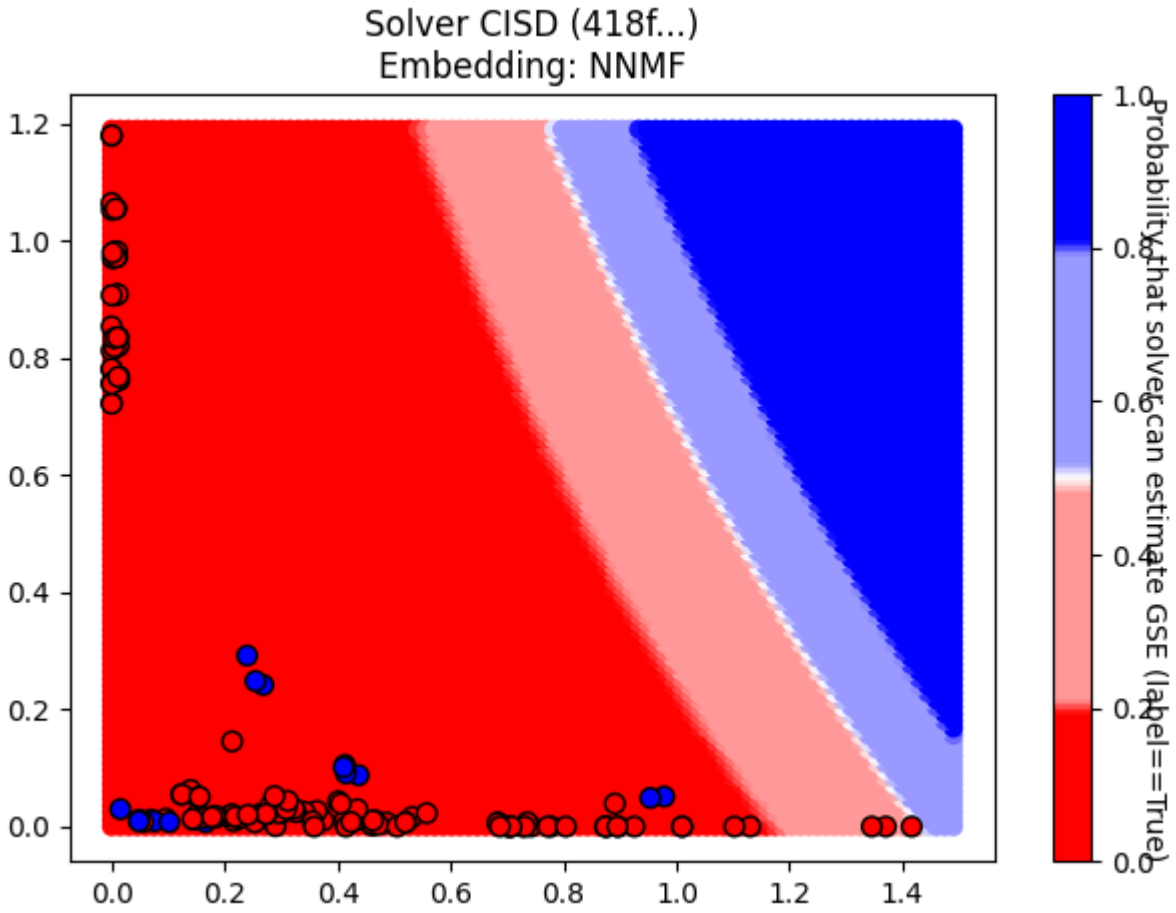


Note: plot only contains `attempted` tasks.

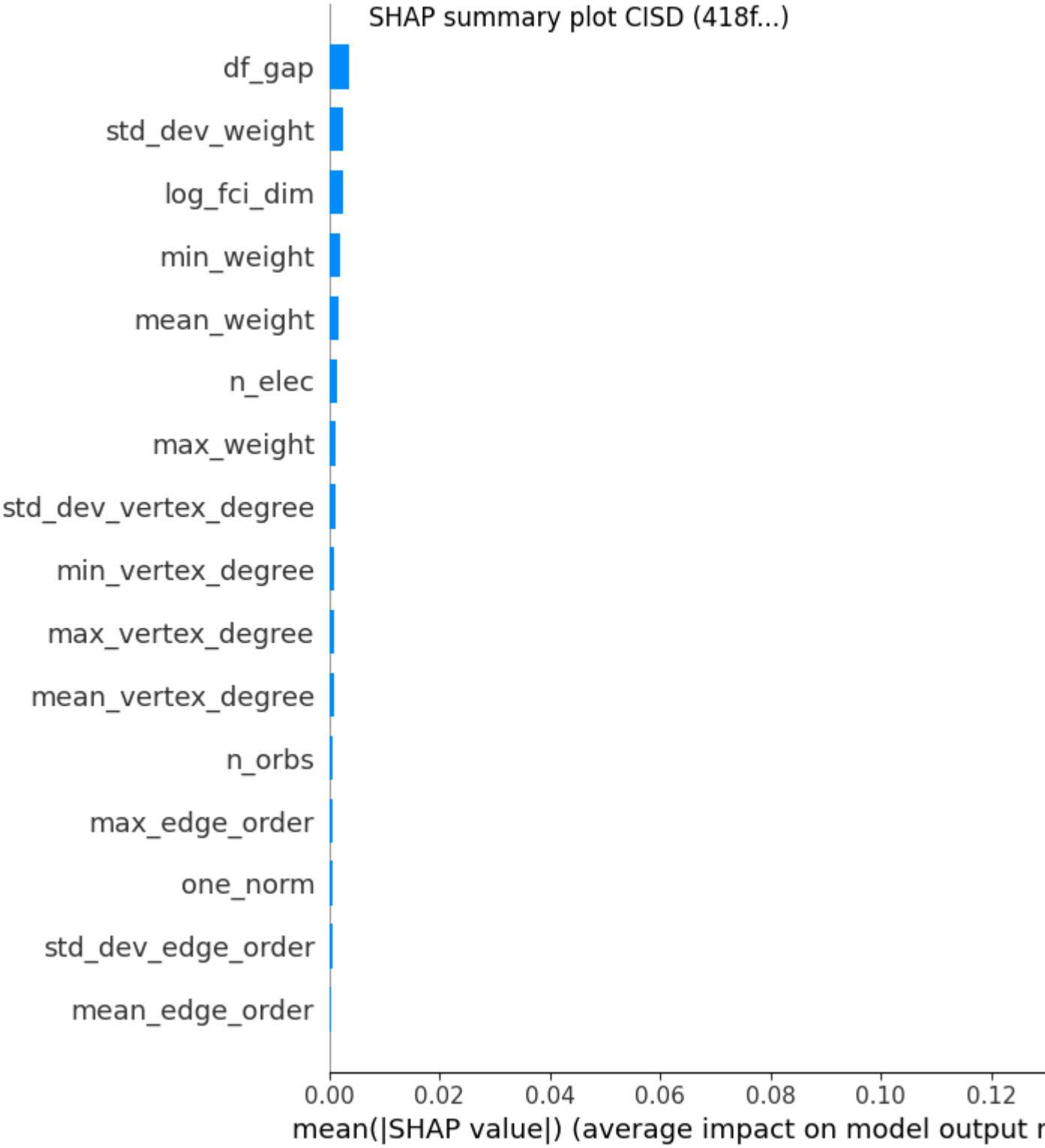


Note: plot only contains `attempted` tasks.


Utility capture from CISD/418f...
(captured: $4.8e-03/1.5e+07, approximately 3.2e-08%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CISD (418f...)
Task failed CISD (418f...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: 55960442-3a06-48c0-a7cb-4841d1f1f871

creation_timestamp: 2025-01-28T17:07:42.747013+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

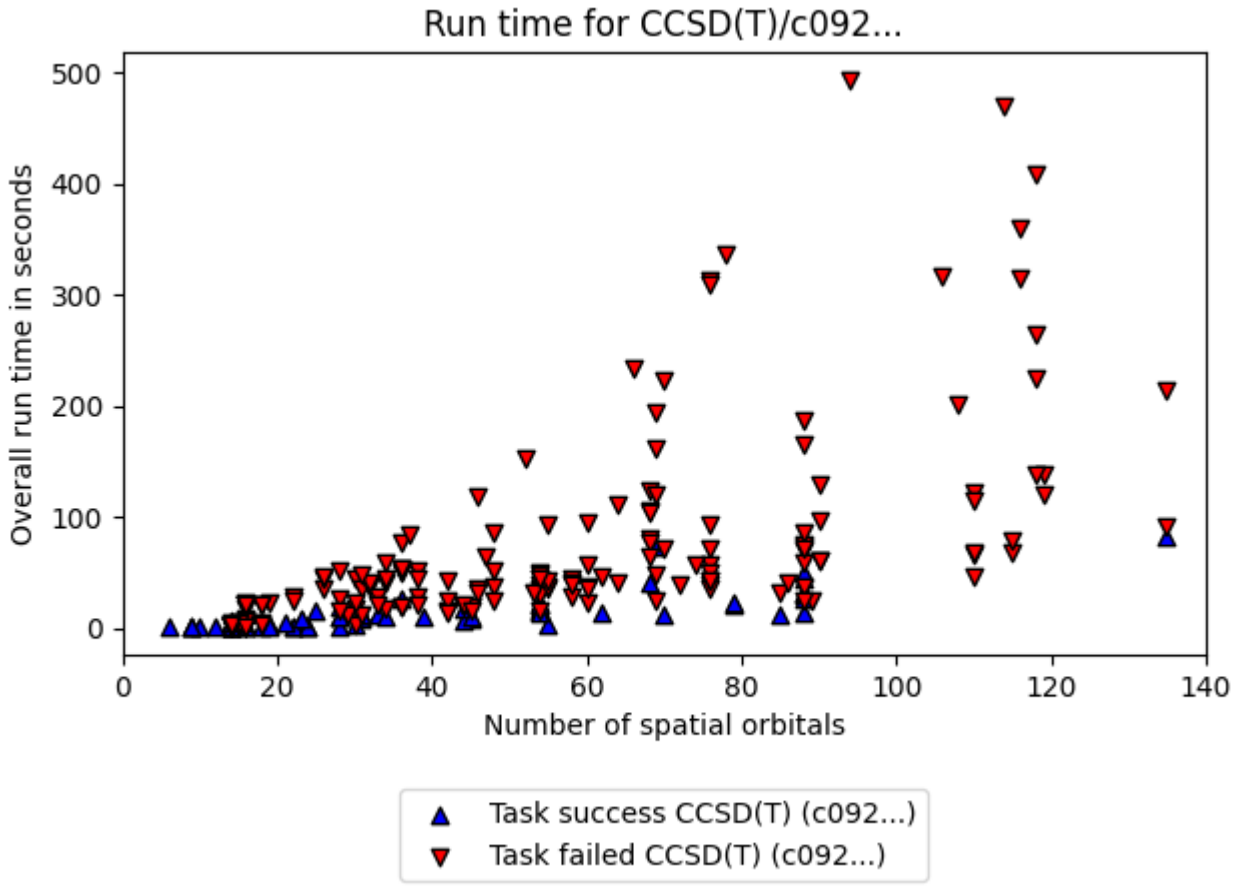
max_run_time_of_attempted_tasks: 493.4080808162689

sum_of_run_time_of_attempted_tasks: 13199.317583084106

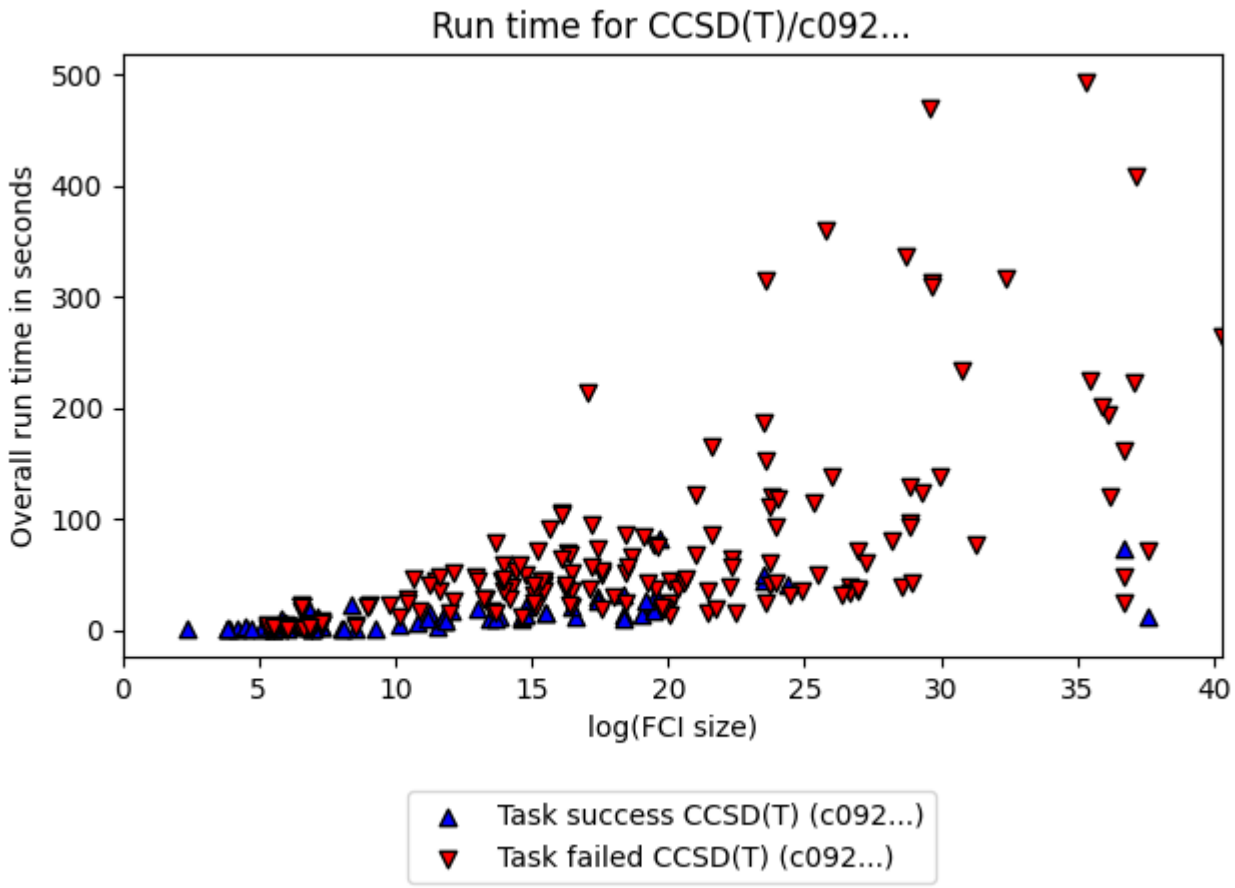
solvability_ratio: 0.8567

f1_score: [0.8795180722891566, 0.8666666666666667]

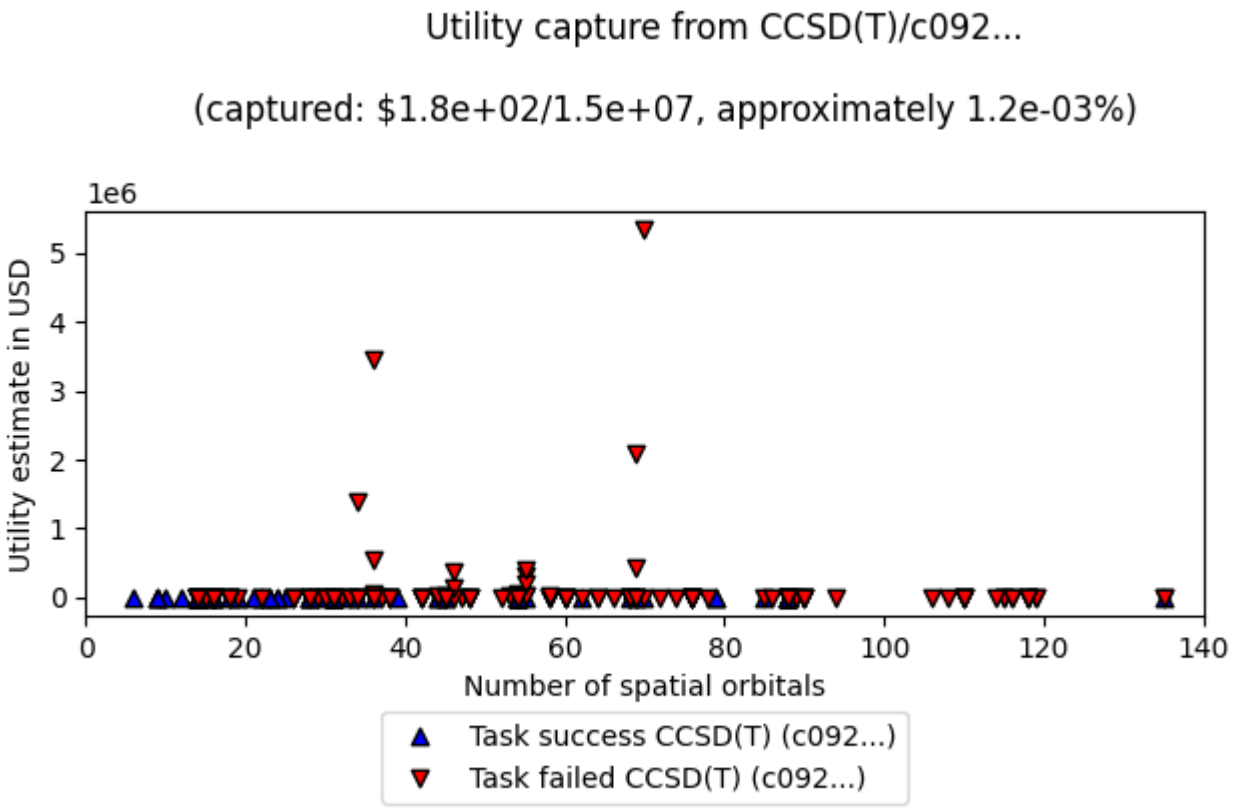
ml_metrics_calculator_version: 1

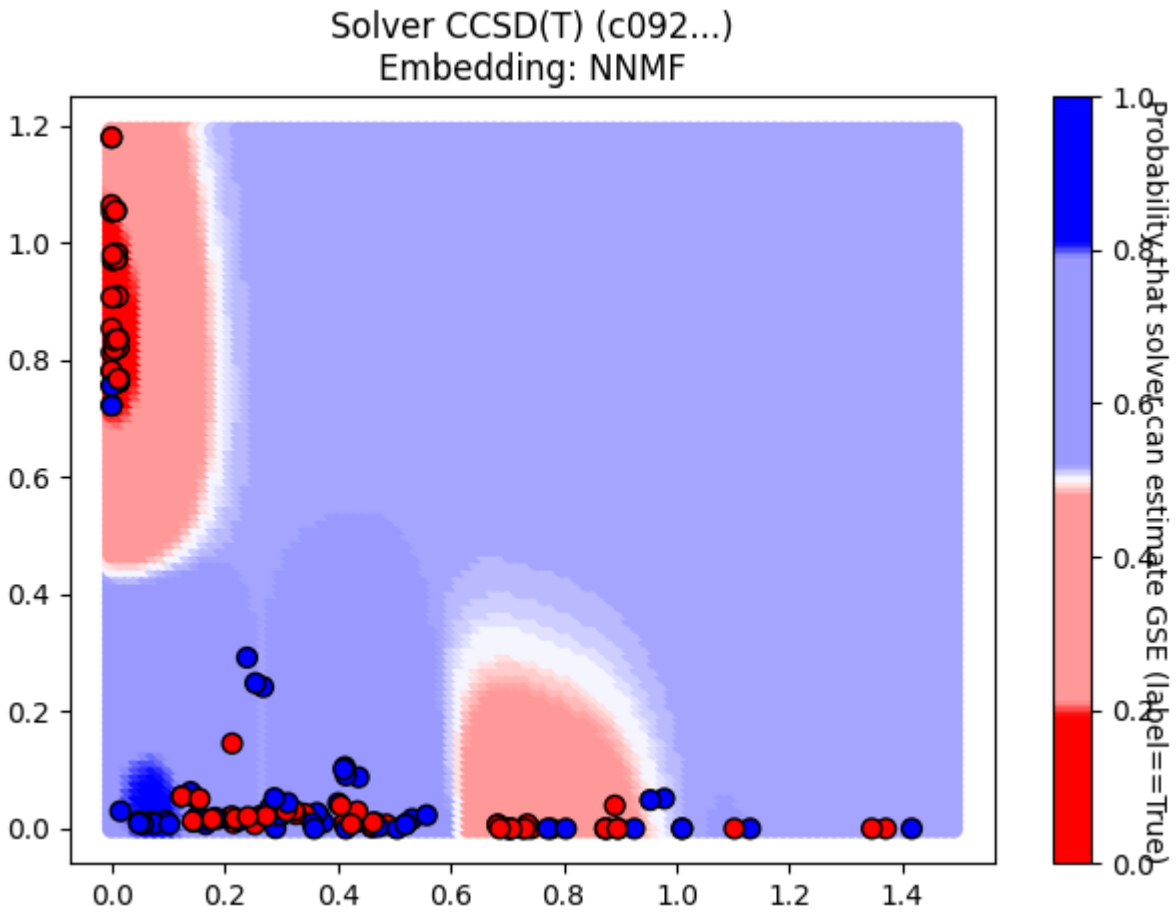


Note: plot only contains `attempted` tasks.

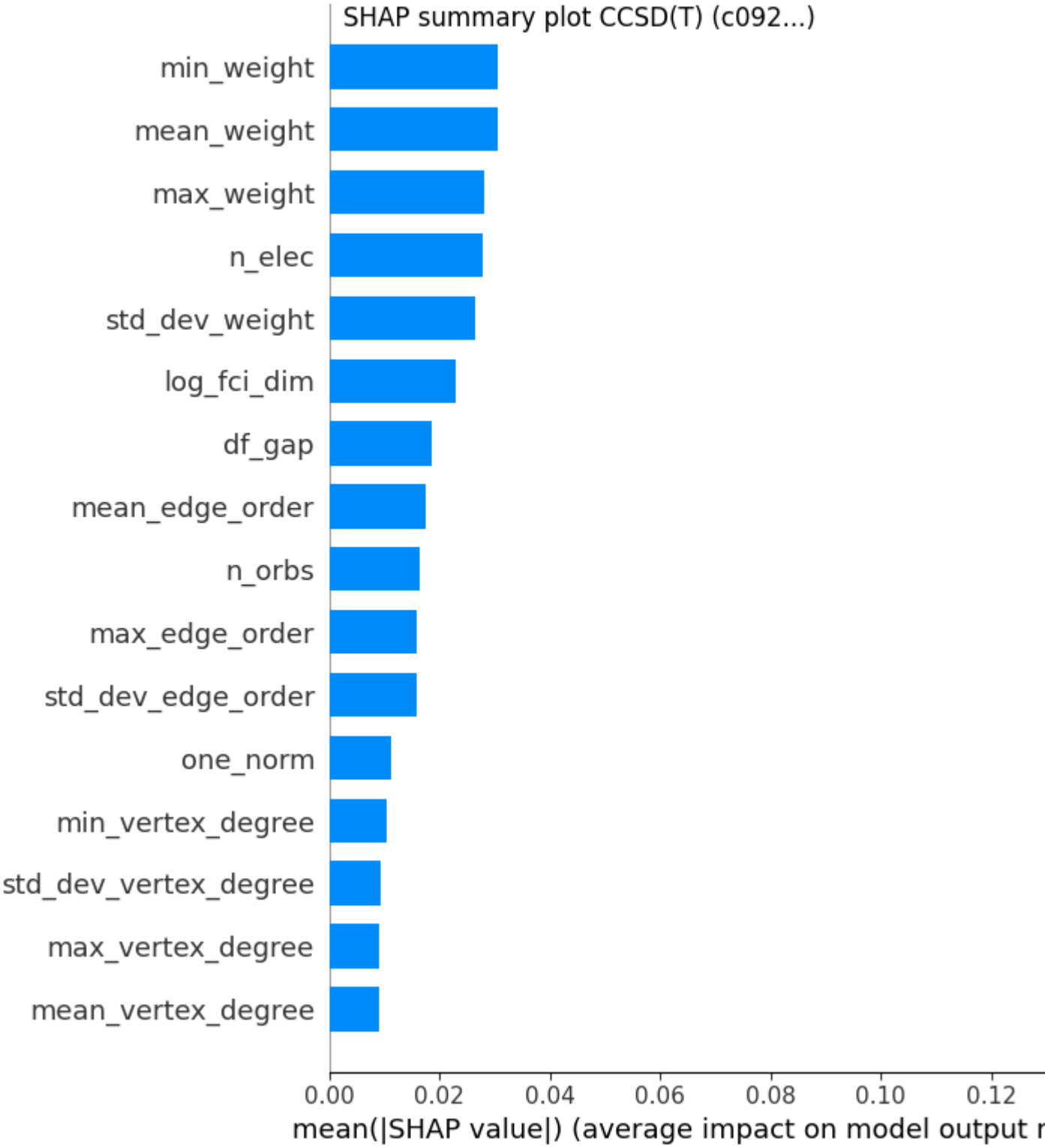


Note: plot only contains `attempted` tasks.


Utility capture from CCSD(T)/c092...
(captured: $1.8e+02/1.5e+07, approximately 1.2e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSD(T) (c092...)
Task failed CCSD(T) (c092...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: d3040414-62ea-470b-8694-23b30cbbe4d8

creation_timestamp: 2025-01-28T17:07:42.747013+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

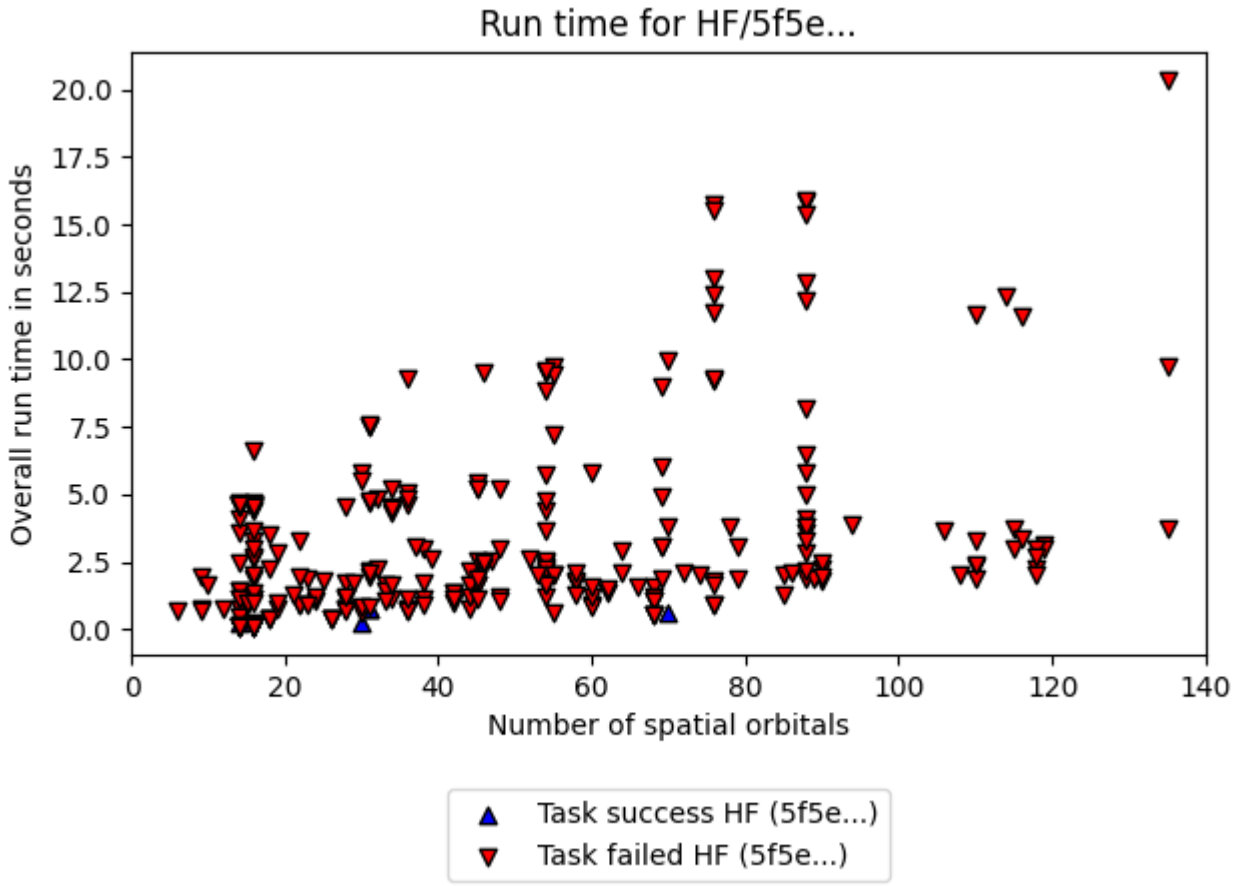
max_run_time_of_attempted_tasks: 20.338801622390747

sum_of_run_time_of_attempted_tasks: 906.4860525131226

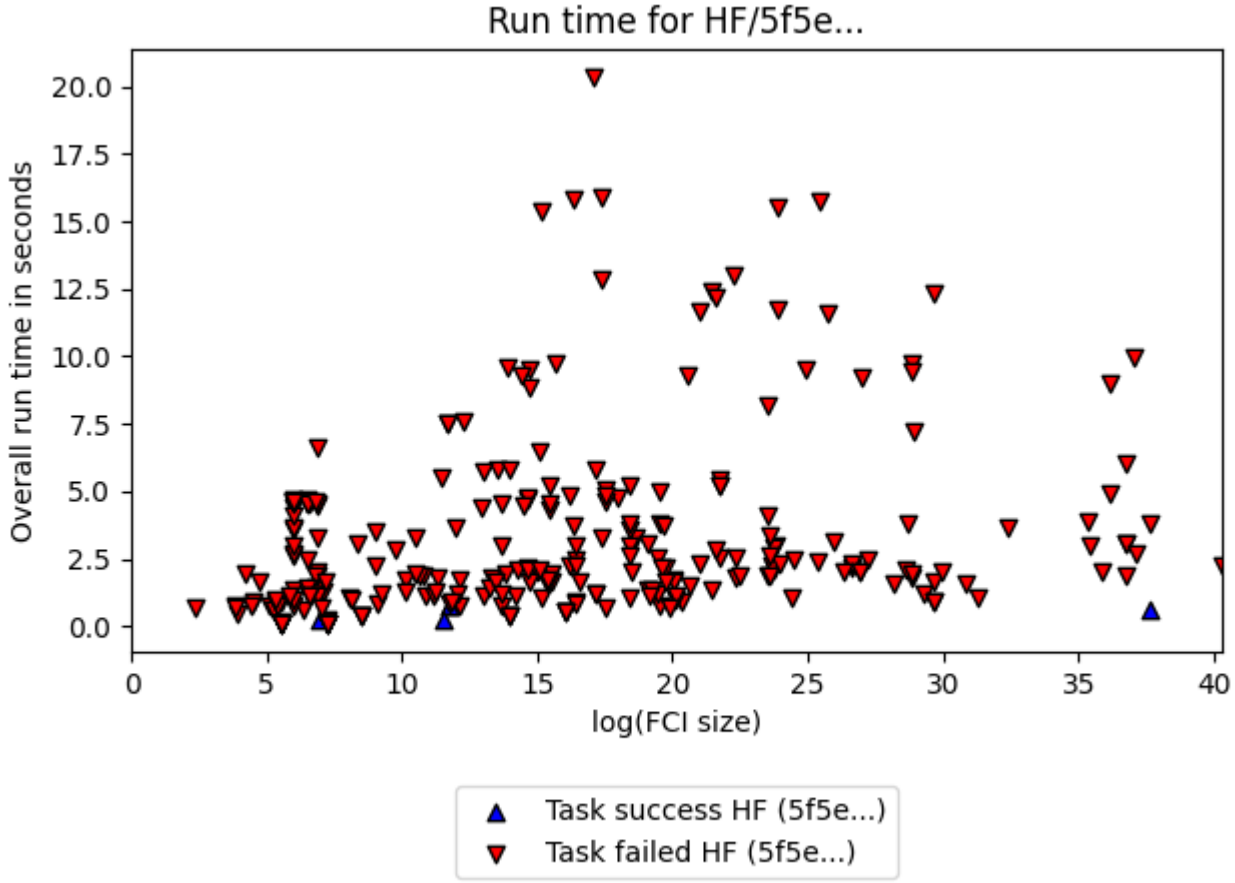
solvability_ratio: 0.0

f1_score: [0.9867549668874173, 0.7142857142857143]

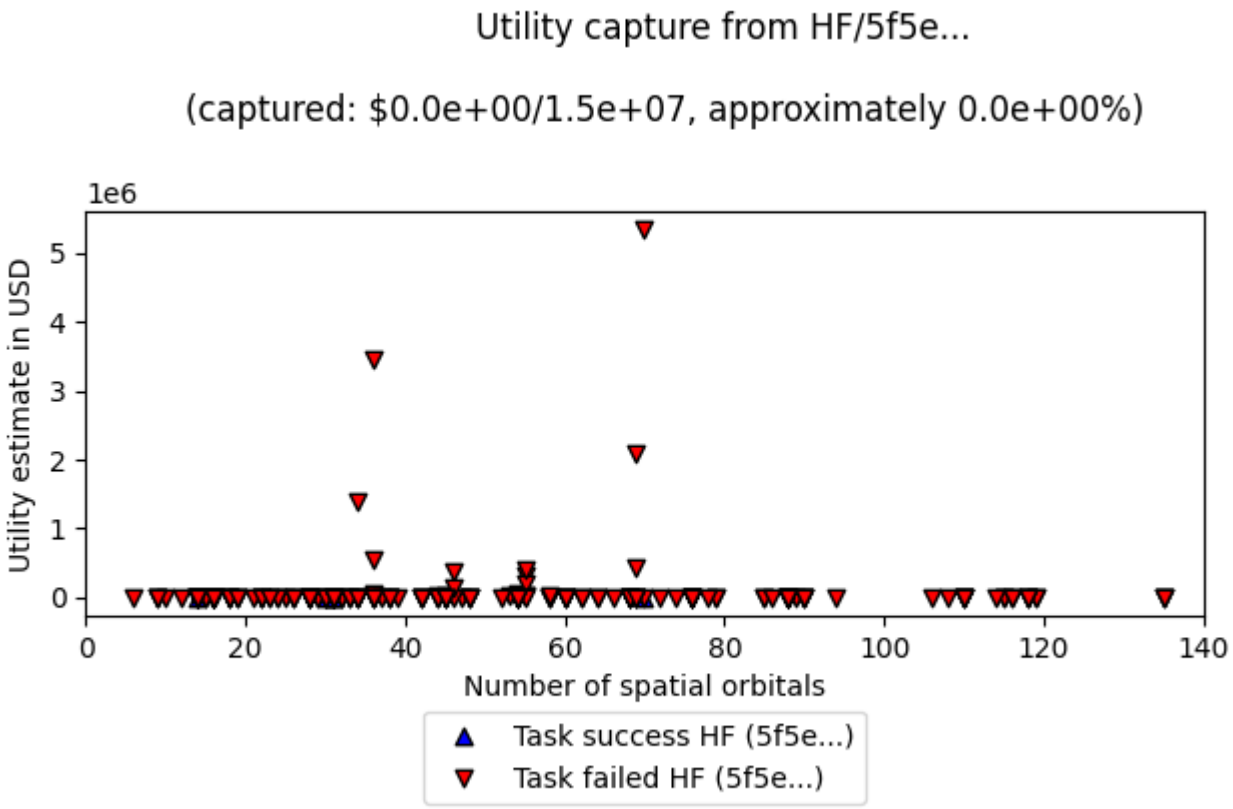
ml_metrics_calculator_version: 1

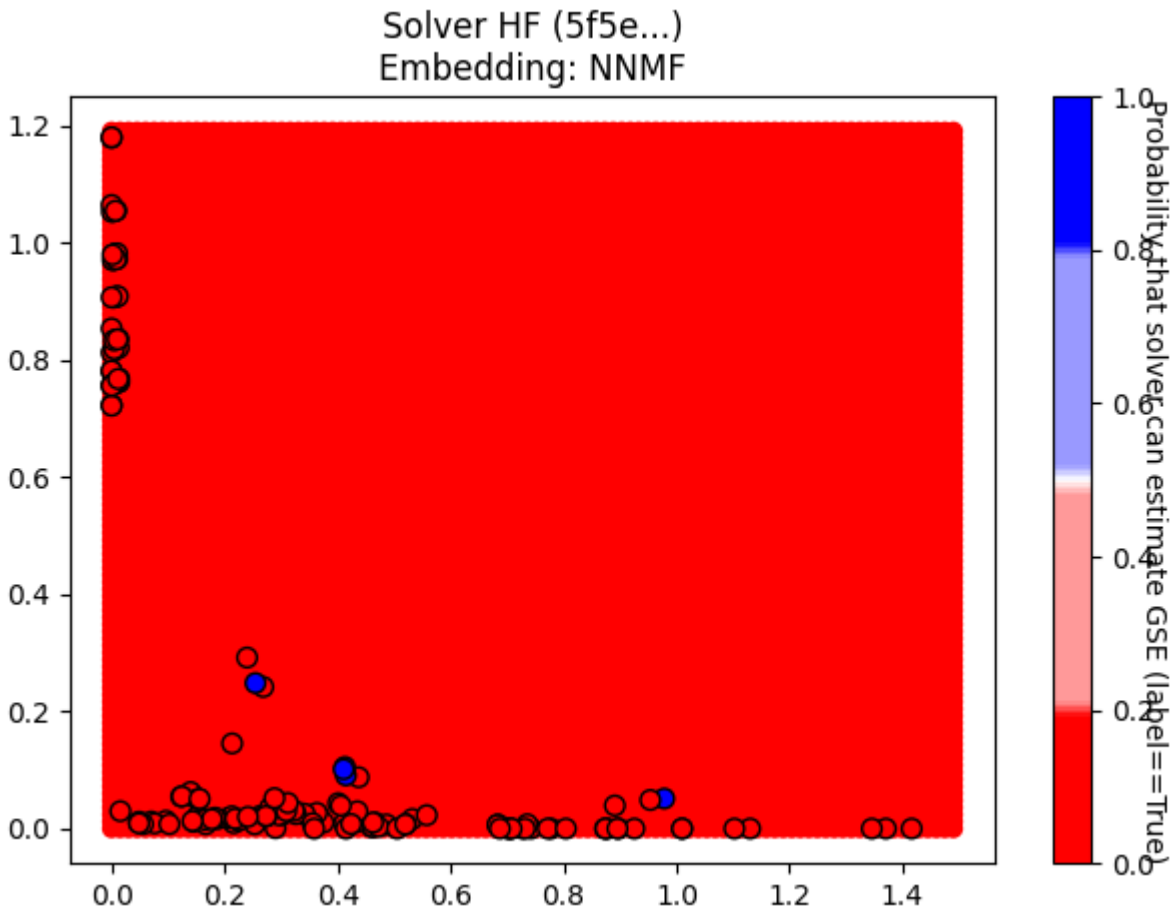


Note: plot only contains `attempted` tasks.

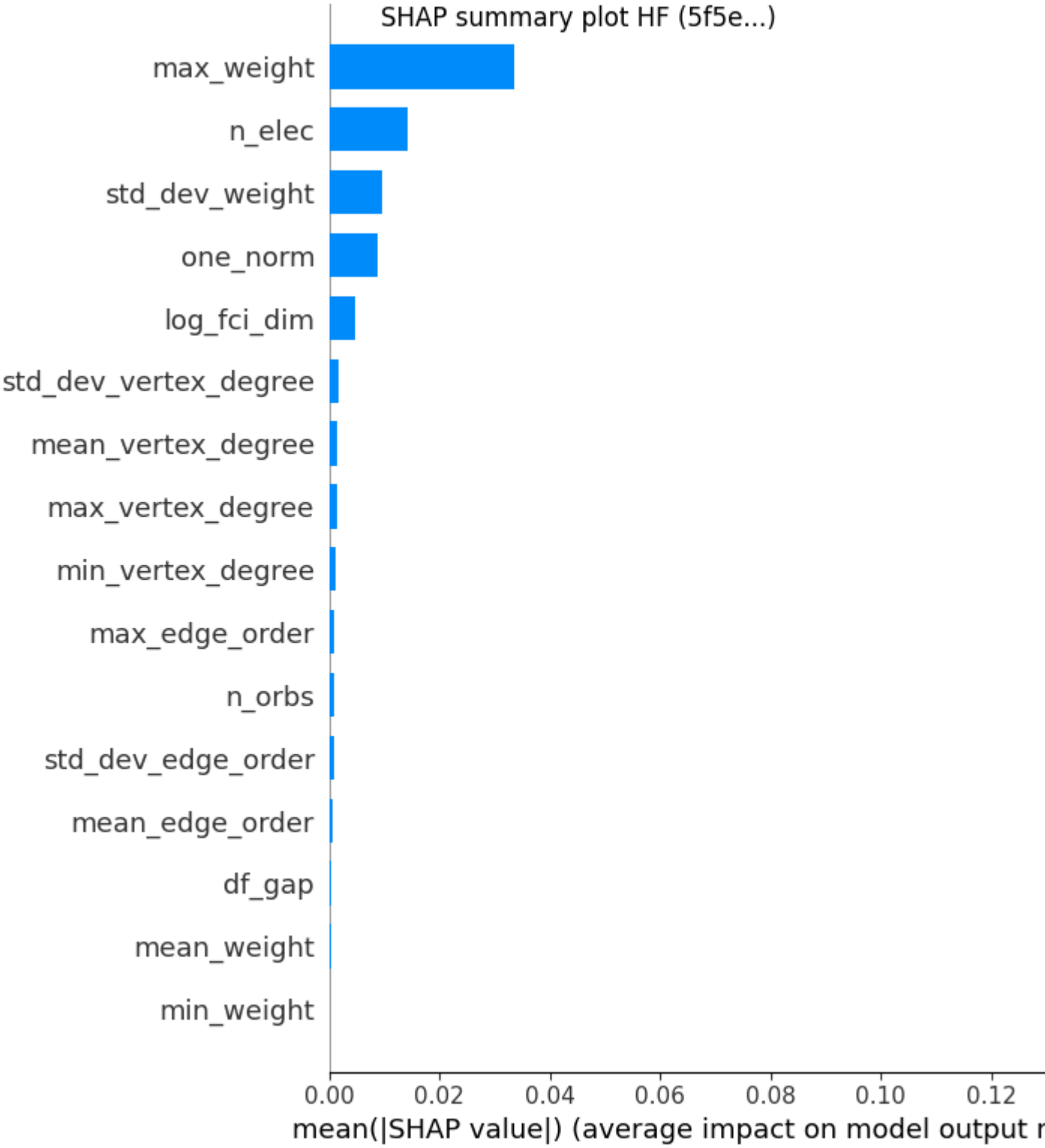


Note: plot only contains `attempted` tasks.


Utility capture from HF/5f5e...
(captured: $0.0e+00/1.5e+07, approximately 0.0e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success HF (5f5e...)
Task failed HF (5f5e...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: e445e548-c86f-4d2f-8772-ae2f1a951f36

creation_timestamp: 2025-01-28T17:07:42.747013+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

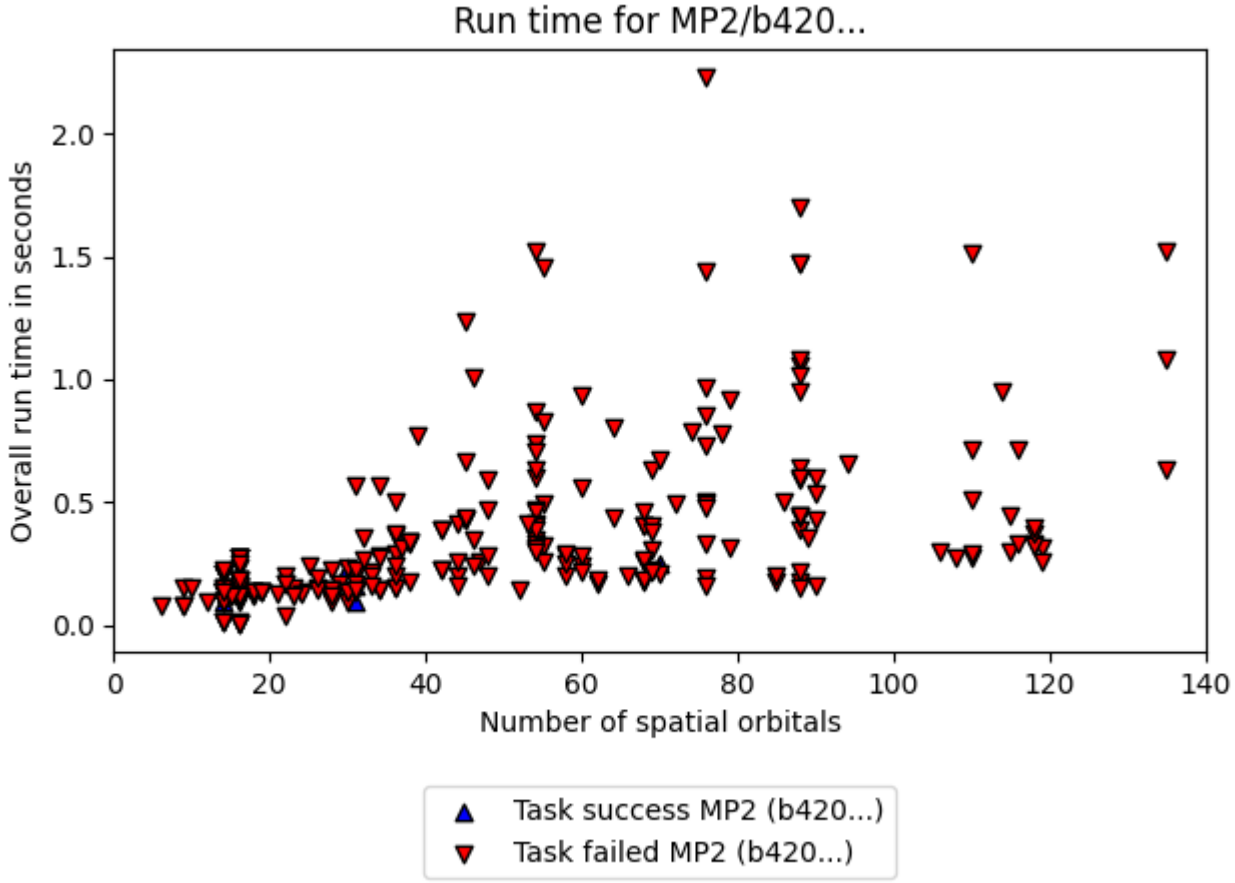
max_run_time_of_attempted_tasks: 2.230440139770508

sum_of_run_time_of_attempted_tasks: 94.7442626953125

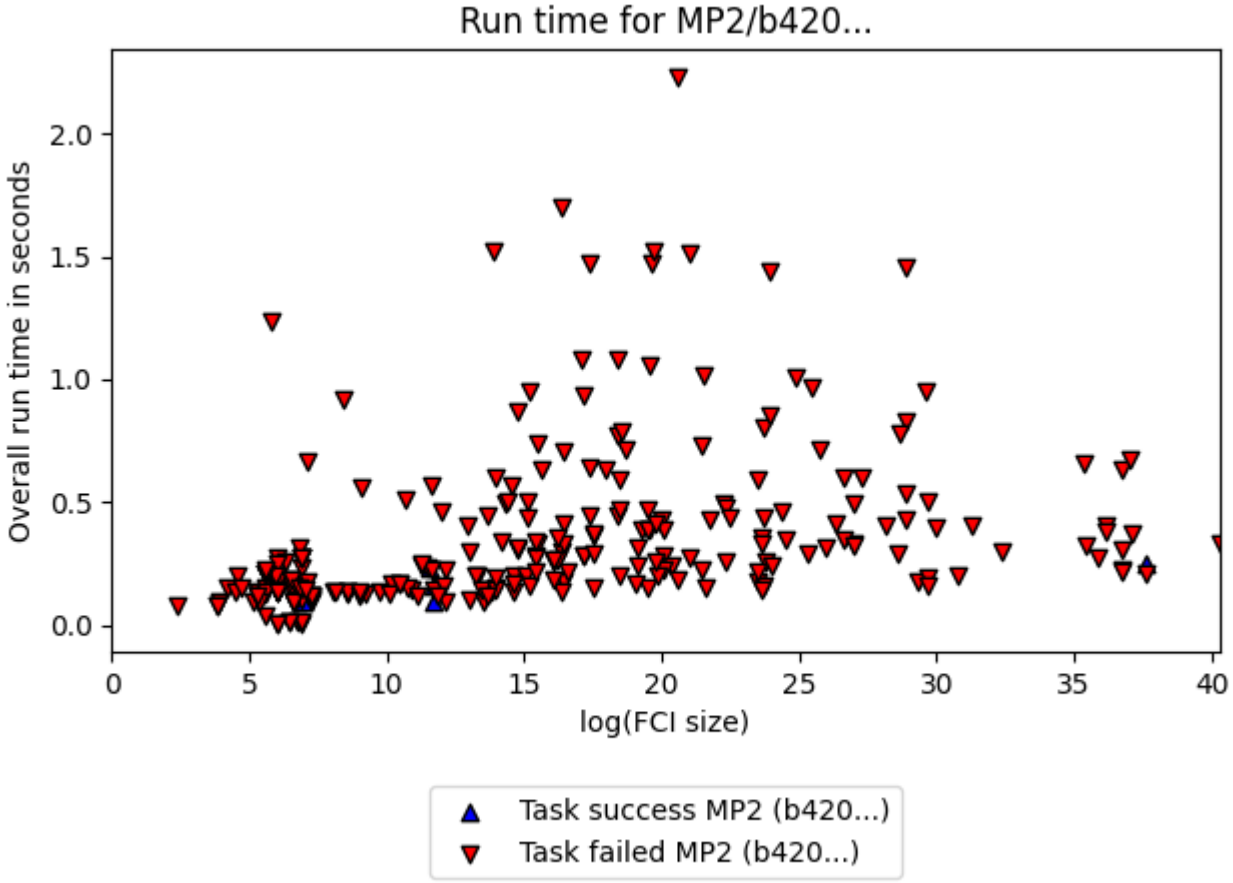
solvability_ratio: 0.0

f1_score: [0.9867549668874173, 0.7142857142857143]

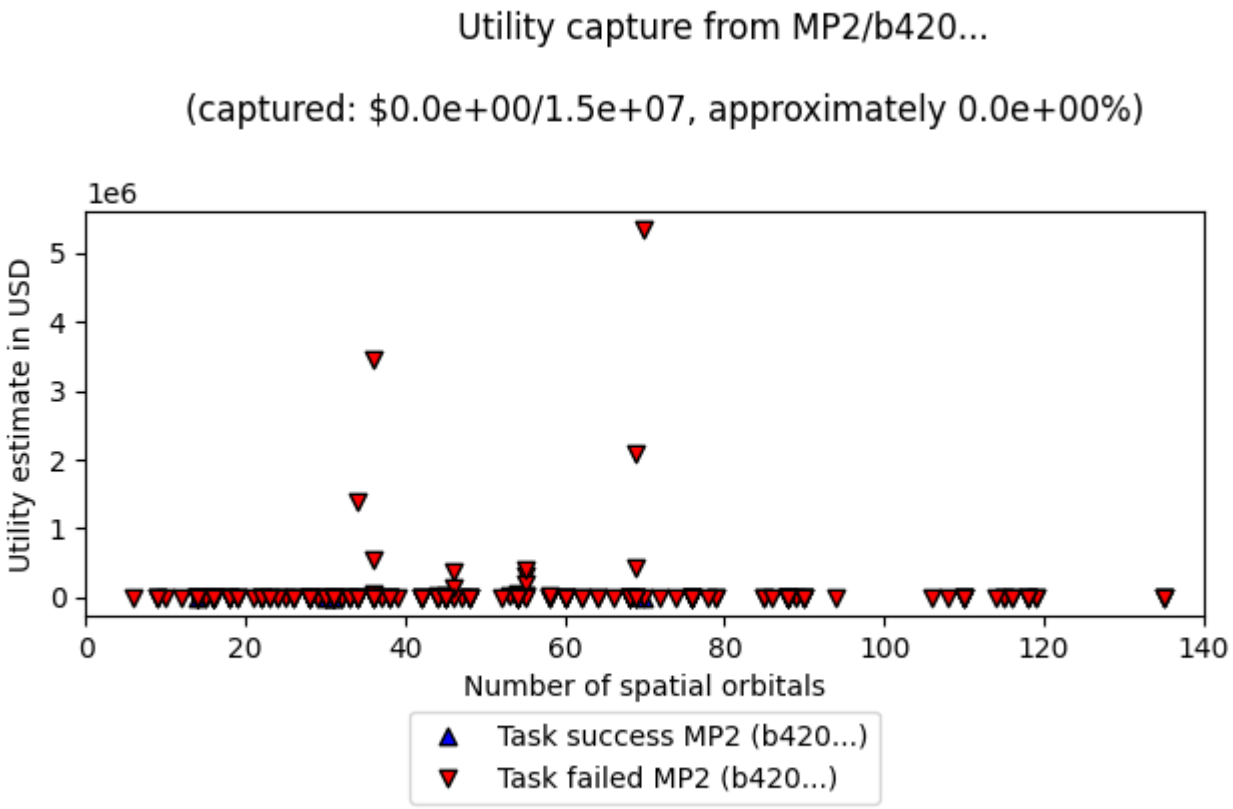
ml_metrics_calculator_version: 1

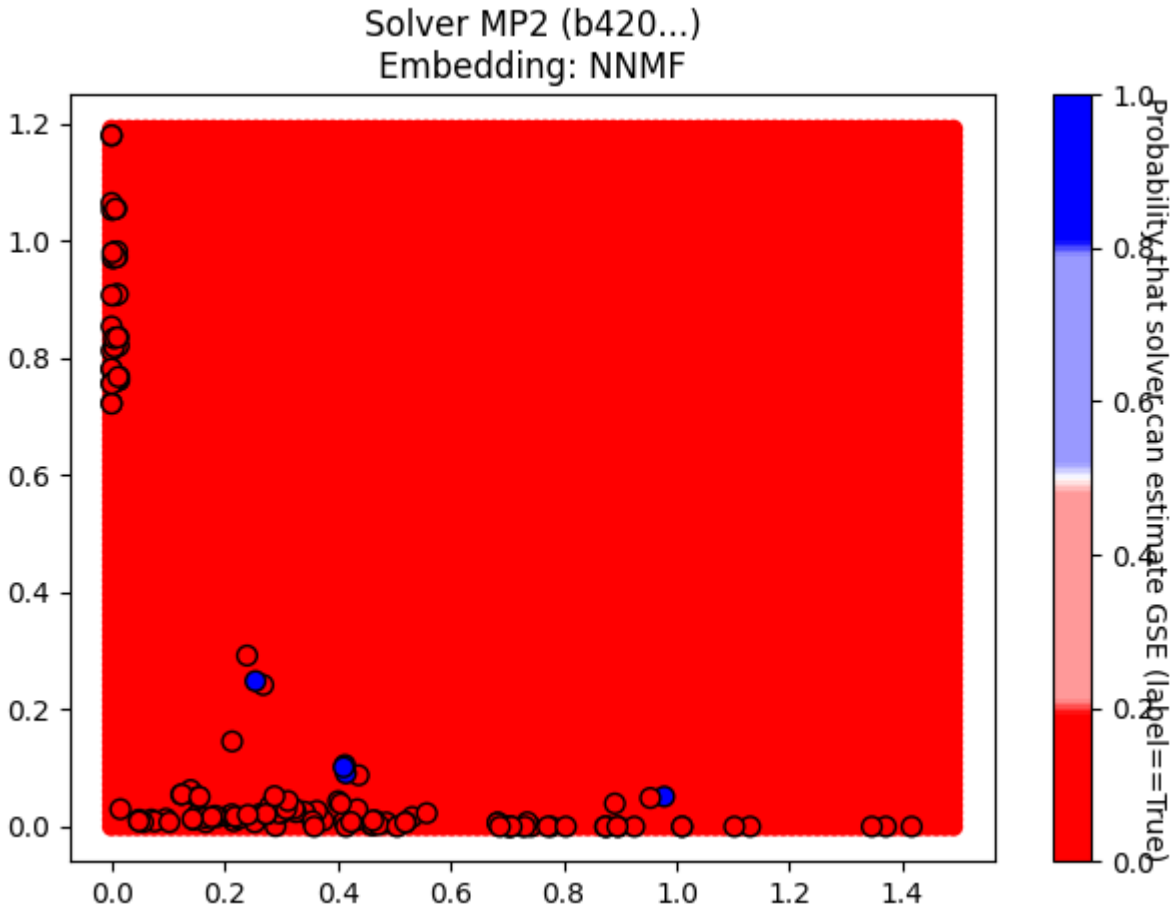


Note: plot only contains `attempted` tasks.

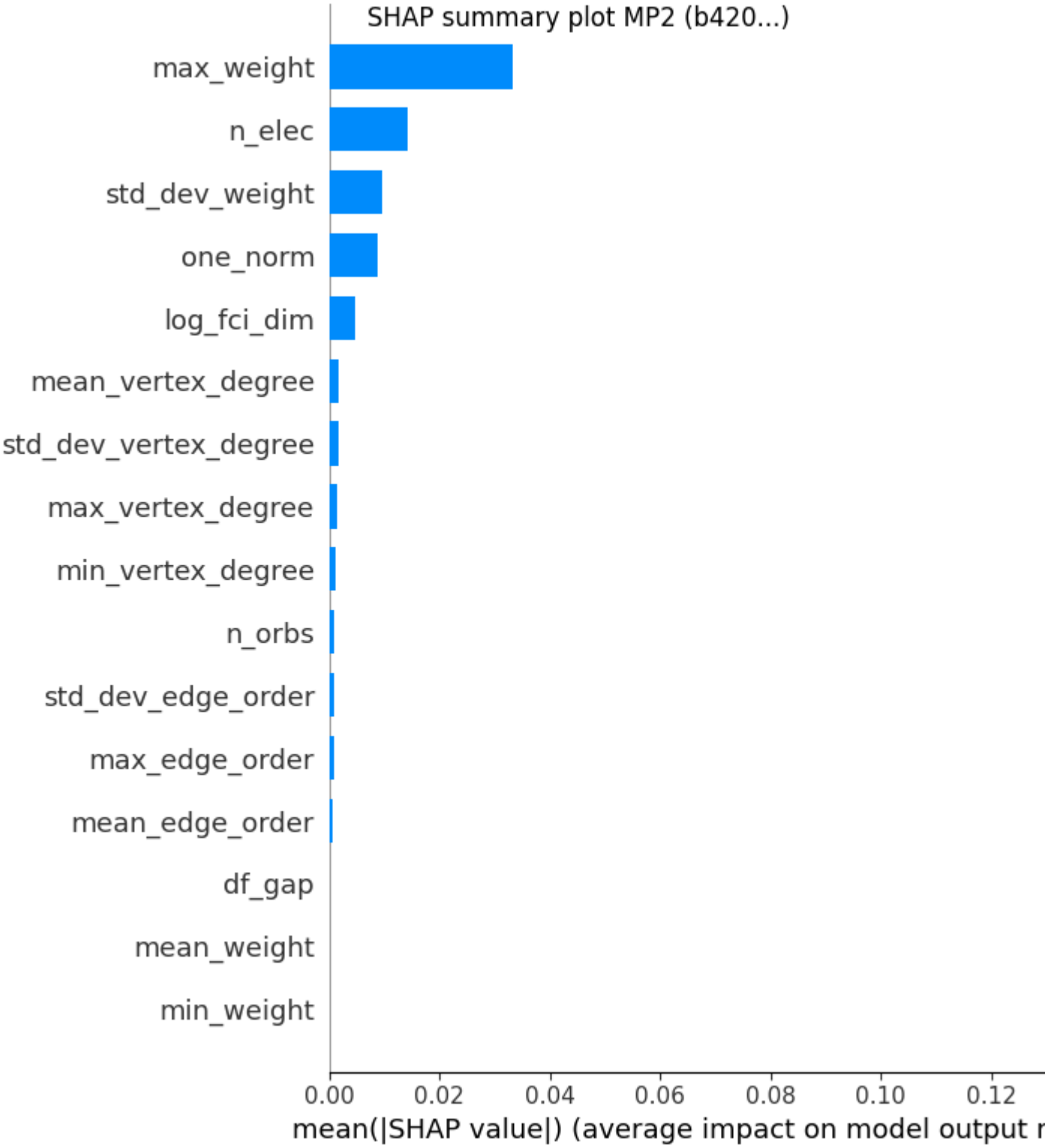


Note: plot only contains `attempted` tasks.


Utility capture from MP2/b420...
(captured: $0.0e+00/1.5e+07, approximately 0.0e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success MP2 (b420...)
Task failed MP2 (b420...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: b1019247-1377-4706-9522-5cb5407e5407

creation_timestamp: 2025-01-28T17:07:42.747013+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

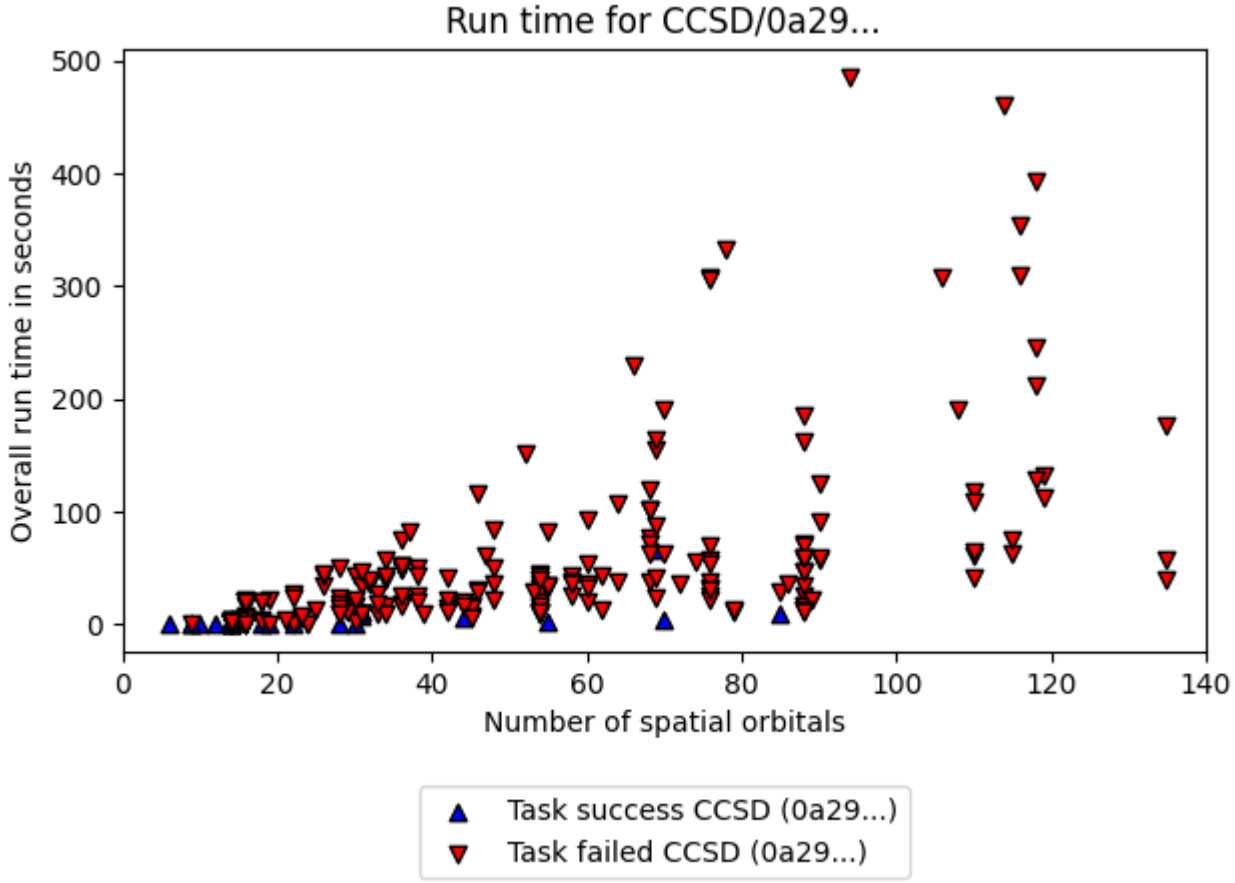
max_run_time_of_attempted_tasks: 485.1982181072235

sum_of_run_time_of_attempted_tasks: 12252.72845697403

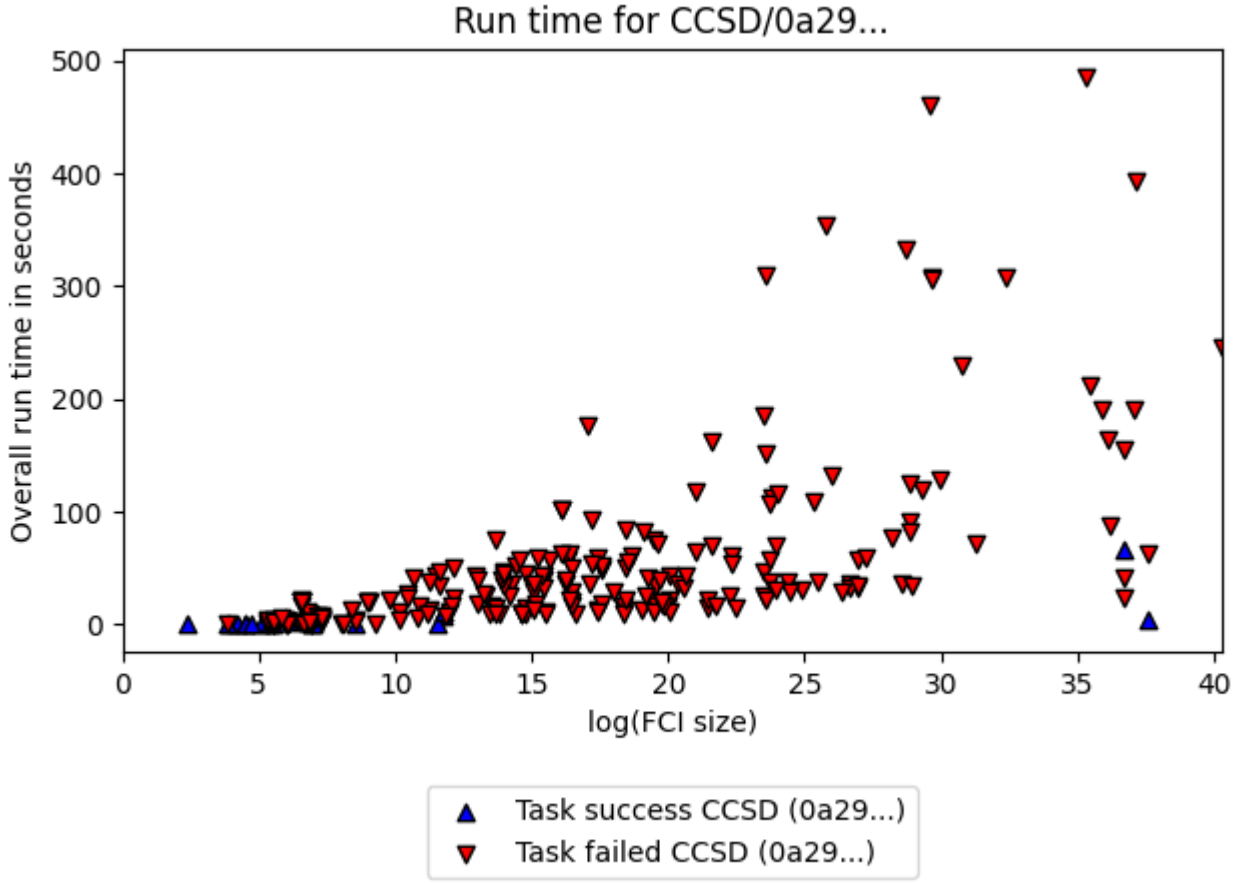
solvability_ratio: 0.0154

f1_score: [0.9777777777777777, 0.8695652173913043]

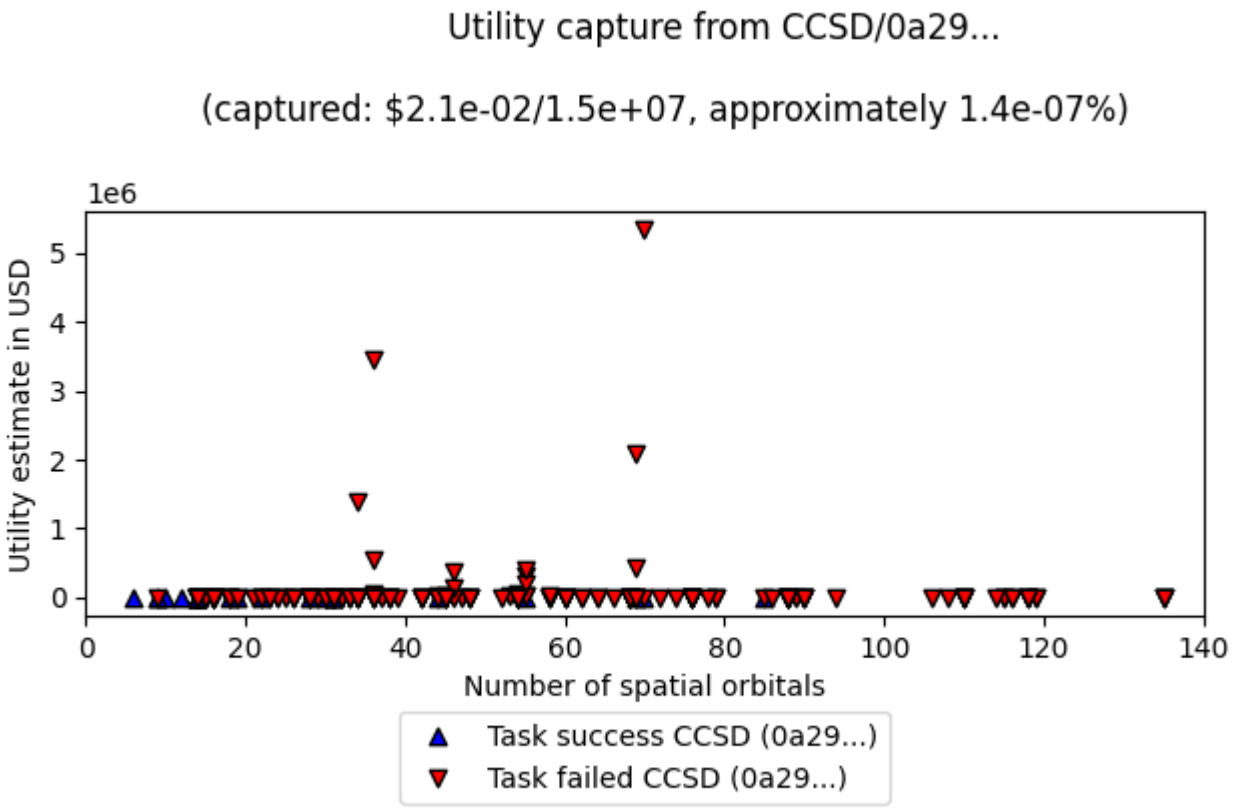
ml_metrics_calculator_version: 1

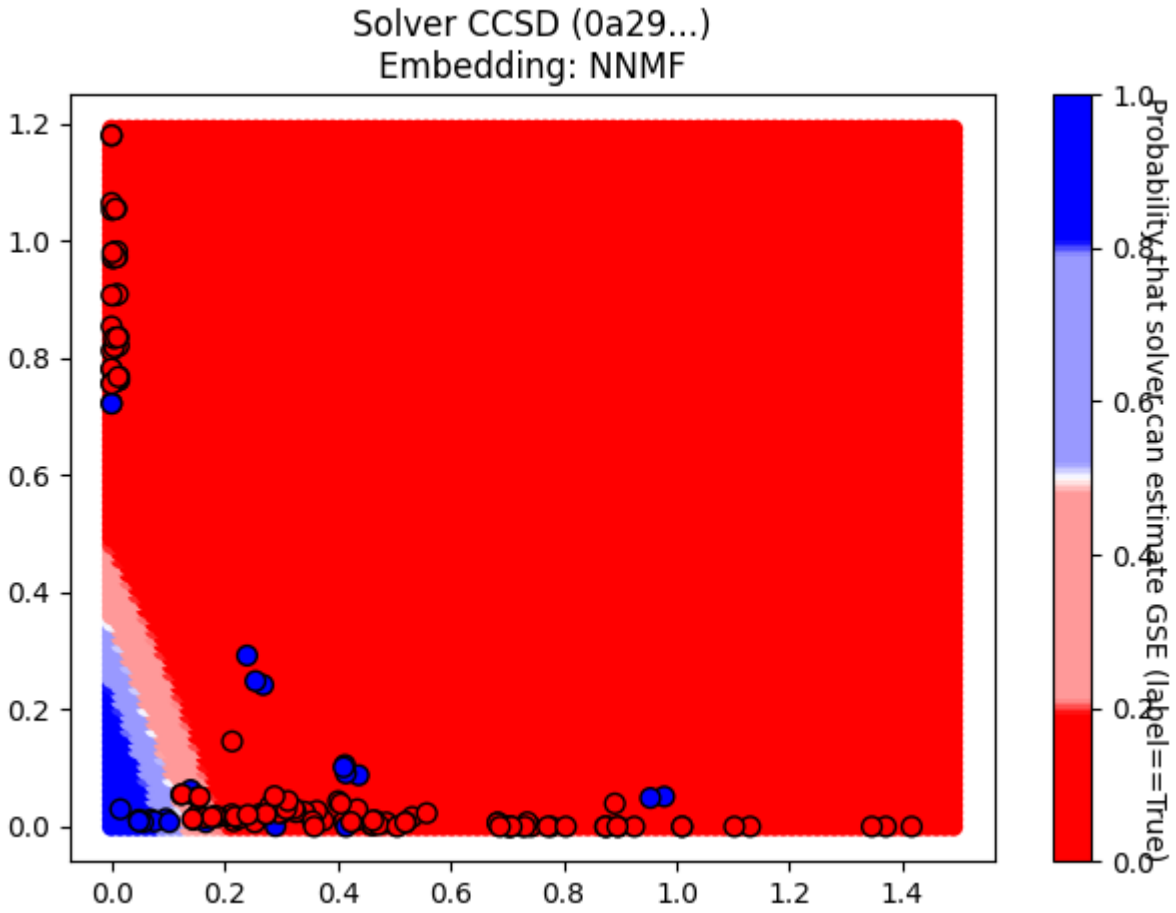


Note: plot only contains `attempted` tasks.

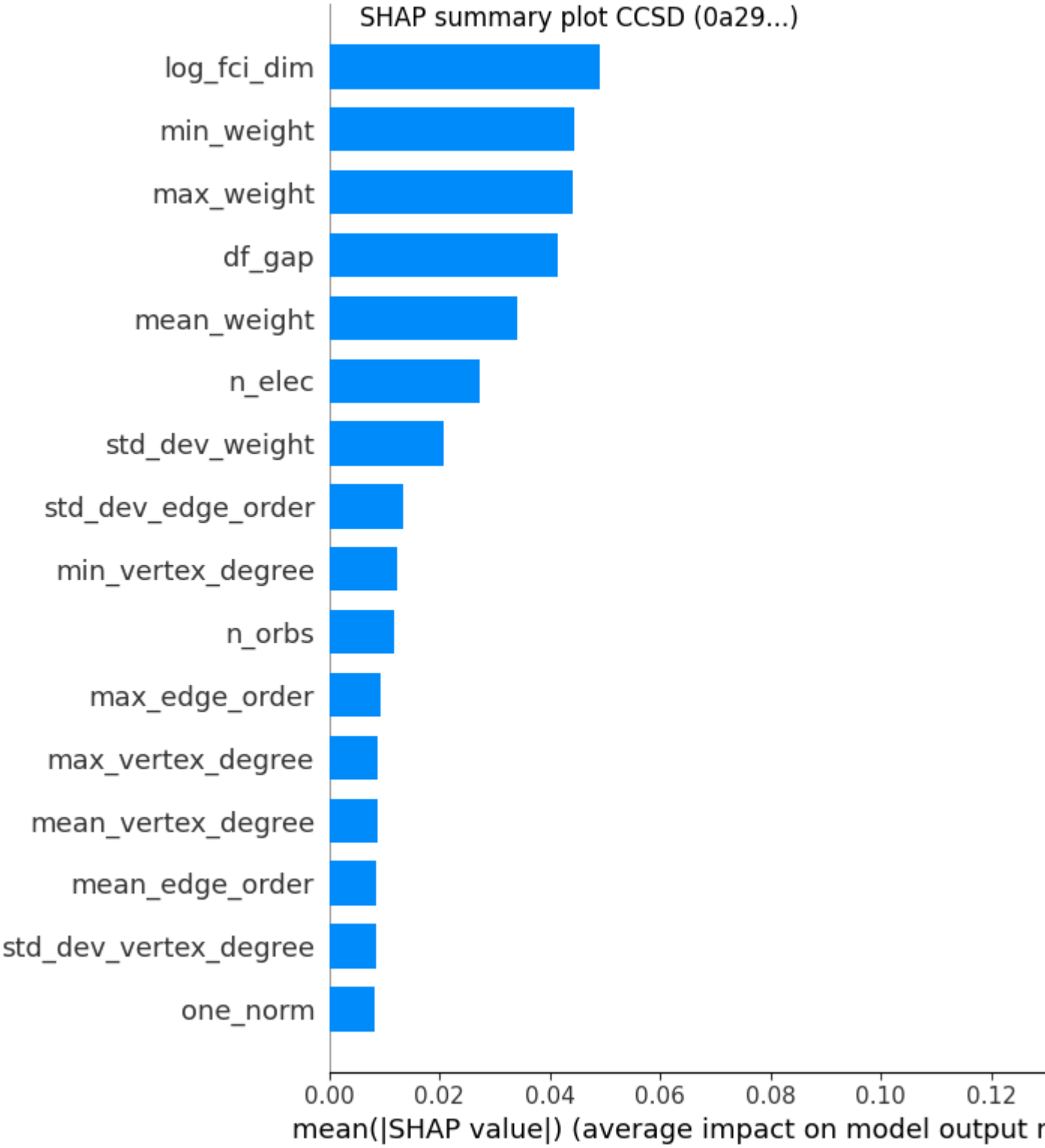


Note: plot only contains `attempted` tasks.


Utility capture from CCSD/0a29...
(captured: $2.1e-02/1.5e+07, approximately 1.4e-07%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSD (0a29...)
Task failed CCSD (0a29...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: 9722e21e-c0ad-4112-b0fb-ce12fe834fbe

creation_timestamp: 2025-01-28T17:07:42.747013+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

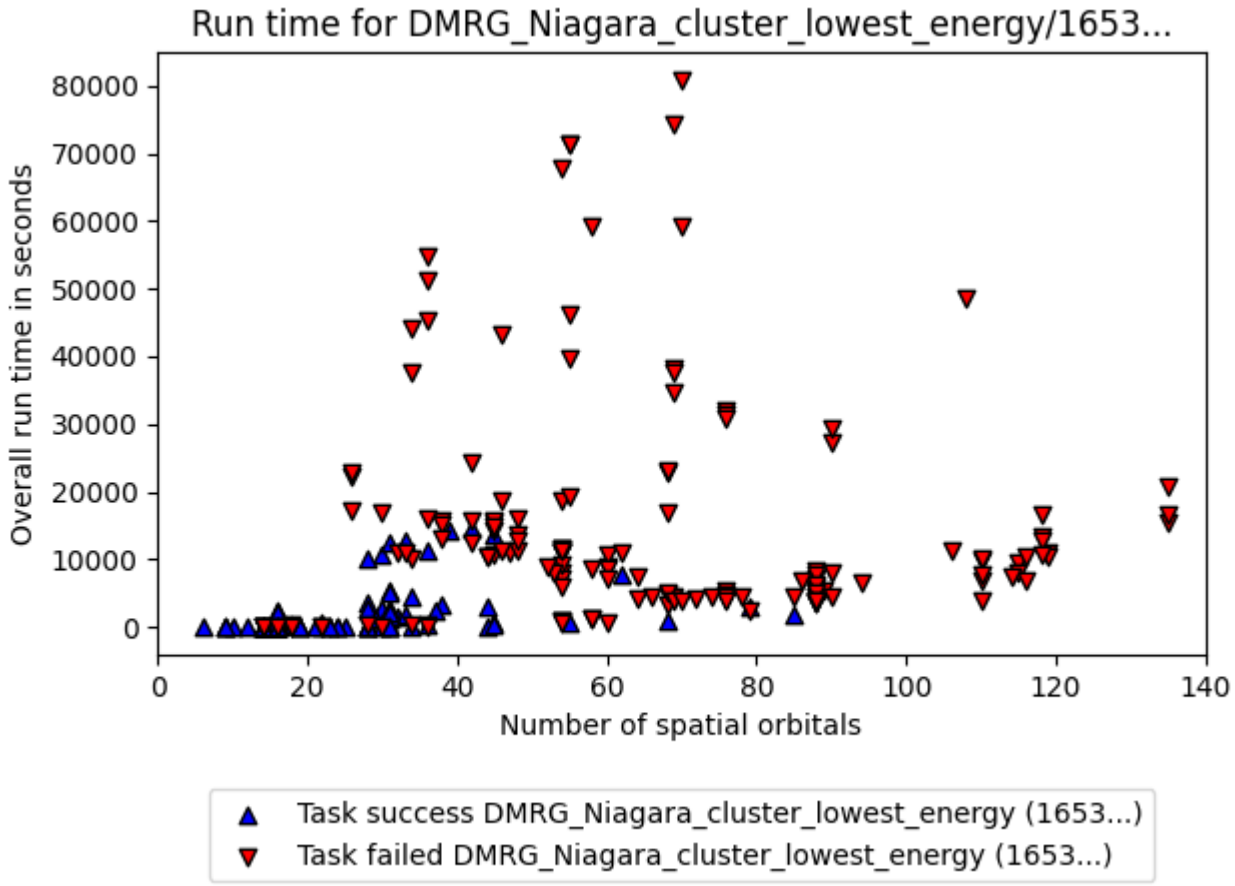
max_run_time_of_attempted_tasks: 80820.729907066

sum_of_run_time_of_attempted_tasks: 2471726.9051446947

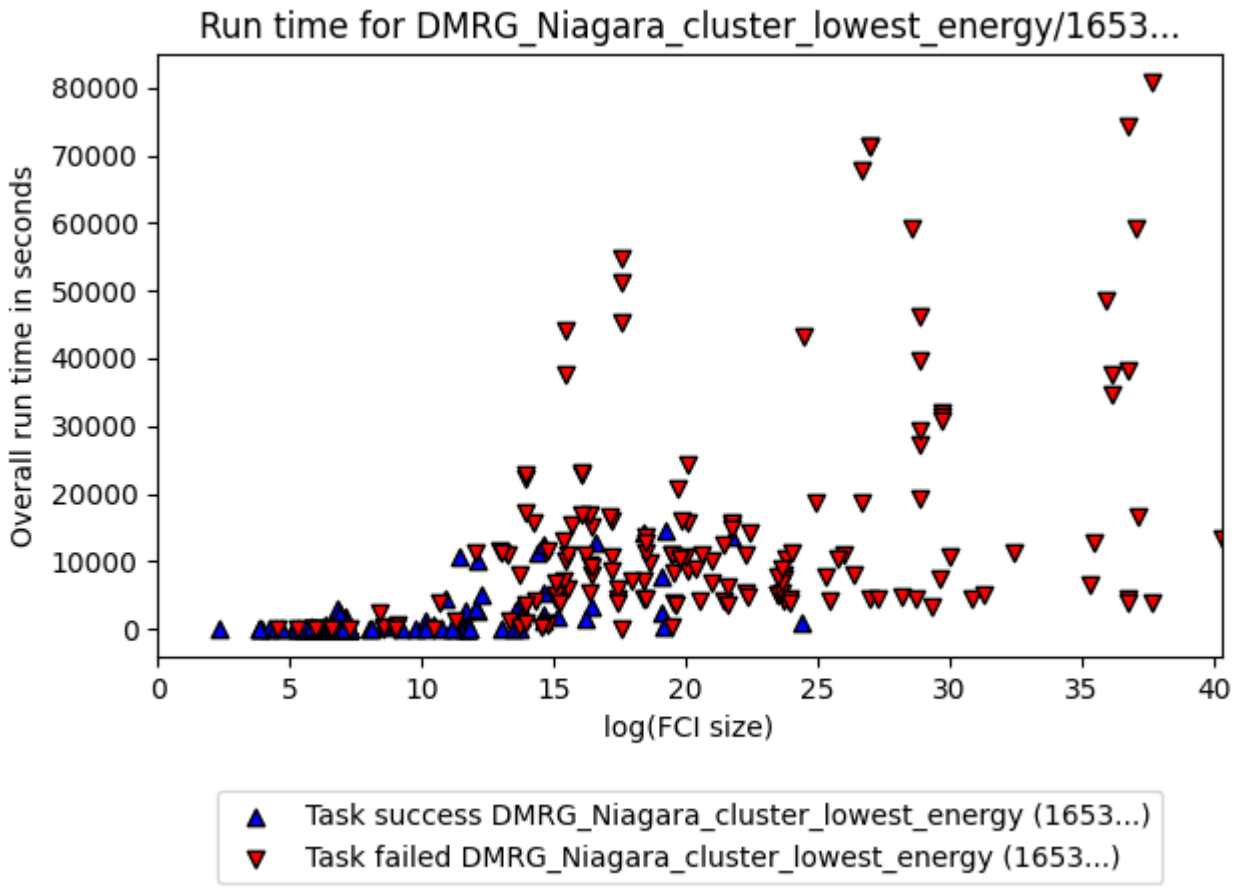
solvability_ratio: 0.3405

f1_score: [0.9662921348314607, 0.986784140969163]

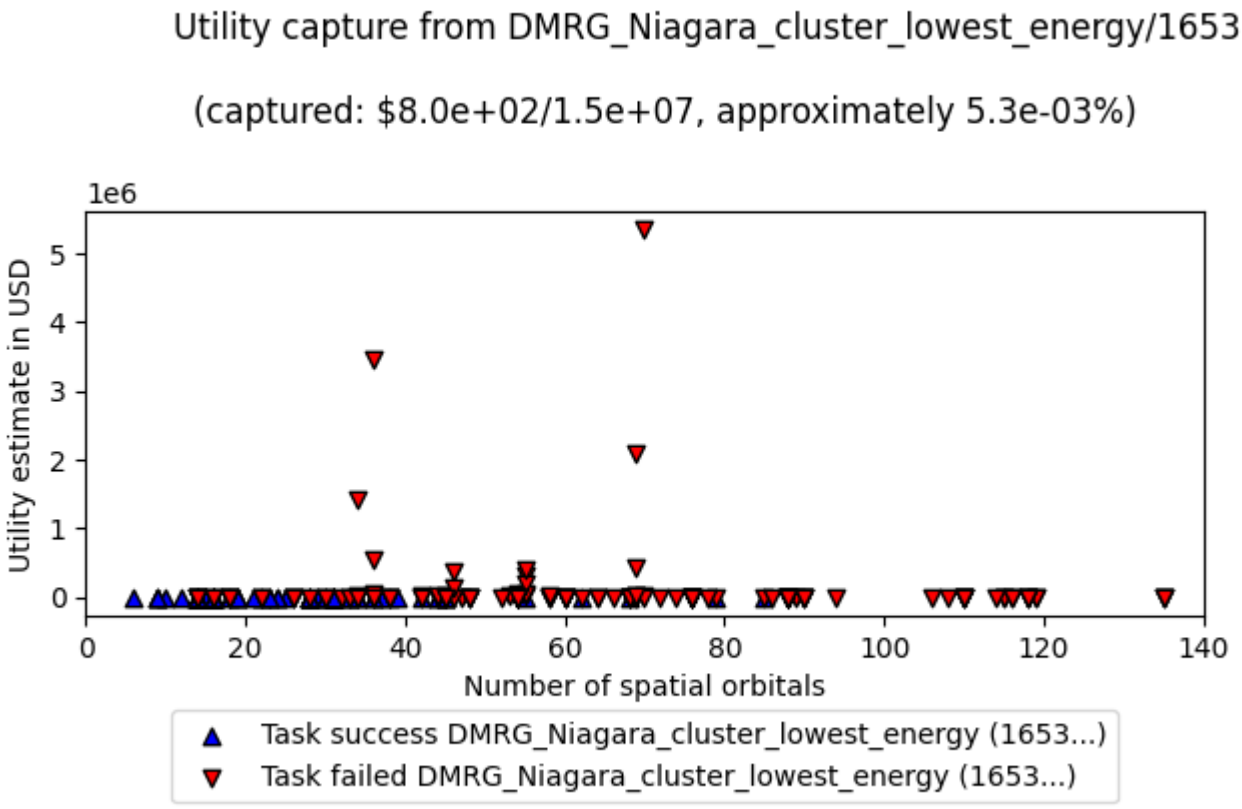
ml_metrics_calculator_version: 1

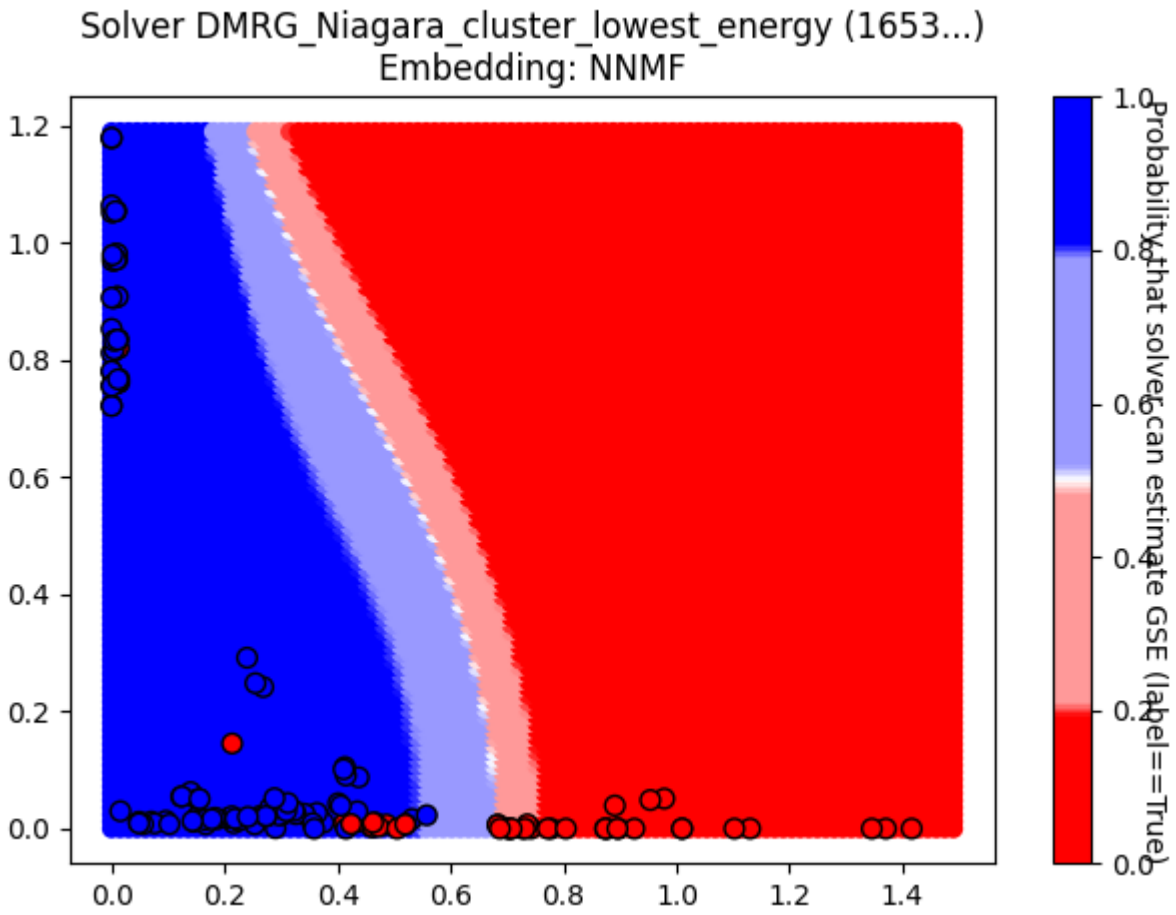


Note: plot only contains `attempted` tasks.

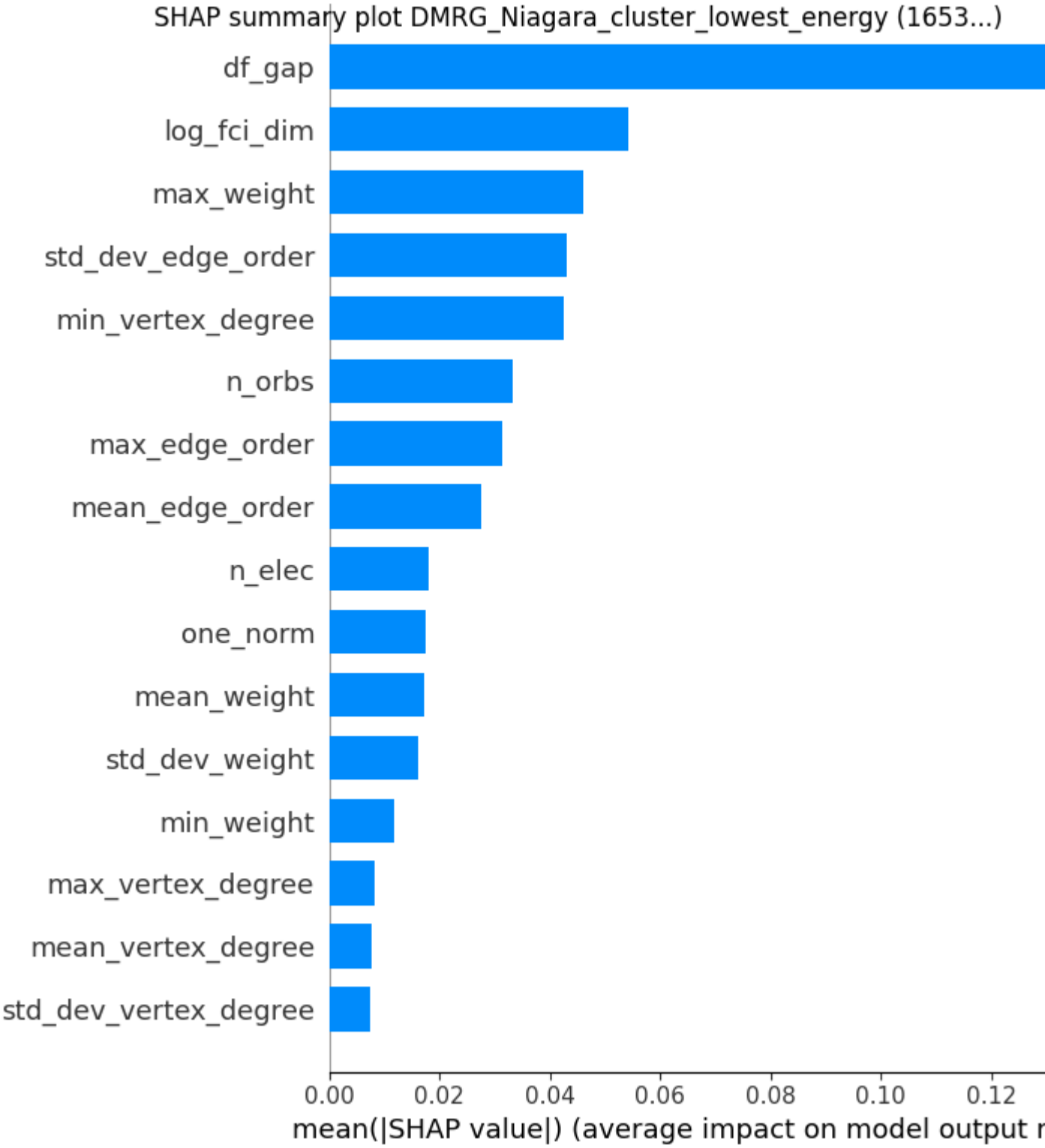


Note: plot only contains `attempted` tasks.


Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..
(captured: $8.0e+02/1.5e+07, approximately 5.3e-03%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success DMRG_Niagara_cluster_lowest_energy (1653...)
Task failed DMRG_Niagara_cluster_lowest_energy (1653...)



Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)



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: cae2d073-ae33-4ef3-8fde-e0b737f1f641

creation_timestamp: 2025-01-28T17:07:42.747013+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

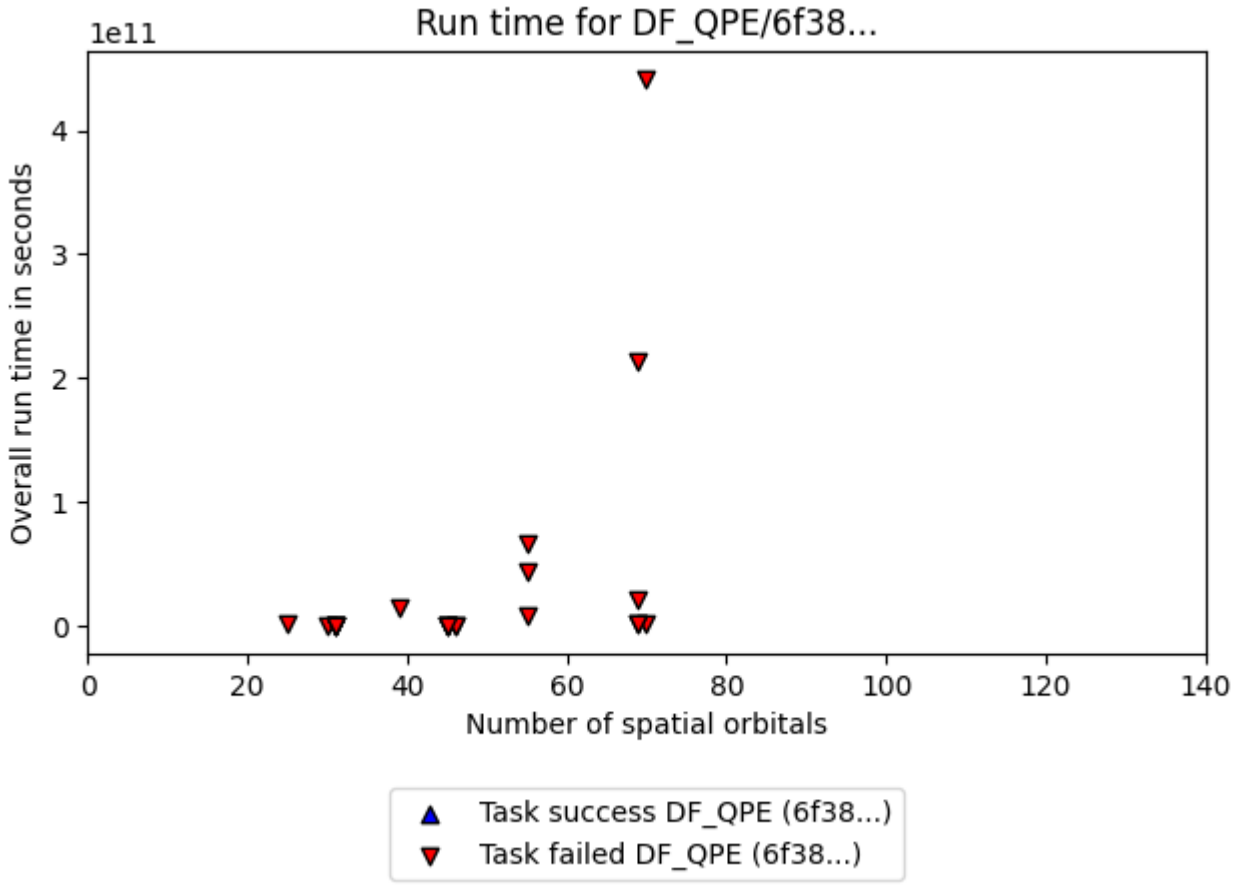
sum_of_run_time_of_attempted_tasks: 819346667619.2955

solvability_ratio: None

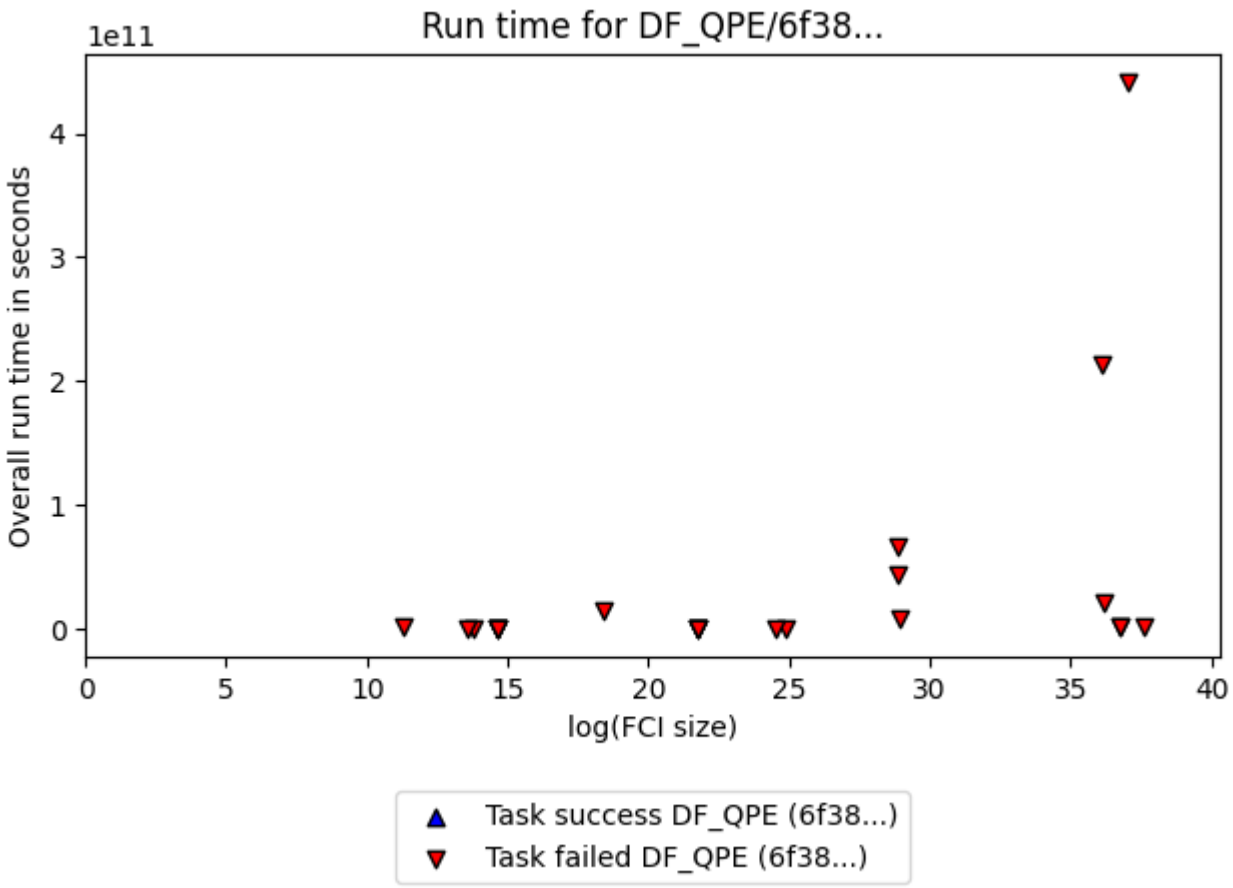
f1_score: None

ml_metrics_calculator_version: 1

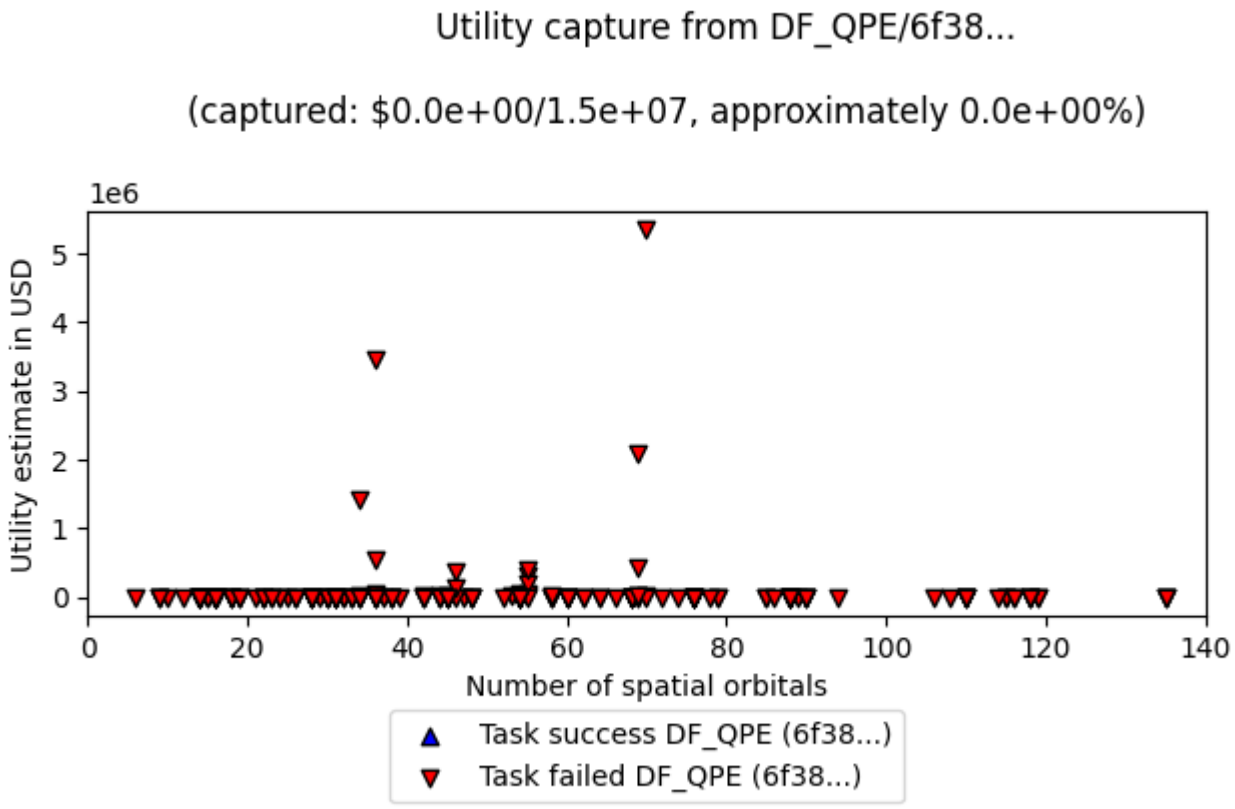
comment: All labels were either all `True` or all `False` and we cannot create an ML model with only one class.



Note: plot only contains `attempted` tasks.



Note: plot only contains `attempted` tasks.

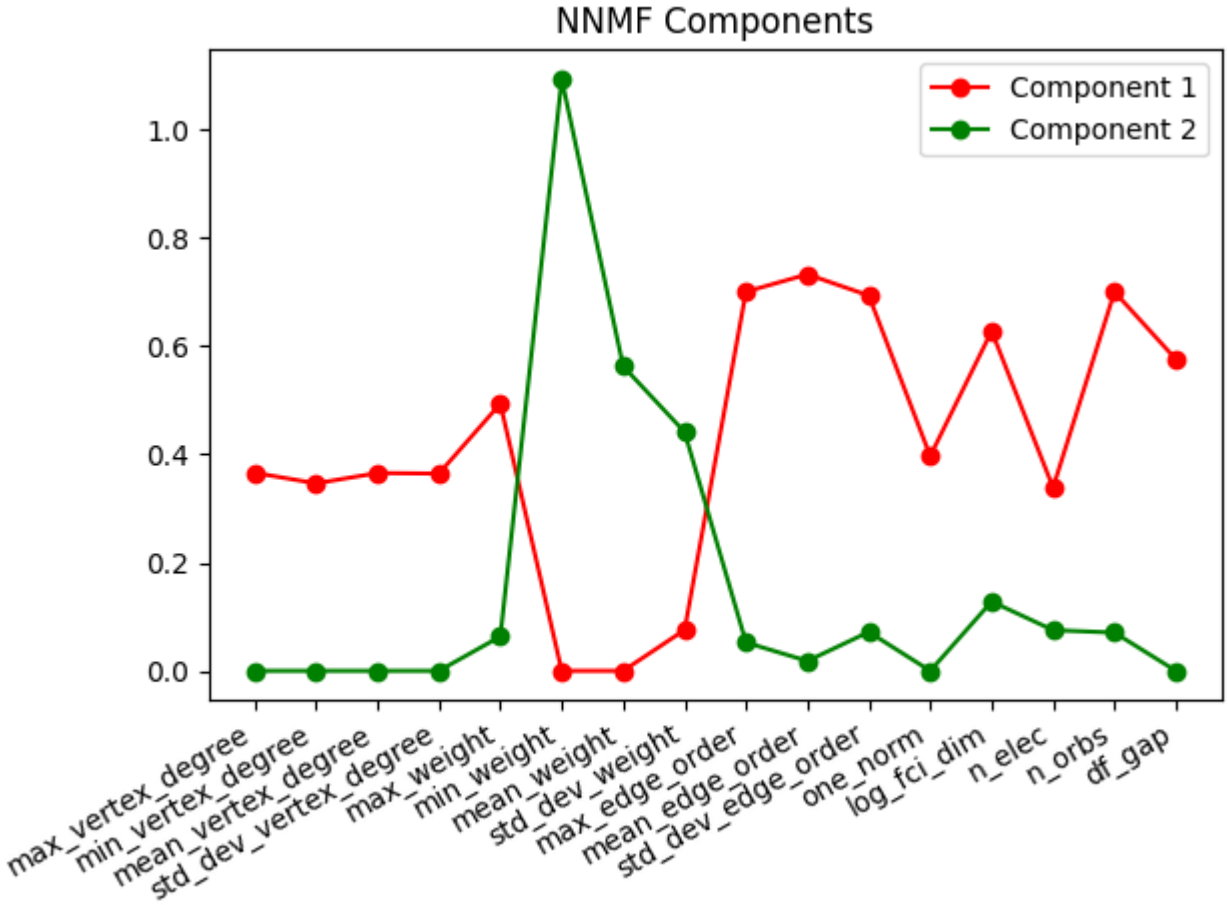


Solver miniML plot

Note: ML surface plot is based on Hamiltonians where a `reference_energy` was provided. (`attempted` may be `True` or `False`.)

SHAP summary plot

Non-negative matrix factorization (ML latent space)



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']

Component 1: [0.36604788 0.3465517 0.3656555 0.36466294 0.49391307 0. 0. 0.07560829 0.70083452 0.73297542 0.69367903 0.39707278 0.62804024 0.33874397 0.7006798 0.57585866]

Component 2: [0. 0. 0. 0. 0.06352889 1.09340886 0.56300493 0.44159773 0.05242832 0.01821226 0.07191467 0. 0.12812831 0.07525071 0.07071245 0.]