GSEE Benchmark Standard Report

Report based on data from 2025-01-23T16:28:43.200733+00:00

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

Input data: `Hamiltonian_features.csv`, last modified Mon Dec 30 16:29:03 2024

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: Wed Jan 22 17:01:13 2025

Latest creation time for a `performance_metrics.json` file: Thu Jan 23 11:38:42 2025

Latest creation time for a `solution.json` file: Wed Jan 22 16:55:50 2025

Problem Instance Summary Statistics

number of `problem_instances`: 82

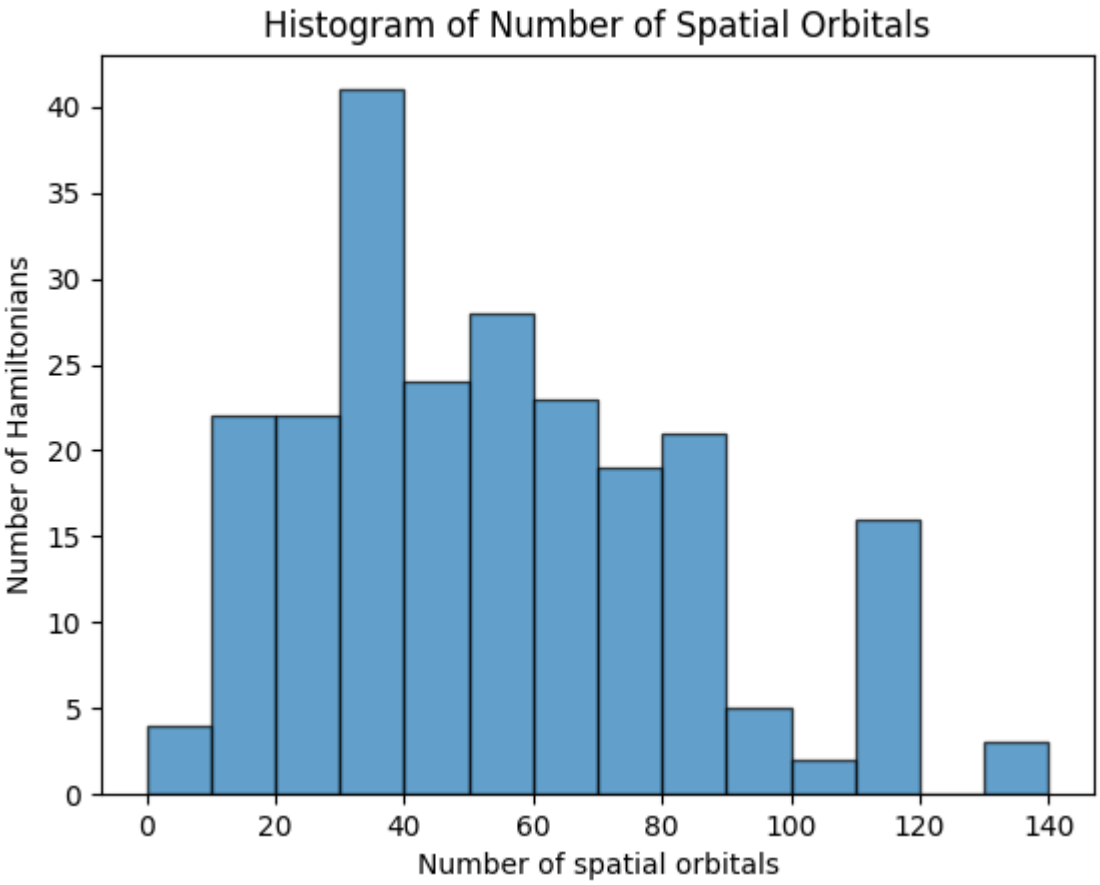
`problem_instance.json` with the most tasks: 30 (hubbard_square/614c4444-a31a-4348-b24d-01040208651c)

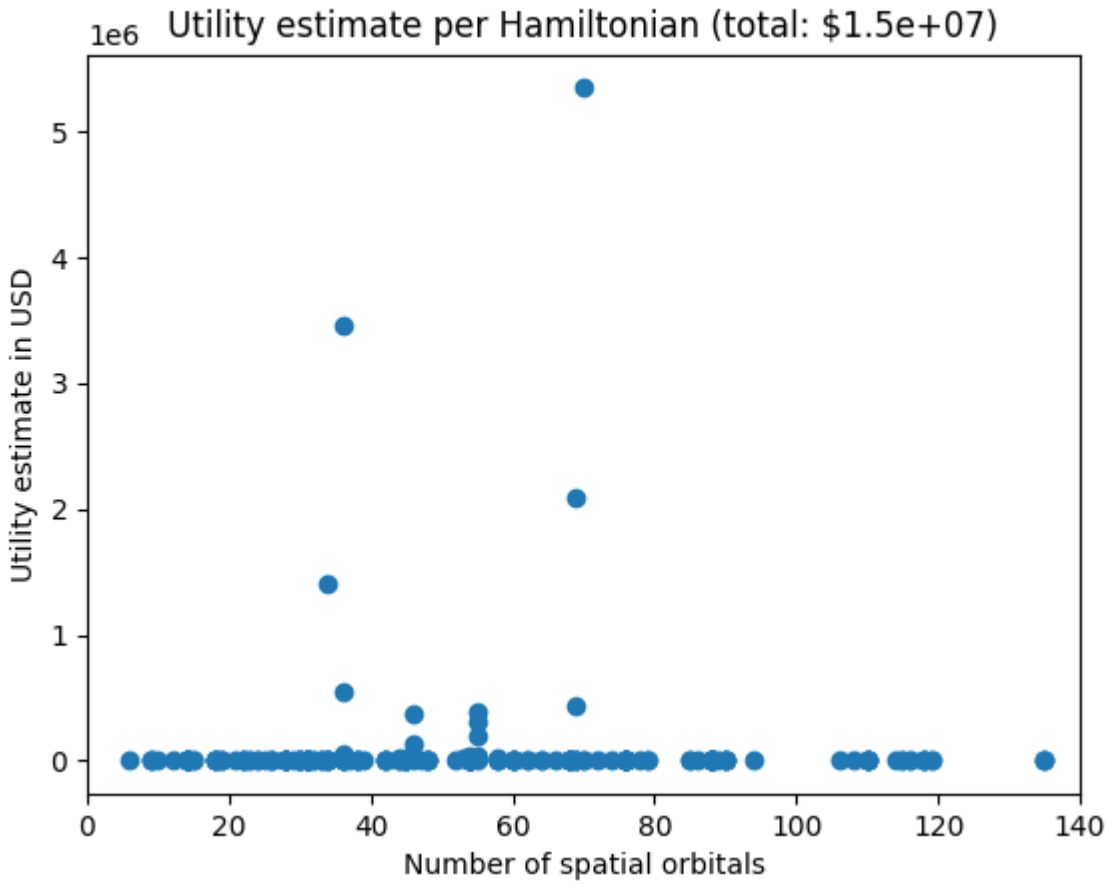
number of Hamiltonians (i.e., tasks): 230

minimum number of orbitals: 6

median number of orbitals: 53.5

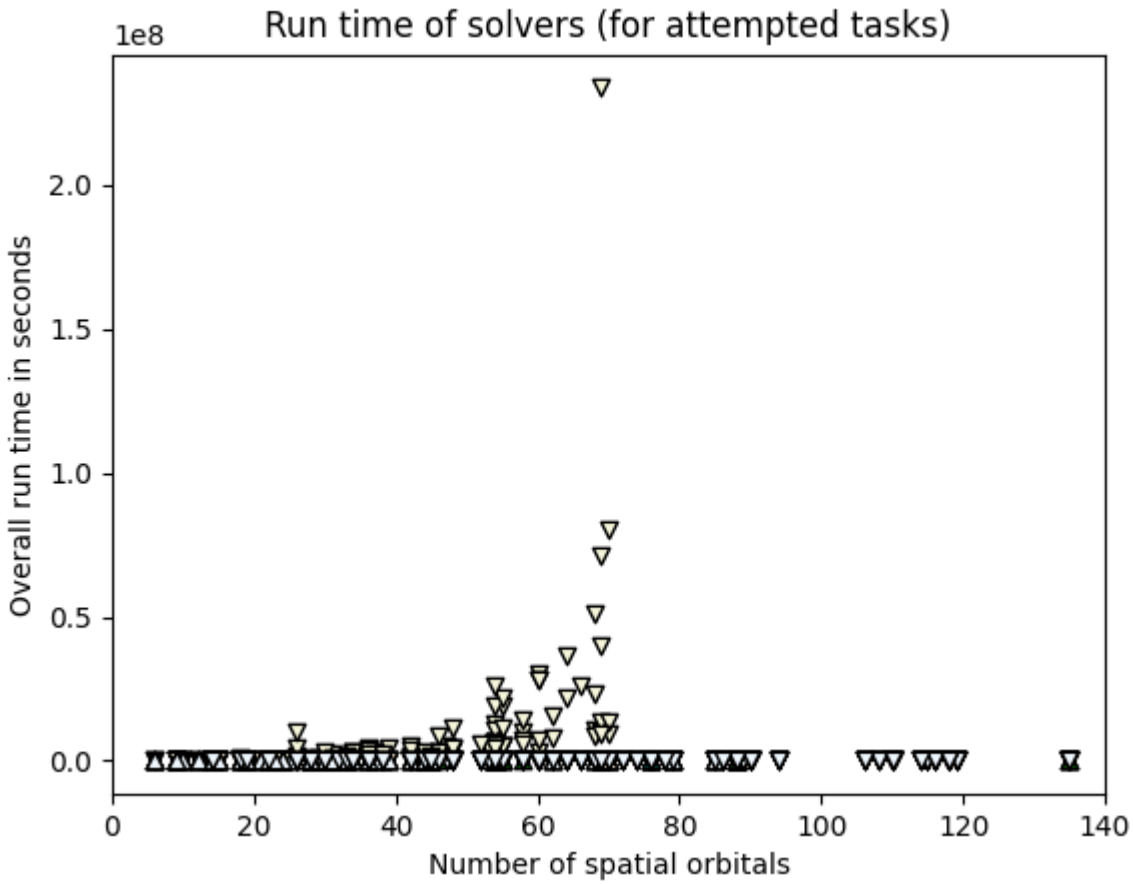
maximum number of orbitals: 135

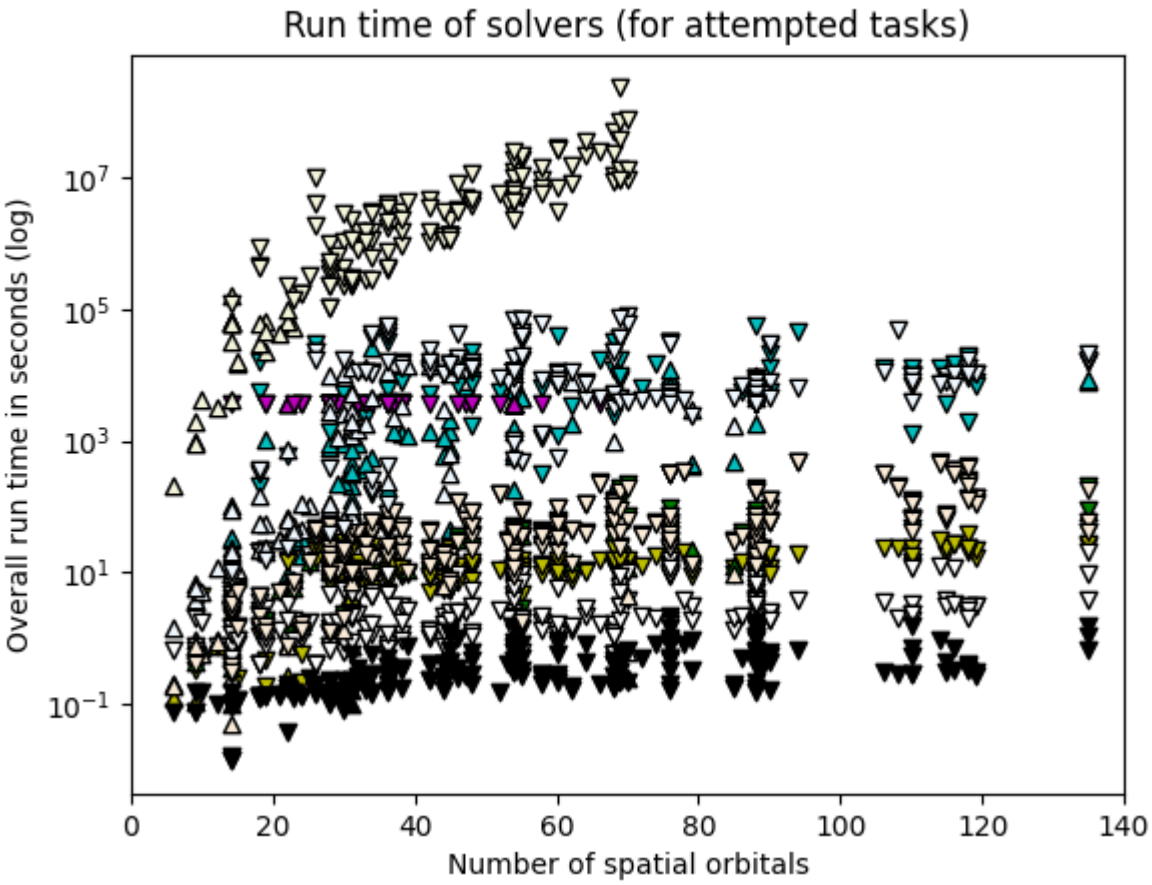

Histogram of Number of Spatial Orbitals
Number of Hamiltonians
Number of spatial orbitals
0
5
10
15
20
25
30
35
40
0
20
40
60
80
100
120
140



Solver Summary Statistics

number of unique participating solvers: 9


Run time of solvers (for attempted tasks)
1e8
2.0
1.5
1.0
0.5
0.0
Overall run time in seconds
0
20
40
60
80
100
120
140
Number of spatial orbitals



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: 80ee05f7-aa48-48e1-ad58-d21baa5cfdd4

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 41

number_of_problem_instances_solved: 14

number_of_tasks: 230

number_of_tasks_attempted: 162

number_of_tasks_solved: 80

number_of_tasks_solved_within_run_time_limit: 162

number_of_tasks_solved_within_accuracy_threshold: 80

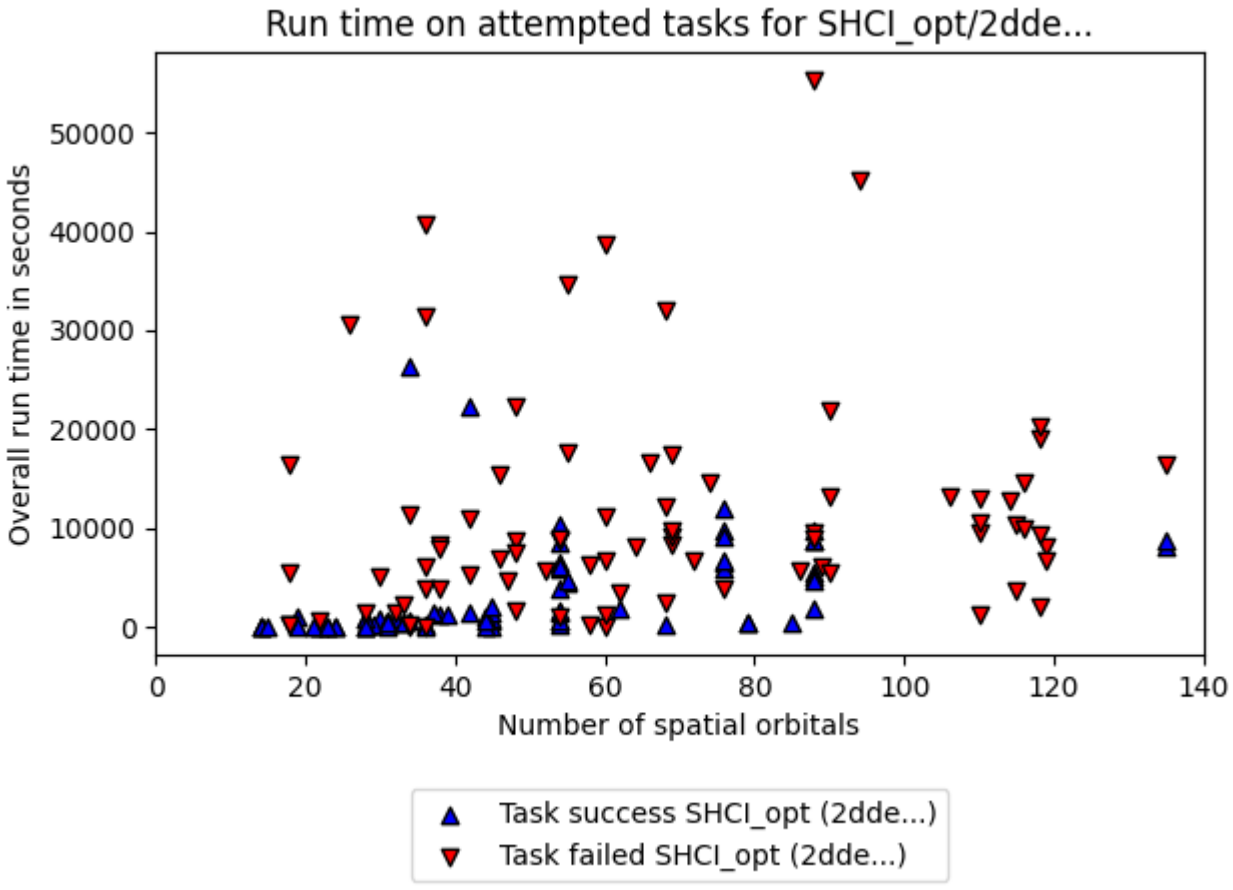
max_run_time_of_attempted_tasks: 55299.387

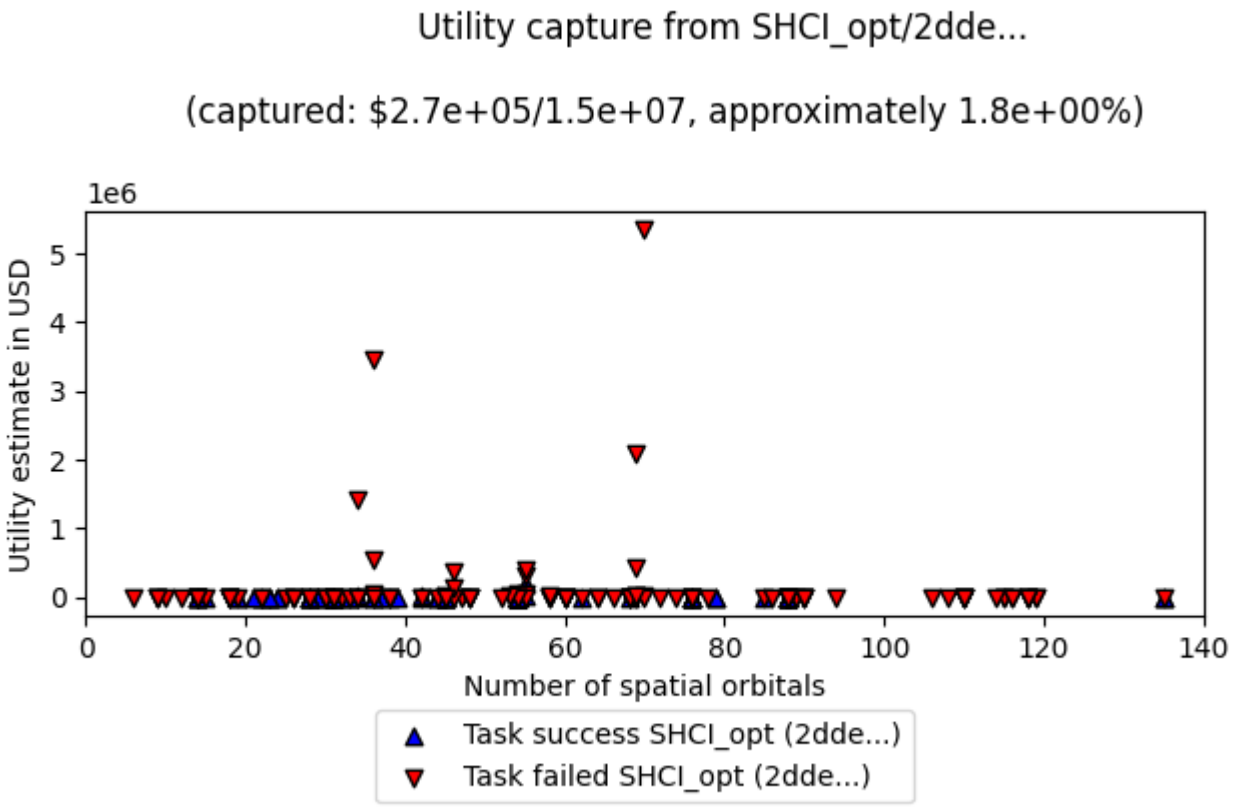
sum_of_run_time_of_attempted_tasks: 1138067.4269999997

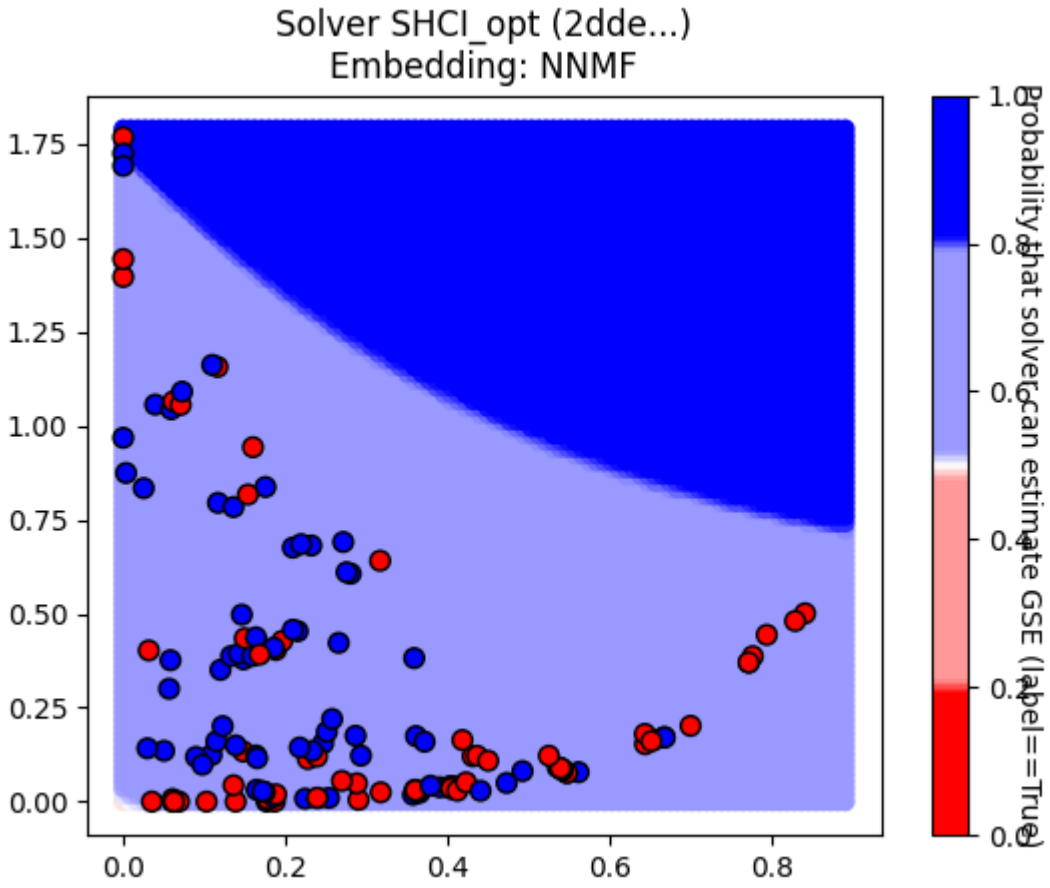
solvability_ratio: 0.9998

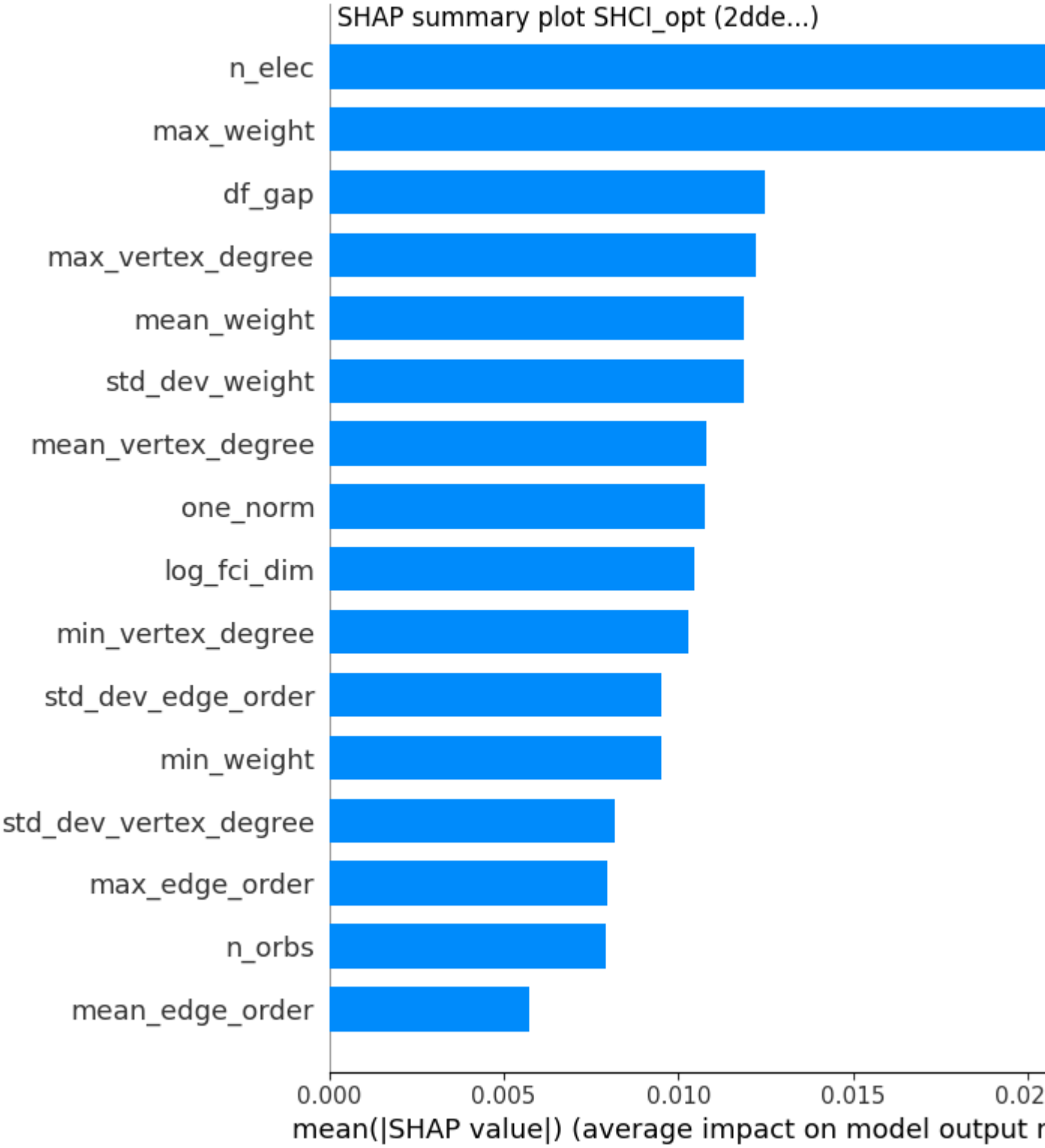
f1_score: [0.7058823529411765, 0.8275862068965517]

ml_metrics_calculator_version: 1




Utility capture from SHCI_opt/2dde...
(captured: $2.7e+05/1.5e+07, approximately 1.8e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_opt (2dde...)
Task failed SHCI_opt (2dde...)


Solver SHCI_opt (2dde...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



Solver CCSDT_PLACEHOLDER, fd13c864-baf1-44de-b52d-0e5dd69f647a

solver_uuid:fd13c864-baf1-44de-b52d-0e5dd69f647a

solver_short_name:CCSDT_PLACEHOLDER

compute_hardware_type:classical_computer

classical_hardware_details:{'cpu_description':
'CCSDT_PLACEHOLDER_cpu_description'}

algorithm_details:CCSDT_PLACEHOLDER_algorithm_details

software_details:CCSDT_PLACEHOLDER_software_details

performance_metrics_uuid: a1a3bd58-31dc-4940-8785-713186a1fa2e

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 4

number_of_problem_instances_solved: 0

number_of_tasks: 230

number_of_tasks_attempted: 53

number_of_tasks_solved: 16

number_of_tasks_solved_within_run_time_limit: 53

number_of_tasks_solved_within_accuracy_threshold: 16

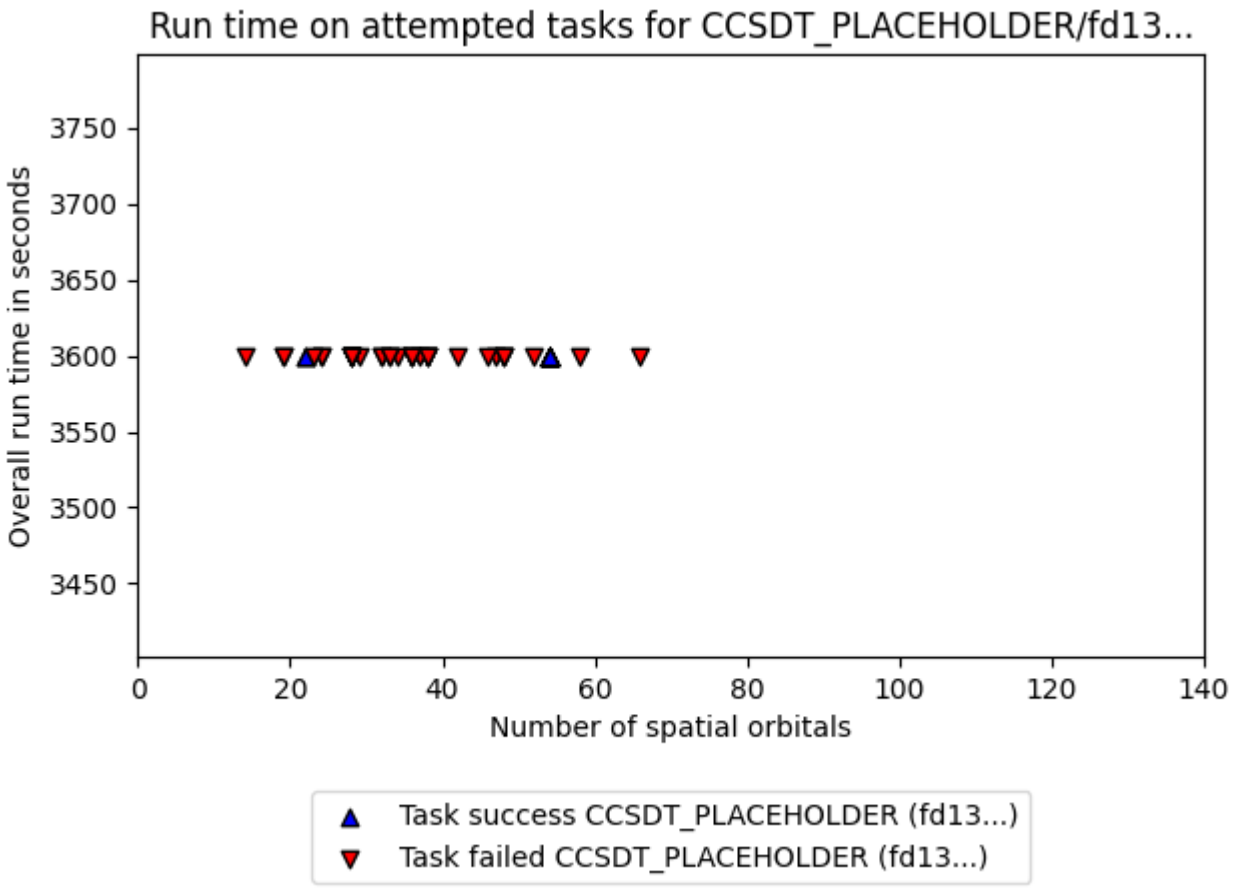
max_run_time_of_attempted_tasks: 3600.0

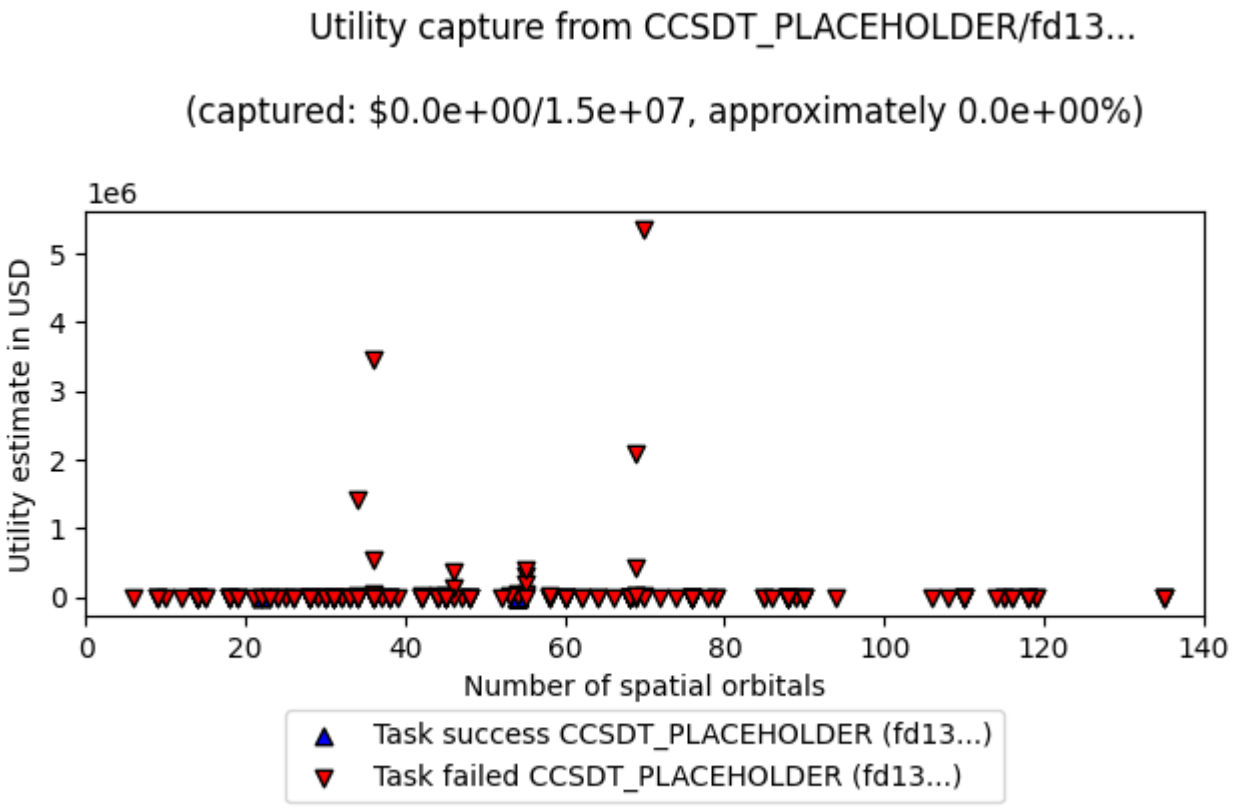
sum_of_run_time_of_attempted_tasks: 190800.0

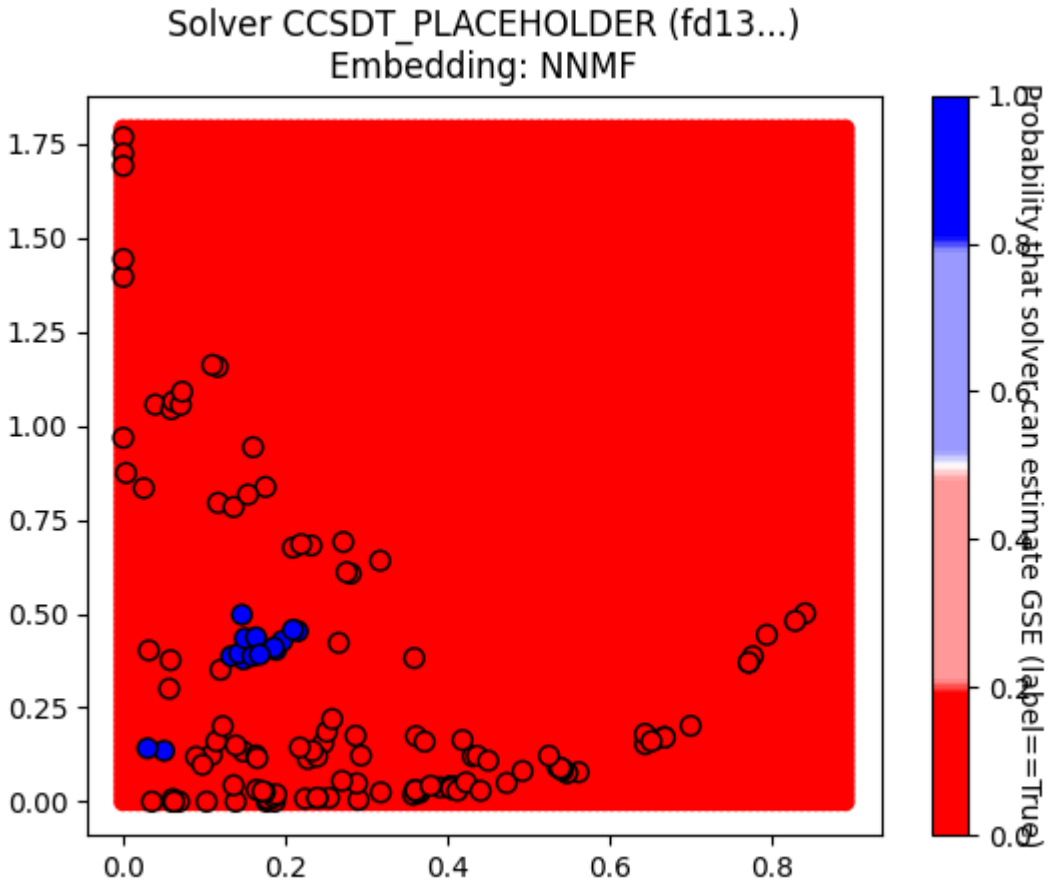
solvability_ratio: 0.0

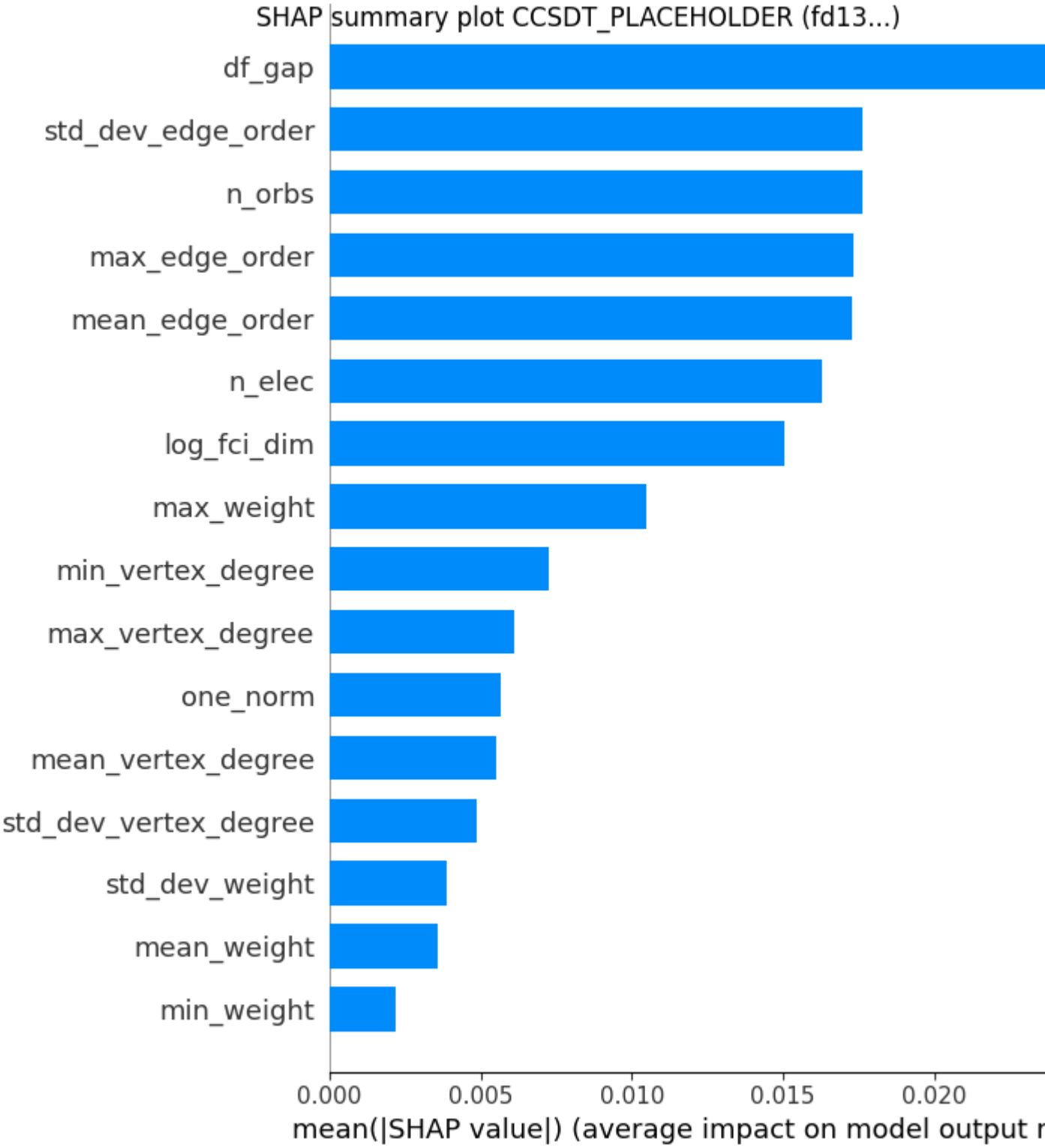
f1_score: [0.9878542510121457, 0.896551724137931]

ml_metrics_calculator_version: 1


Run time on attempted tasks for CCSDT_PLACEHOLDER/fd13...
Overall run time in seconds
3750
3700
3650
3600
3550
3500
3450
0
20
40
60
80
100
120
140
Number of spatial orbitals
Task success CCSDT_PLACEHOLDER (fd13...)
Task failed CCSDT_PLACEHOLDER (fd13...)


Utility capture from CCSDT_PLACEHOLDER/fd13...
(captured: $0.0e+00/1.5e+07, approximately 0.0e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSDT_PLACEHOLDER (fd13...)
Task failed CCSDT_PLACEHOLDER (fd13...)


Solver CCSDT_PLACEHOLDER (fd13...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



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: 1ea2d124-f609-43a3-831a-d09a02f770d3

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 82

number_of_problem_instances_solved: 9

number_of_tasks: 230

number_of_tasks_attempted: 230

number_of_tasks_solved: 14

number_of_tasks_solved_within_run_time_limit: 230

number_of_tasks_solved_within_accuracy_threshold: 14

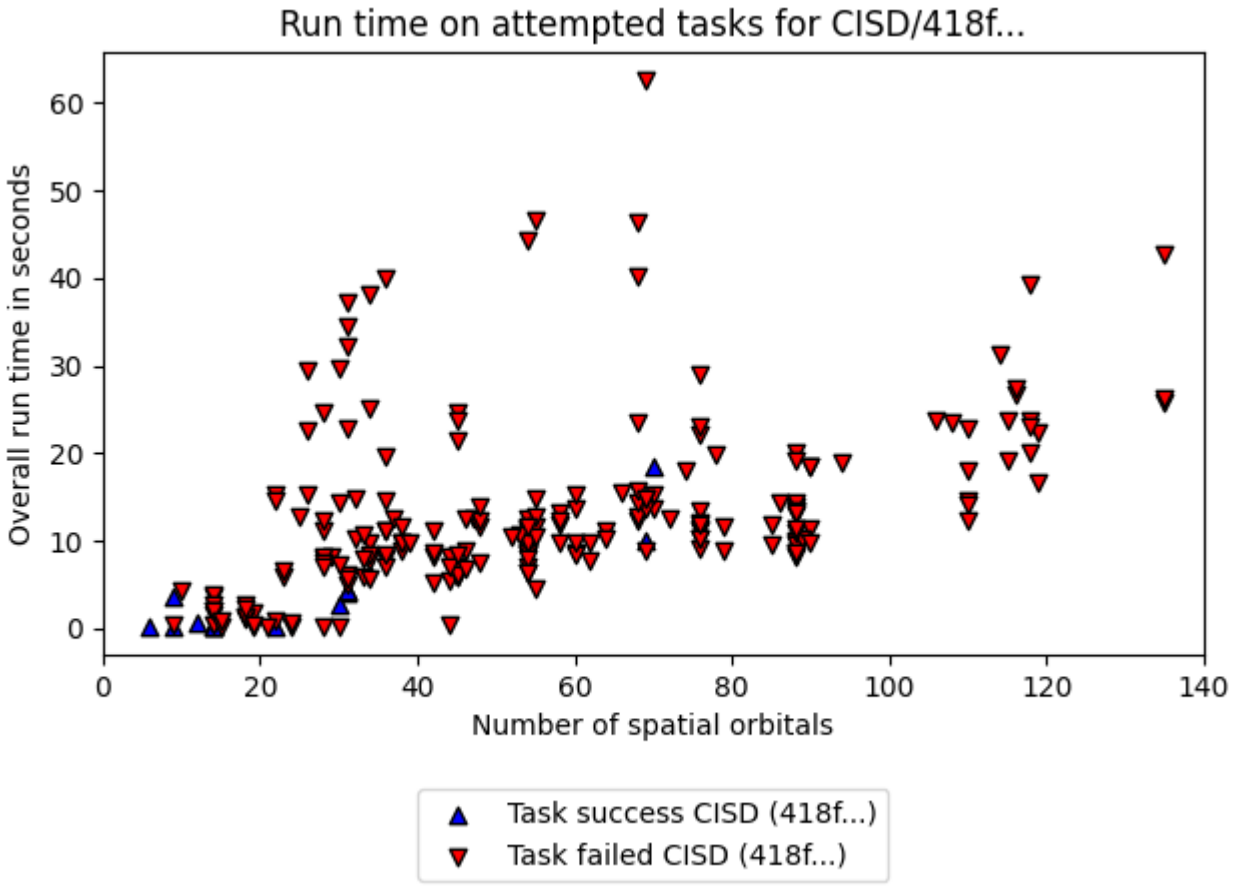
max_run_time_of_attempted_tasks: 62.58296537399292

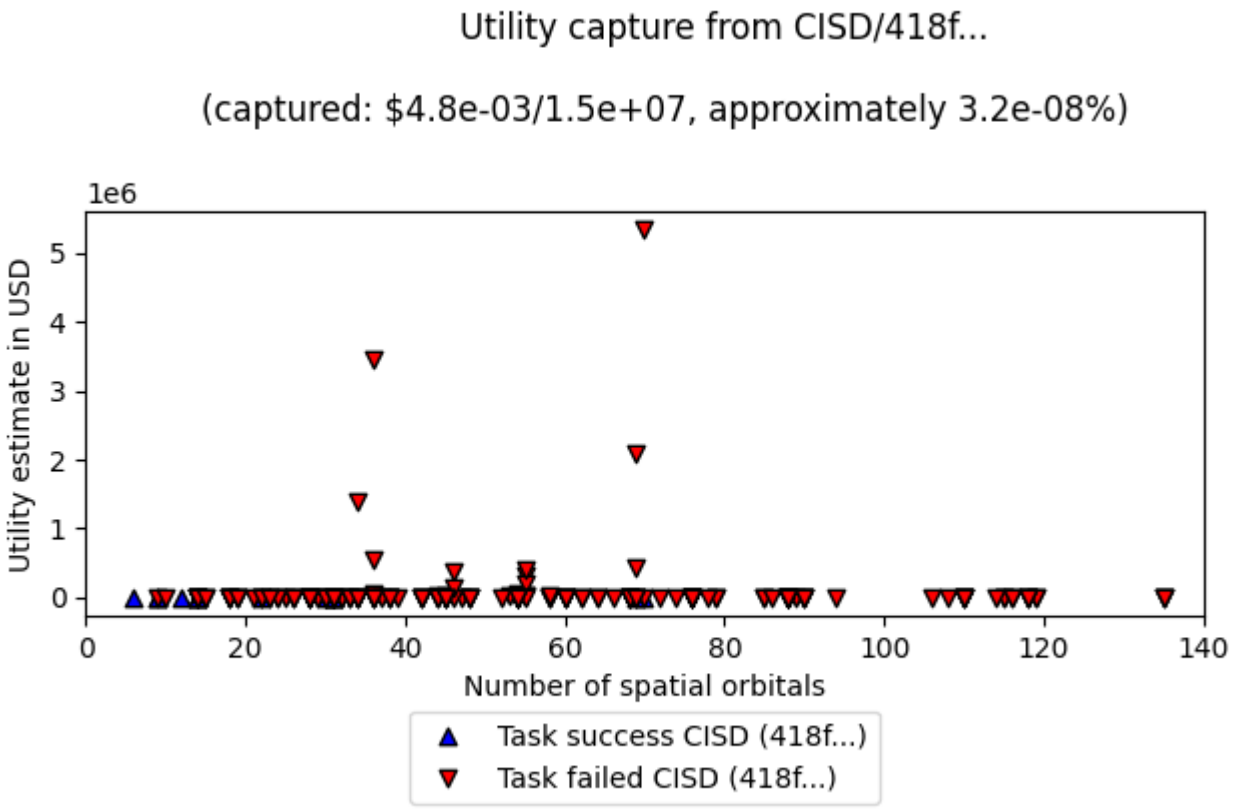
sum_of_run_time_of_attempted_tasks: 2895.8530027866364

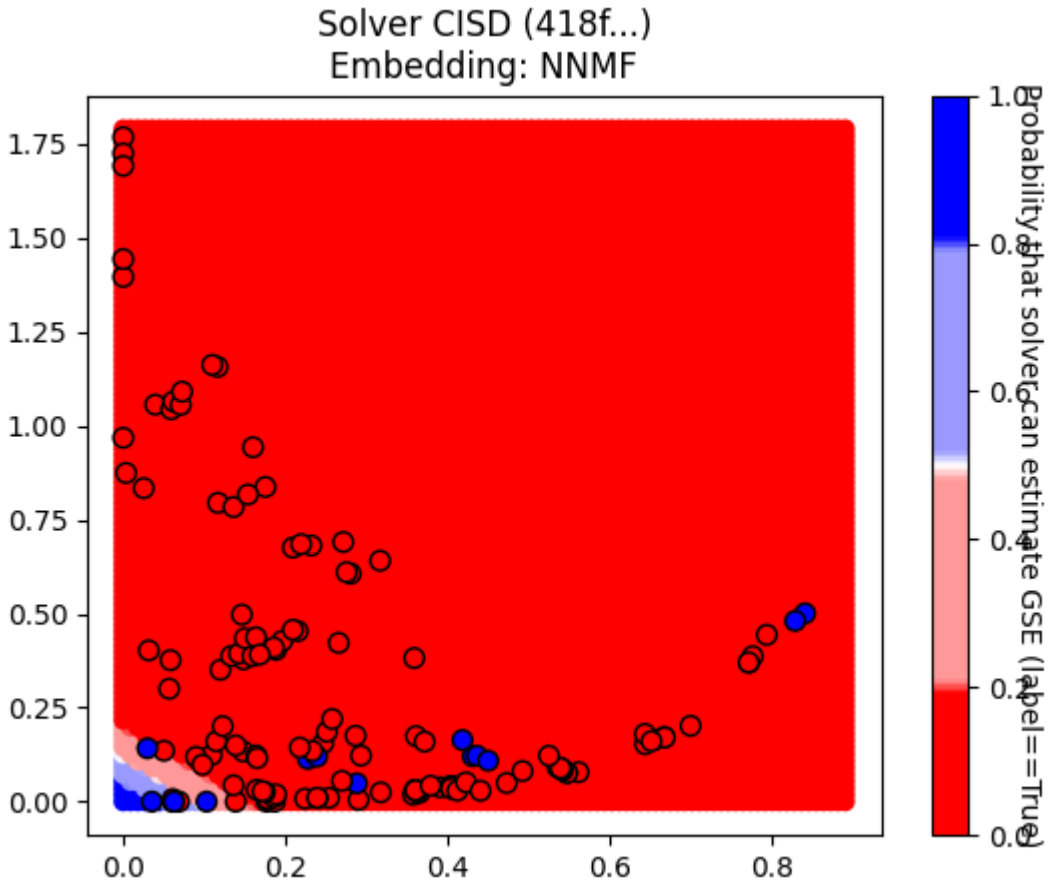
solvability_ratio: 0.0047

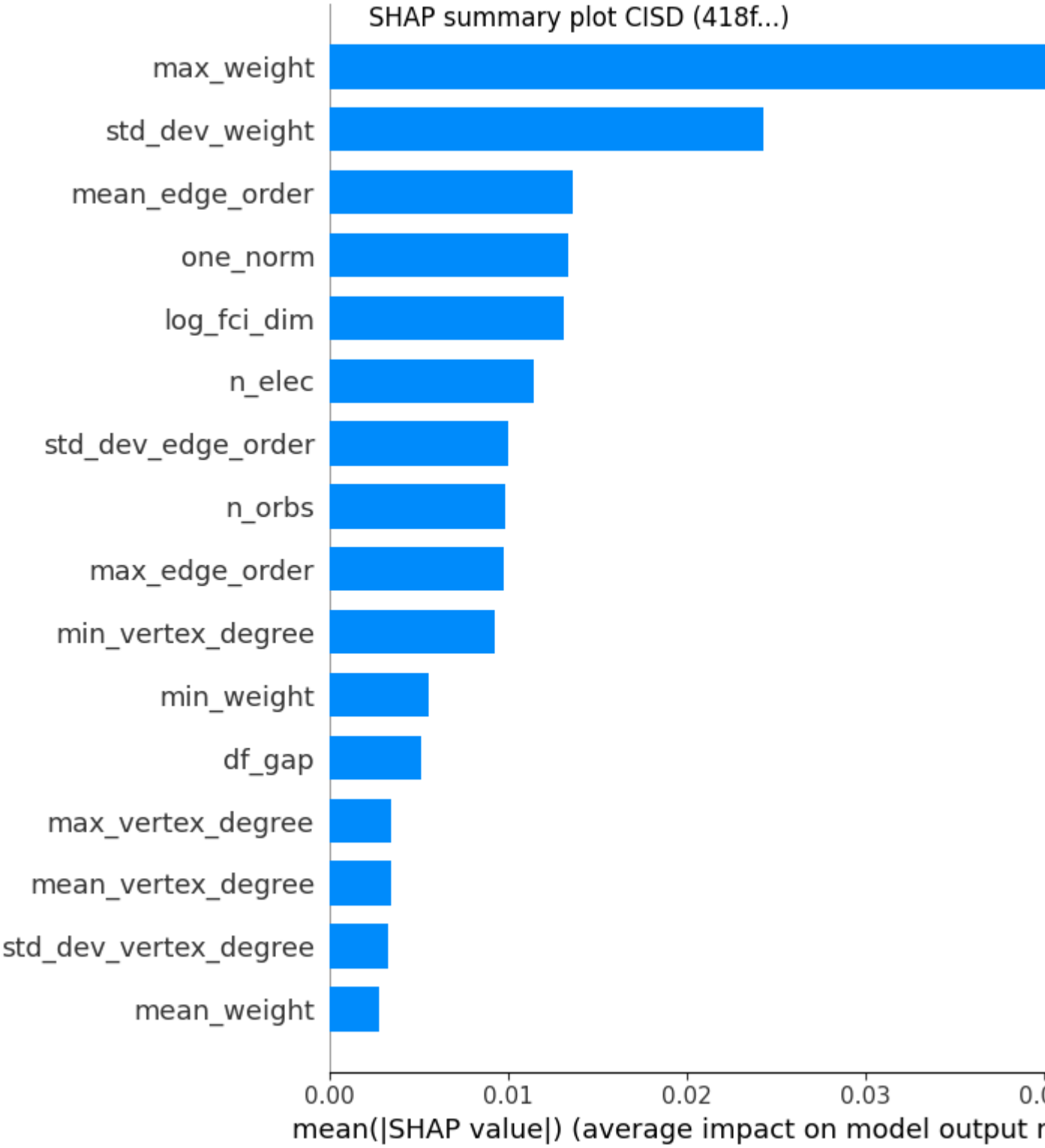
f1_score: [0.9919354838709677, 0.9285714285714286]

ml_metrics_calculator_version: 1


Run time on attempted tasks for CISD/418f...
Overall run time in seconds
Number of spatial orbitals
0
10
20
30
40
50
60
0
20
40
60
80
100
120
140
Task success CISD (418f...)
Task failed CISD (418f...)


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...)


Solver CISD (418f...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



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: 82e77fa6-bd75-4e86-ab35-b17898dc6834

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 78

number_of_problem_instances_solved: 19

number_of_tasks: 230

number_of_tasks_attempted: 221

number_of_tasks_solved: 64

number_of_tasks_solved_within_run_time_limit: 221

number_of_tasks_solved_within_accuracy_threshold: 64

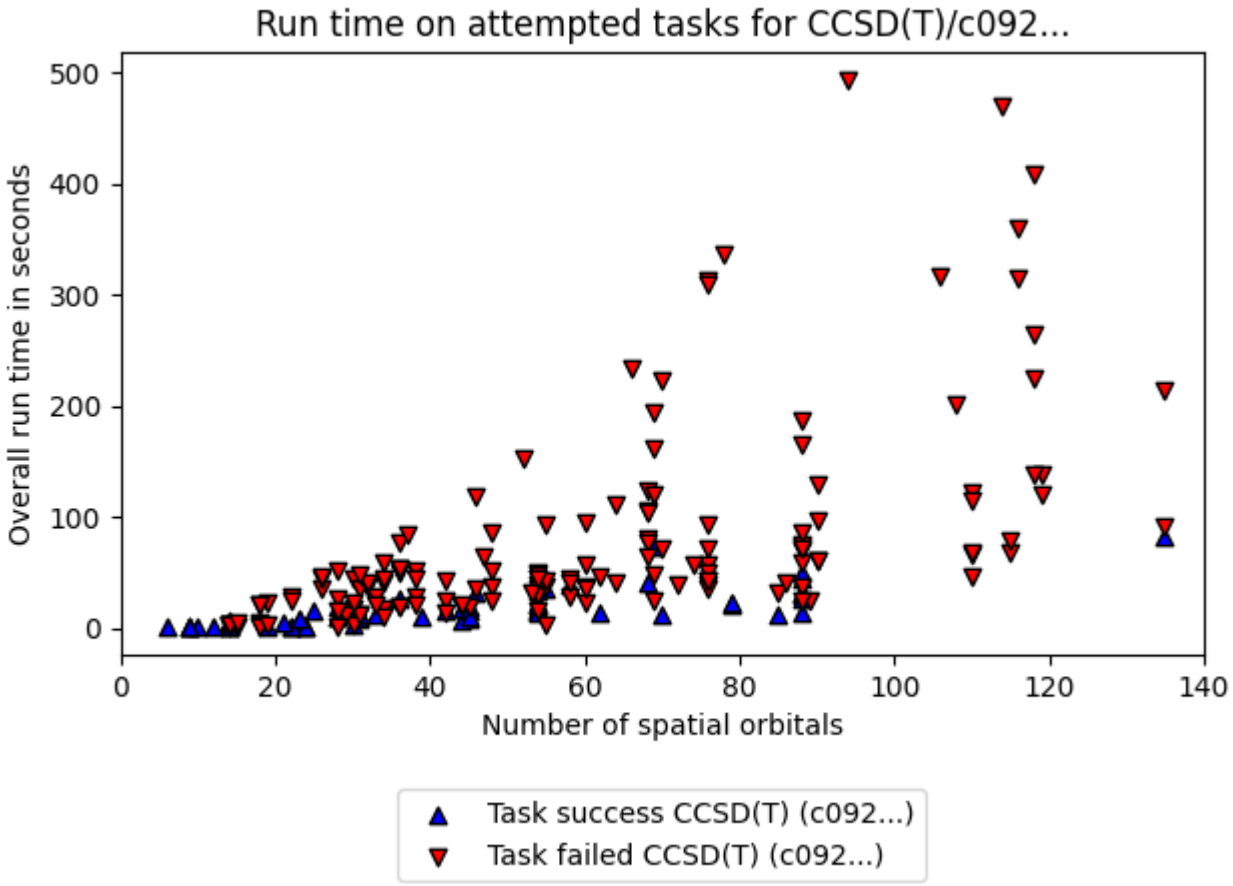
max_run_time_of_attempted_tasks: 493.4080808162689

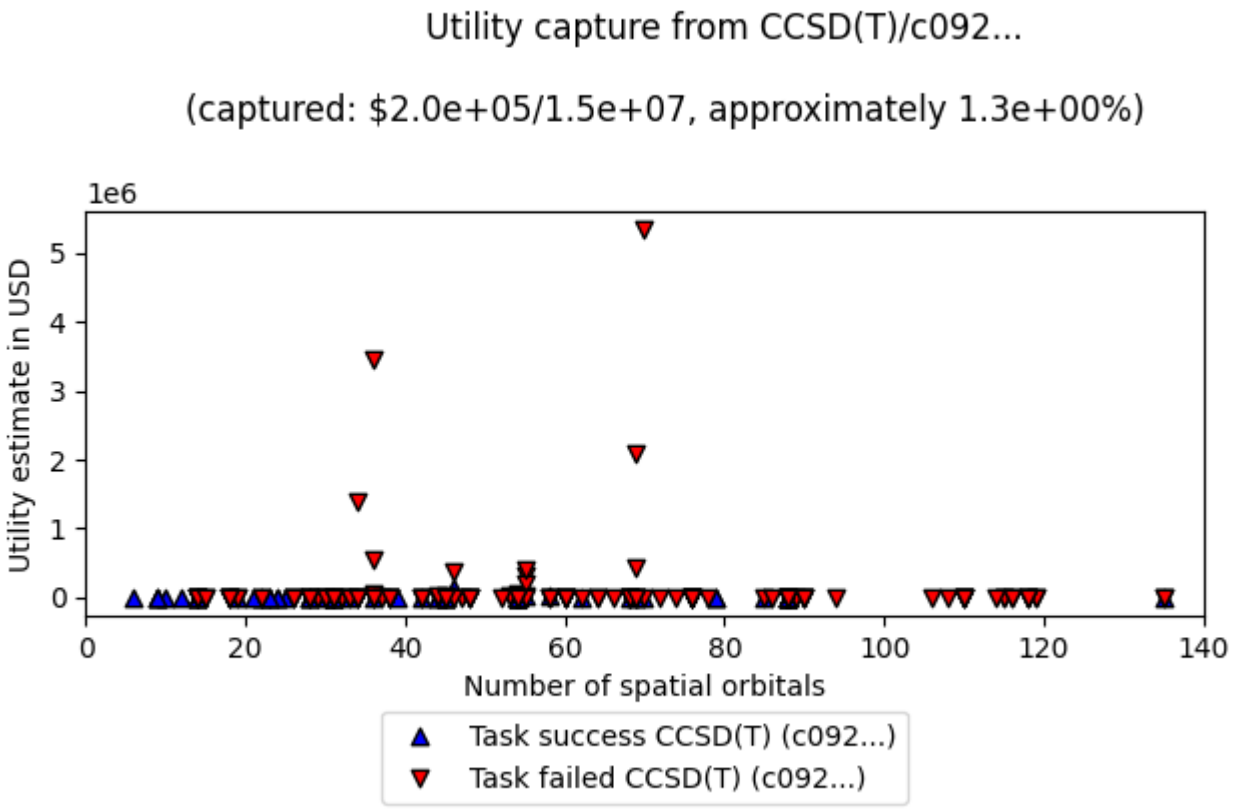
sum_of_run_time_of_attempted_tasks: 12968.4871737957

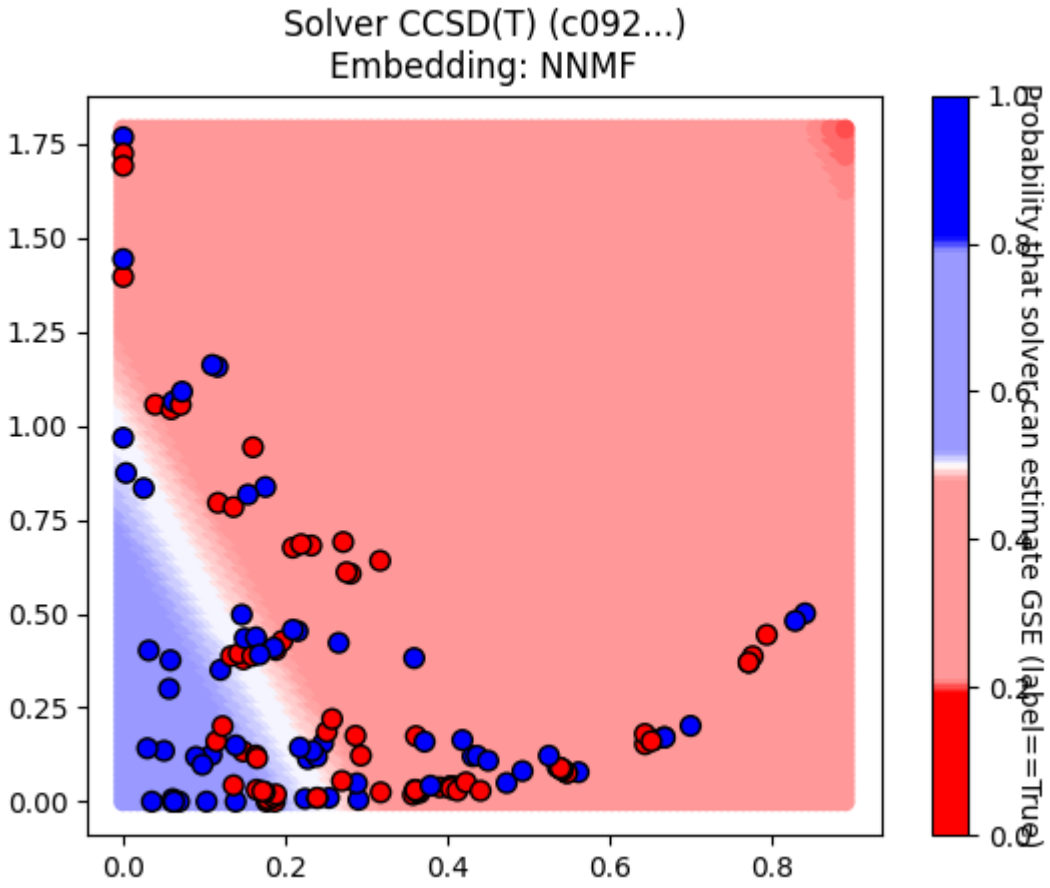
solvability_ratio: 0.0715

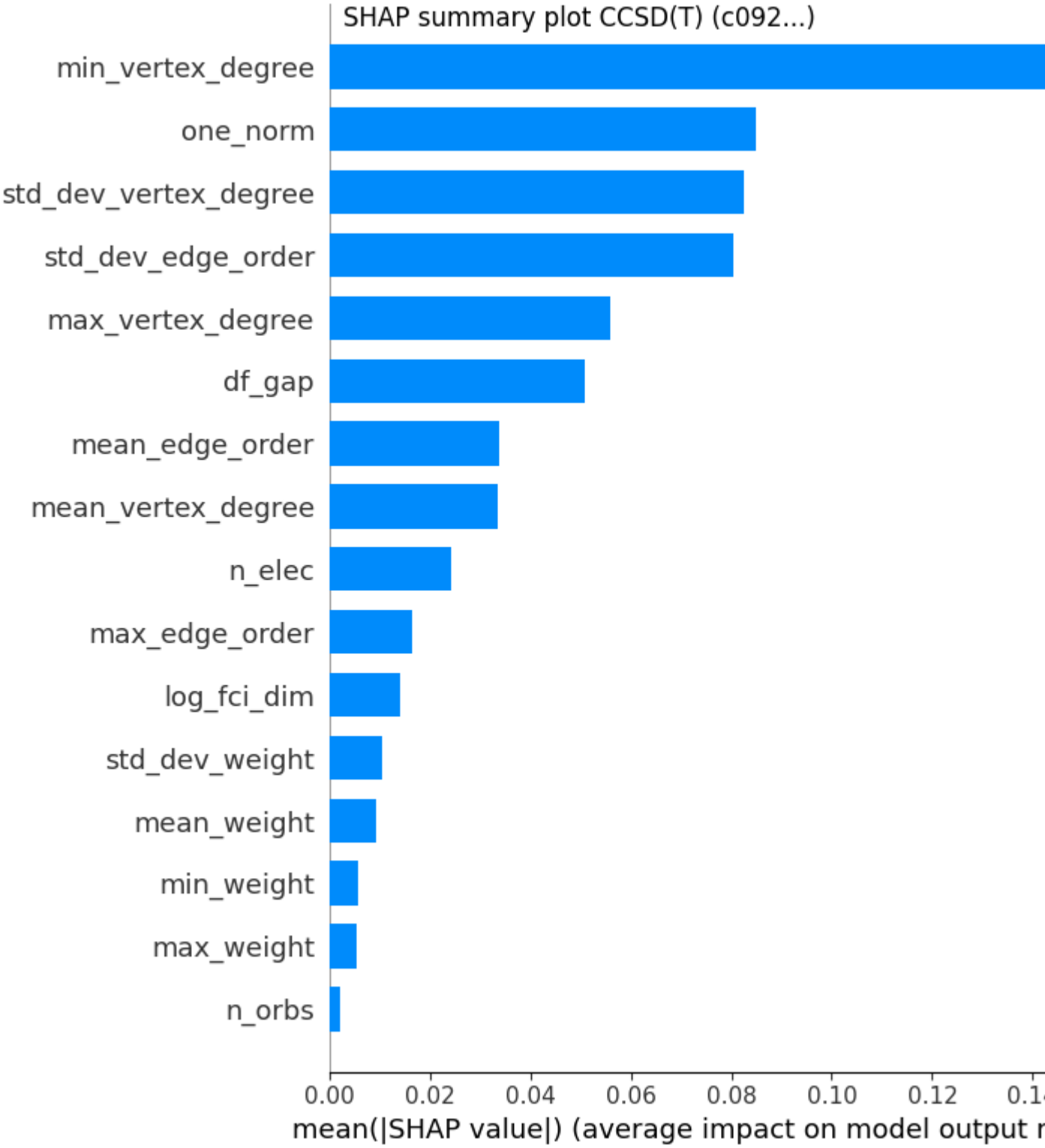
f1_score: [0.759493670886076, 0.6779661016949152]

ml_metrics_calculator_version: 1


Run time on attempted tasks for CCSD(T)/c092...
Overall run time in seconds
Number of spatial orbitals
0
100
200
300
400
500
0
20
40
60
80
100
120
140
Task success CCSD(T) (c092...)
Task failed CCSD(T) (c092...)


Utility capture from CCSD(T)/c092...
(captured: $2.0e+05/1.5e+07, approximately 1.3e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSD(T) (c092...)
Task failed CCSD(T) (c092...)


Solver CCSD(T) (c092...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
Probability that solver can estimate GSE (label==True)



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: 84ecadfc-b2d8-47a8-a9fe-28fd5a212dee

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 82

number_of_problem_instances_solved: 5

number_of_tasks: 230

number_of_tasks_attempted: 230

number_of_tasks_solved: 5

number_of_tasks_solved_within_run_time_limit: 230

number_of_tasks_solved_within_accuracy_threshold: 5

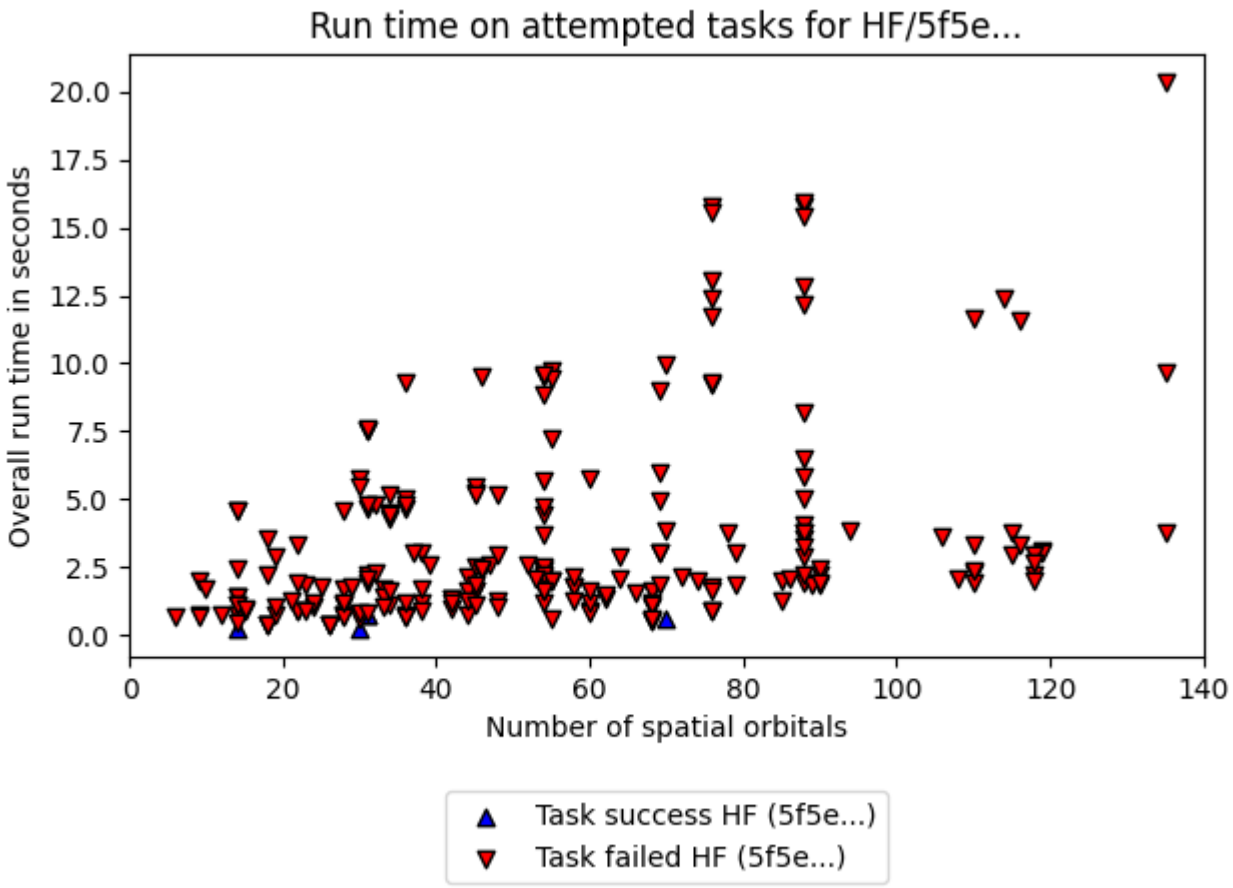
max_run_time_of_attempted_tasks: 20.338801622390747

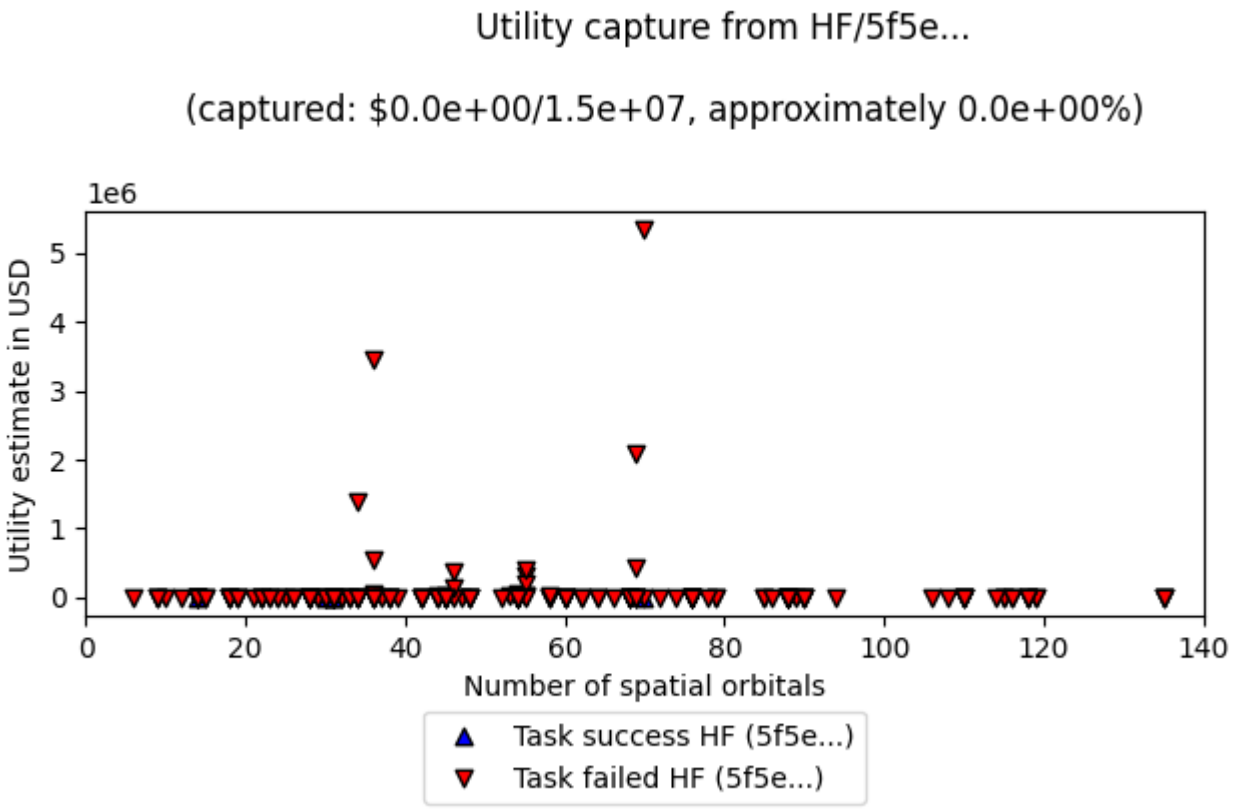
sum_of_run_time_of_attempted_tasks: 792.8028435707092

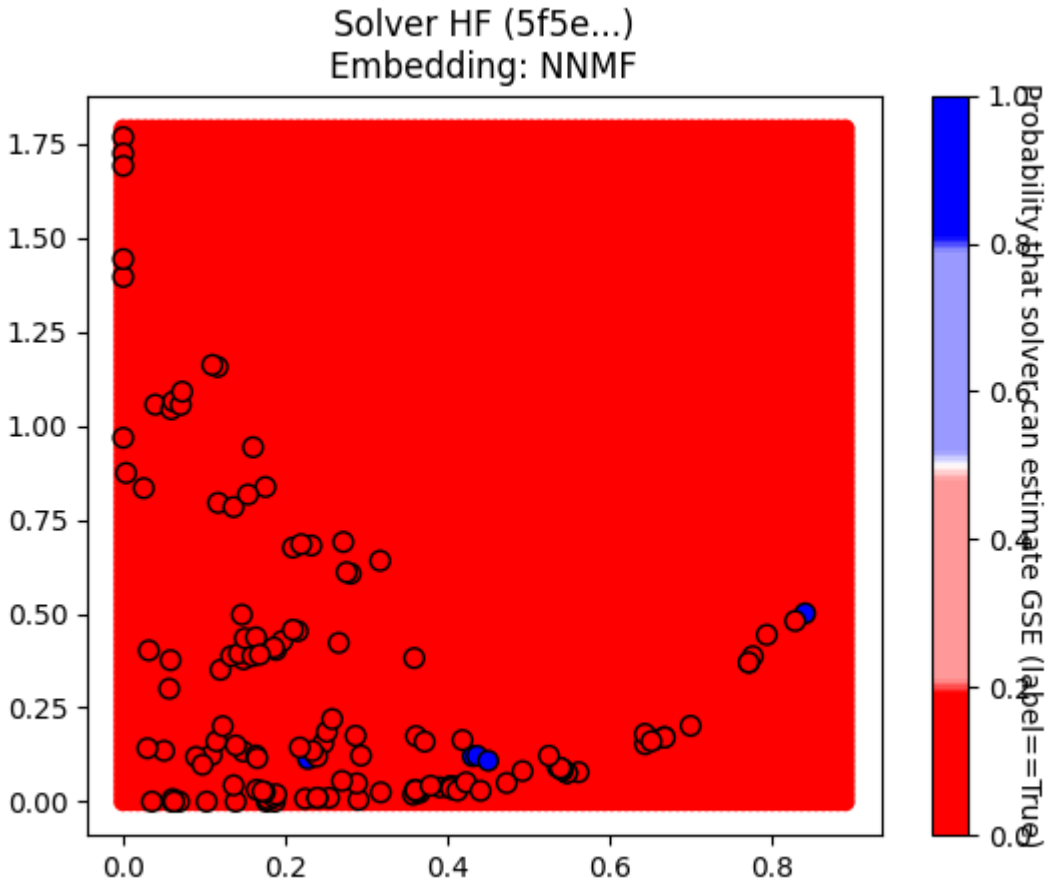
solvability_ratio: 0.0

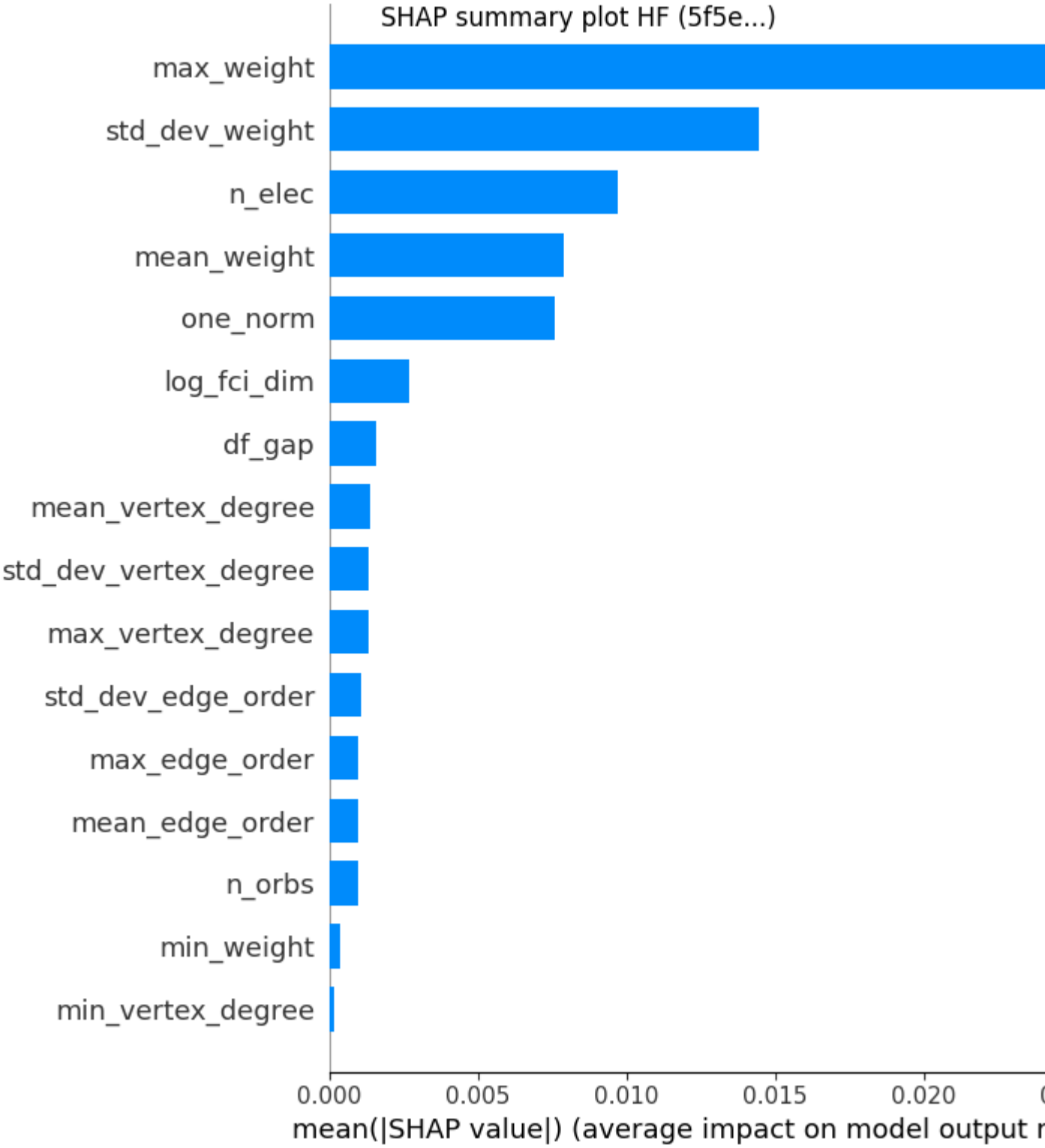
f1_score: [0.9847328244274809, 0.7142857142857143]

ml_metrics_calculator_version: 1


Run time on attempted tasks for HF/5f5e...
Overall run time in seconds
Number of spatial orbitals
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
0
20
40
60
80
100
120
140
Task success HF (5f5e...)
Task failed HF (5f5e...)


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...)


Solver HF (5f5e...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



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: d791e295-64ee-4806-bc59-2bac79f92611

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 79

number_of_problem_instances_solved: 5

number_of_tasks: 230

number_of_tasks_attempted: 222

number_of_tasks_solved: 5

number_of_tasks_solved_within_run_time_limit: 222

number_of_tasks_solved_within_accuracy_threshold: 5

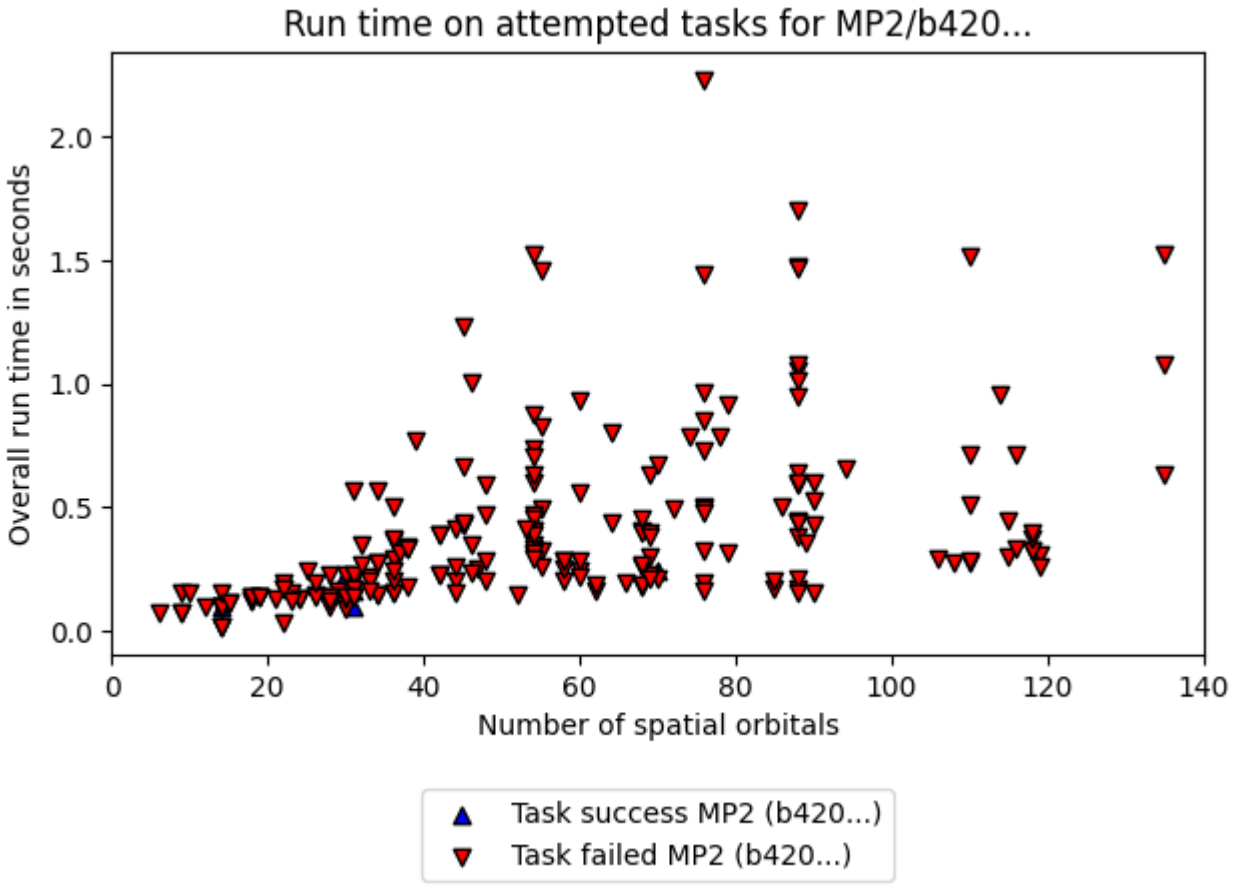
max_run_time_of_attempted_tasks: 2.230440139770508

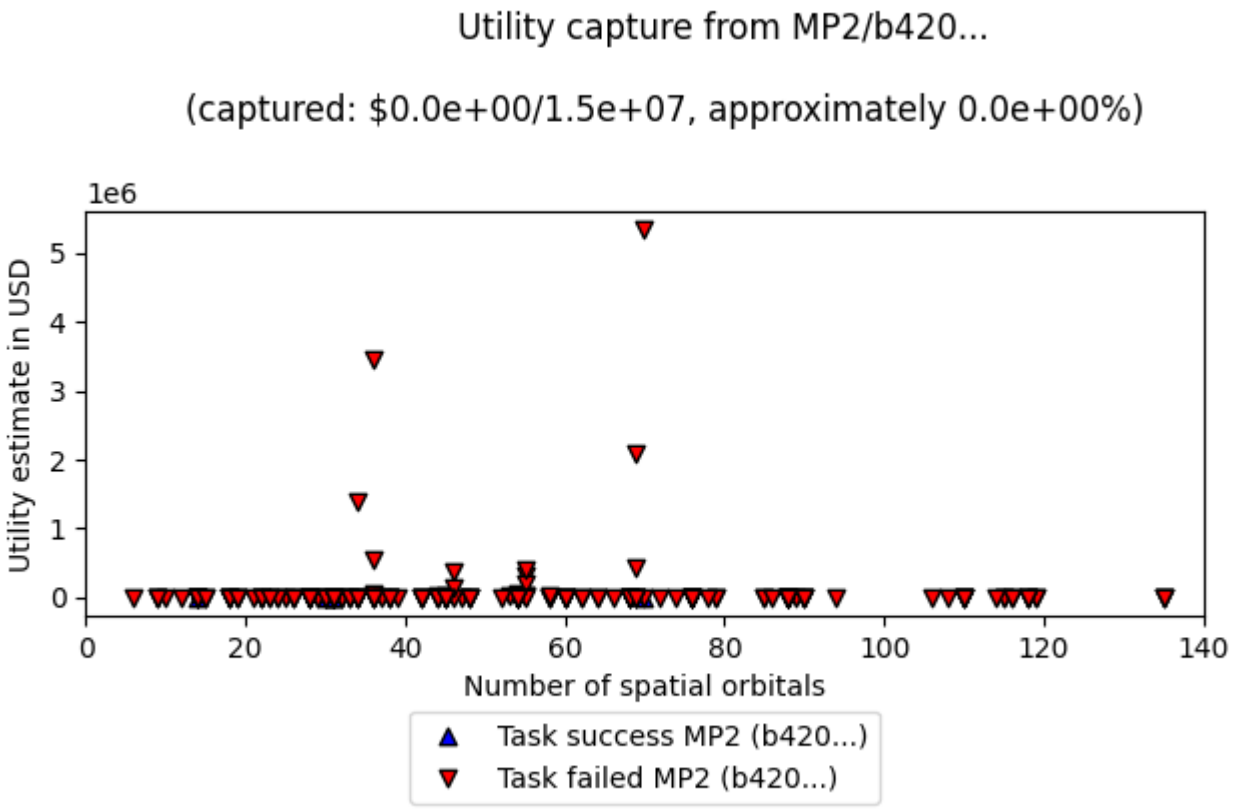
sum_of_run_time_of_attempted_tasks: 87.6544258594513

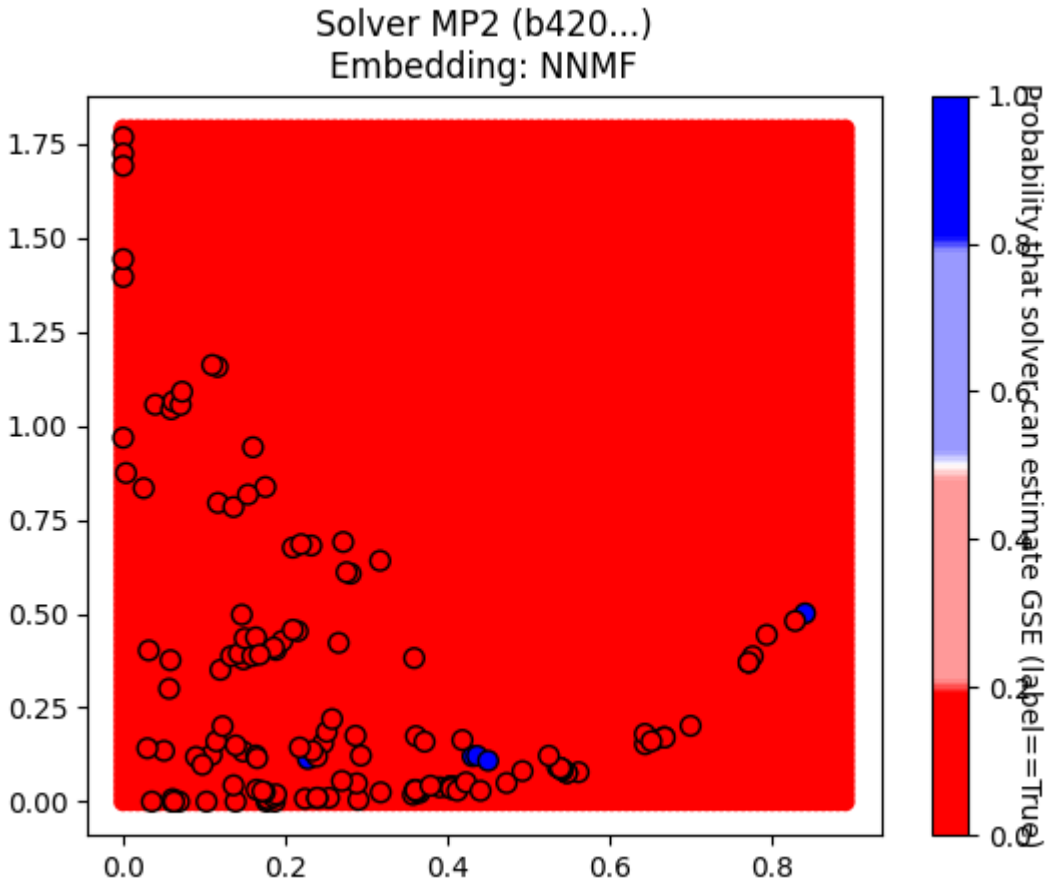
solvability_ratio: 0.0

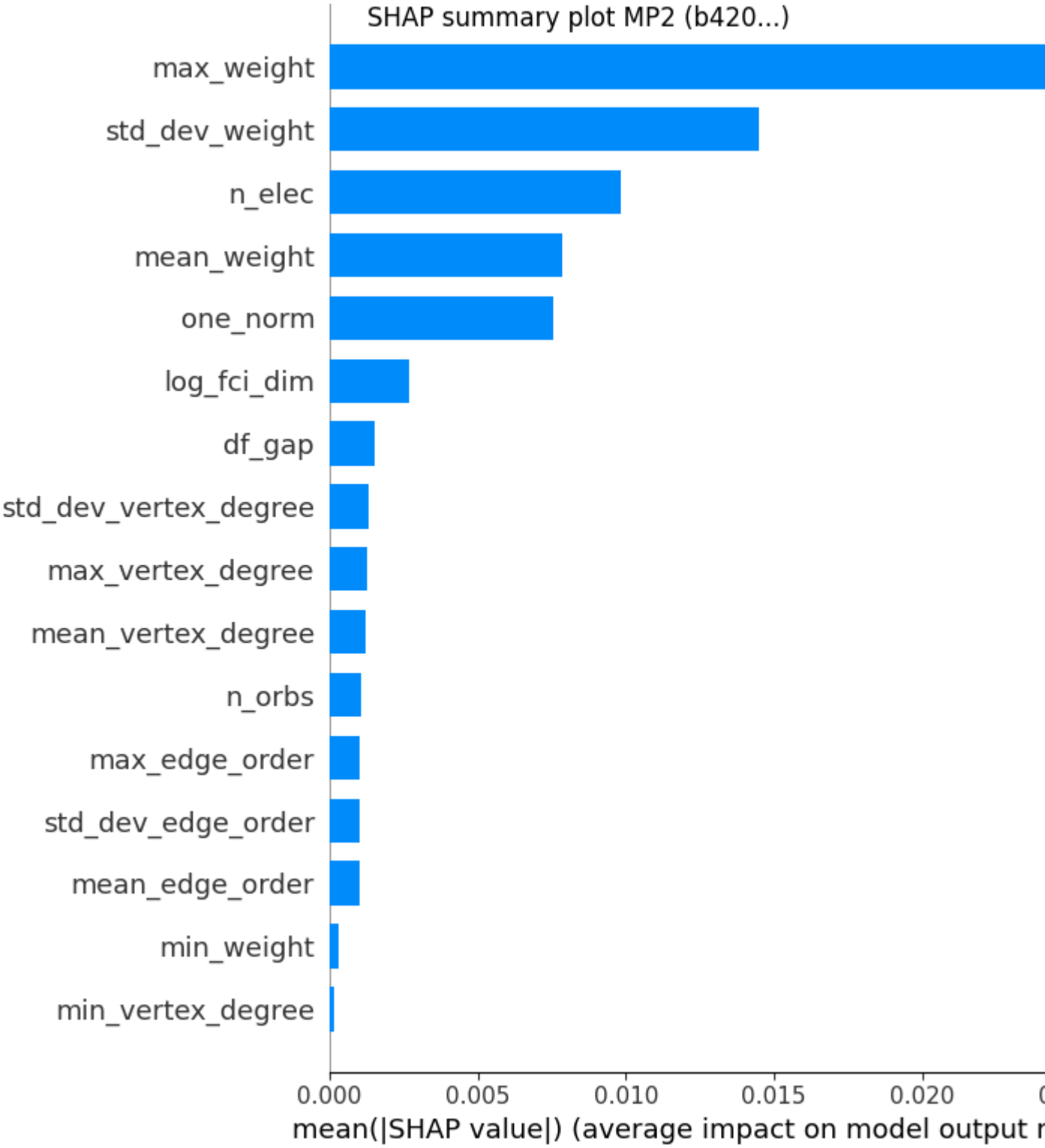
f1_score: [0.9847328244274809, 0.7142857142857143]

ml_metrics_calculator_version: 1


Run time on attempted tasks for MP2/b420...
Overall run time in seconds
0.0
0.5
1.0
1.5
2.0
0
20
40
60
80
100
120
140
Number of spatial orbitals
Task success MP2 (b420...)
Task failed MP2 (b420...)


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...)


Solver MP2 (b420...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



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: d80a29c2-1b9f-418d-bc65-de1ed7c499a5

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 78

number_of_problem_instances_solved: 9

number_of_tasks: 230

number_of_tasks_attempted: 221

number_of_tasks_solved: 17

number_of_tasks_solved_within_run_time_limit: 221

number_of_tasks_solved_within_accuracy_threshold: 17

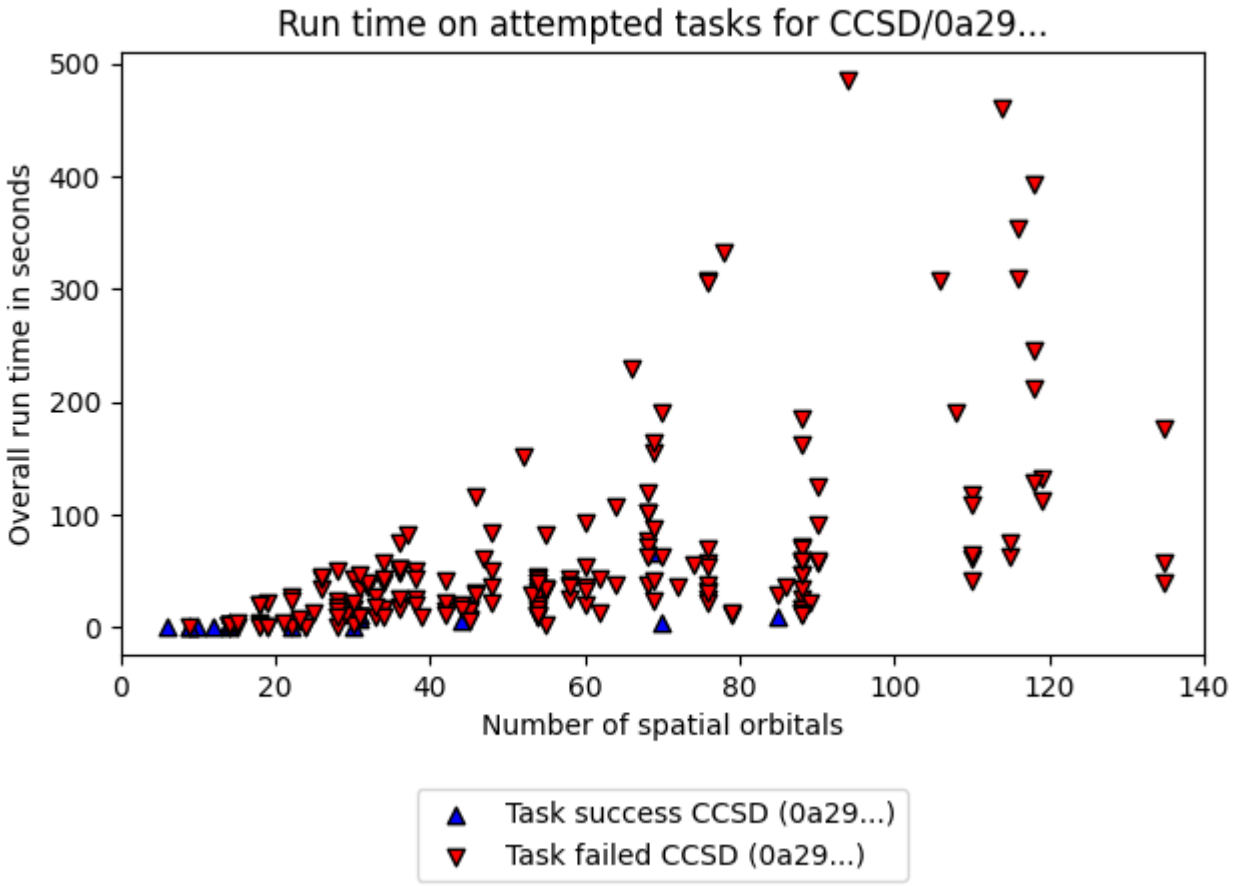
max_run_time_of_attempted_tasks: 485.1982181072235

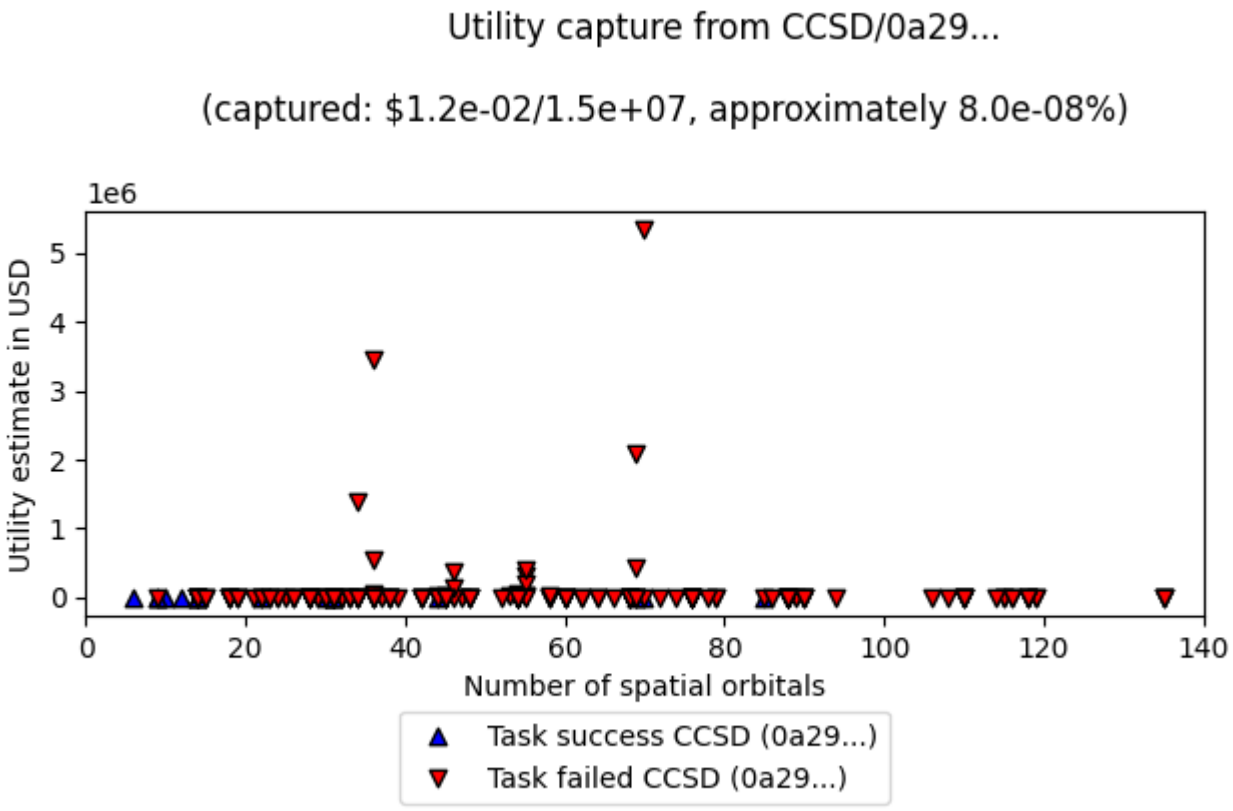
sum_of_run_time_of_attempted_tasks: 12029.76450586319

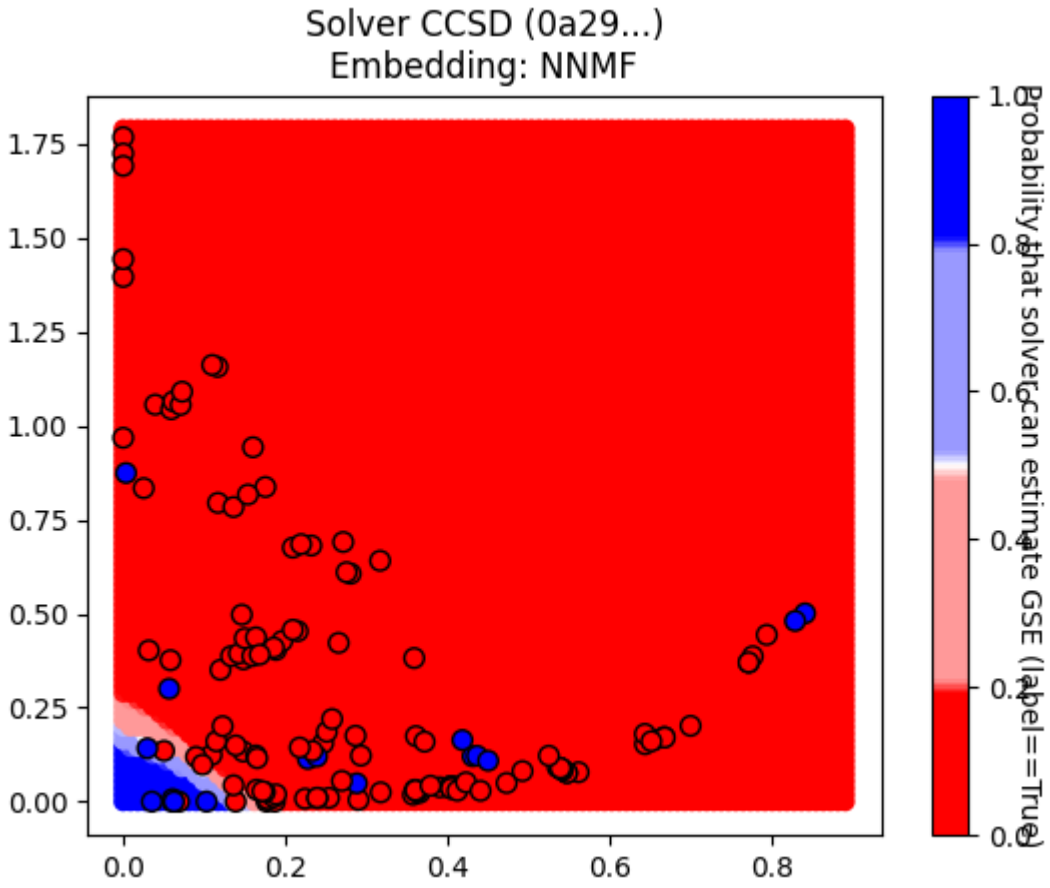
solvability_ratio: 0.0122

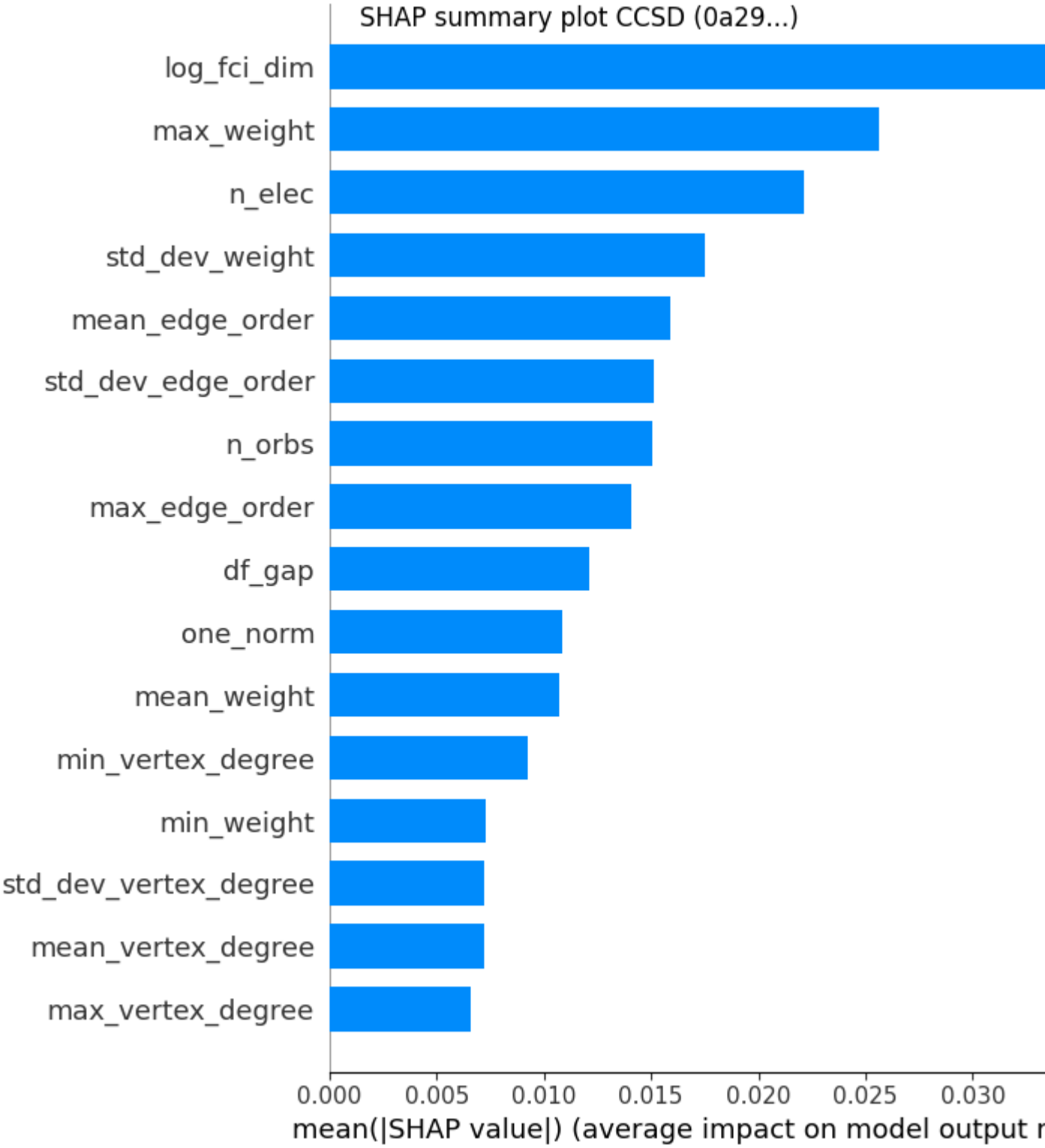
f1_score: [0.995850622406639, 0.9714285714285714]

ml_metrics_calculator_version: 1


Run time on attempted tasks for CCSD/0a29...
Overall run time in seconds
Number of spatial orbitals
0
100
200
300
400
500
0
20
40
60
80
100
120
140
Task success CCSD (0a29...)
Task failed CCSD (0a29...)


Utility capture from CCSD/0a29...
(captured: $1.2e-02/1.5e+07, approximately 8.0e-08%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSD (0a29...)
Task failed CCSD (0a29...)


Solver CCSD (0a29...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



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': '1.2.1'}, {'software_name': 'qb-gsee-benchmark', 'software_version': '0.1.0a2.dev71+g5d9efab.d20241230'}, {'software_name': 'Python', 'software_version': '3.10.12 (main, Nov 6 2024, 20:22:13) [GCC 11.4.0]'}, {'software_name': 'qualtran', 'software_version': '0.2.0'}]

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:72dea71b-fb03-43f0-8086-eb37605ba3db

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

performance_metrics_uuid: 8332924f-3b1d-421f-a35b-78d6d593ec4d

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 24

number_of_problem_instances_solved: 3

number_of_tasks: 230

number_of_tasks_attempted: 163

number_of_tasks_solved: 26

number_of_tasks_solved_within_run_time_limit: 26

number_of_tasks_solved_within_accuracy_threshold: 163

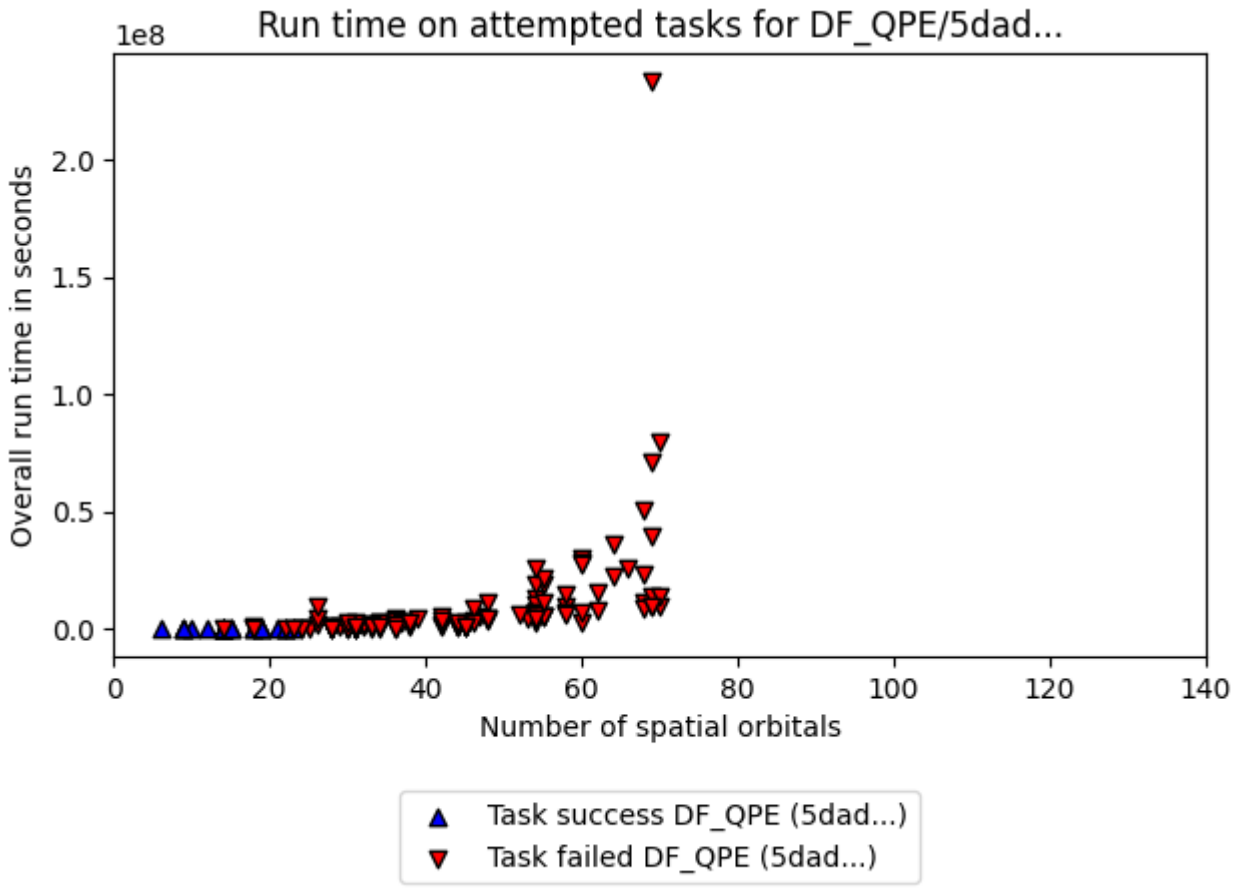
max_run_time_of_attempted_tasks: 233737829.40462503

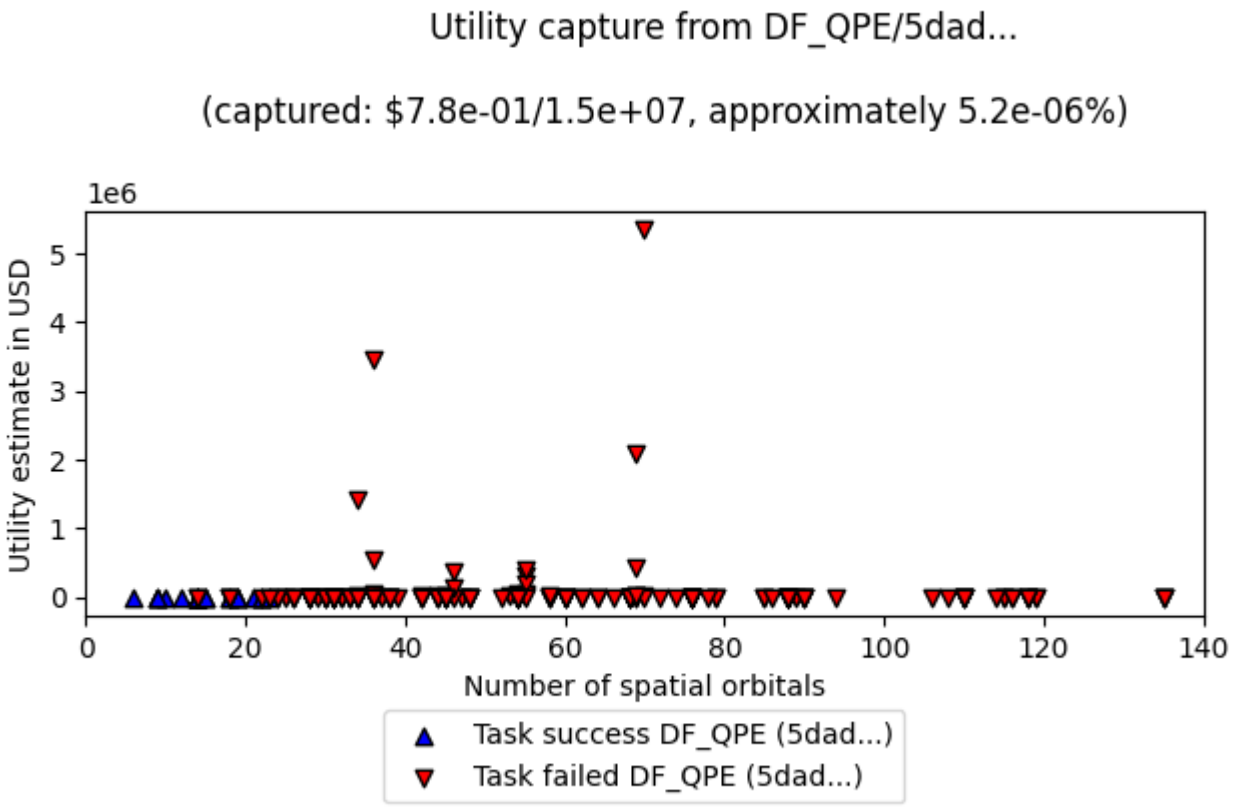
sum_of_run_time_of_attempted_tasks: 1180589418.3385448

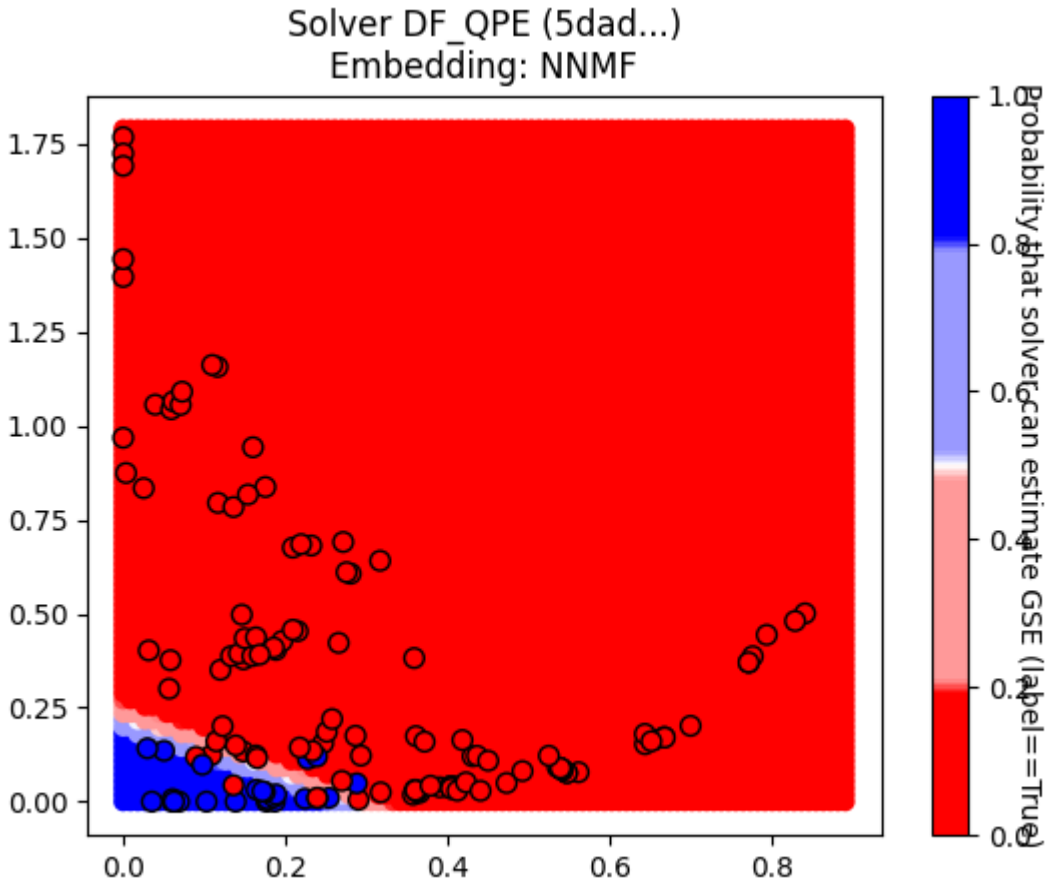
solvability_ratio: 0.0235

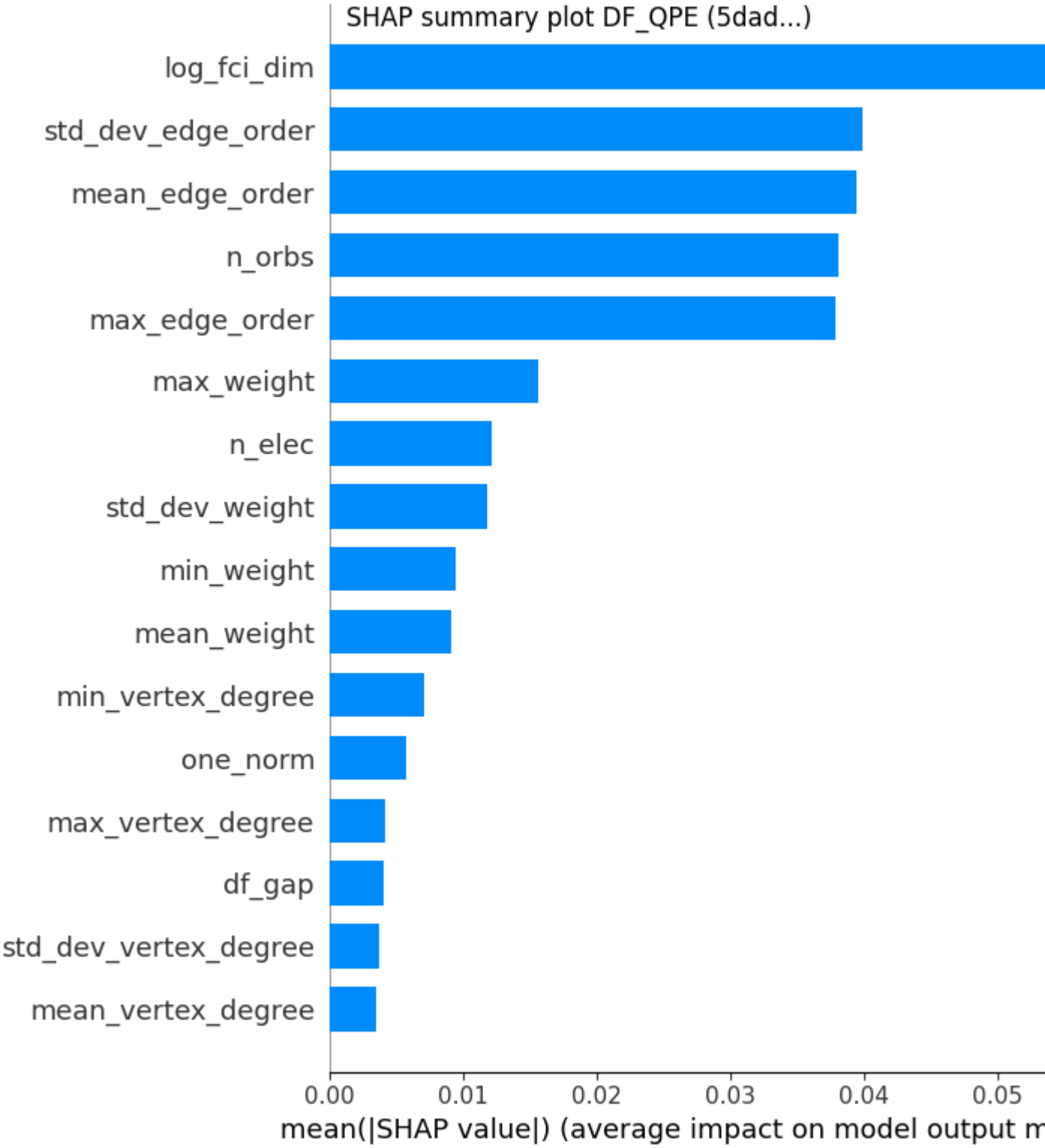
f1_score: [0.9819819819819819, 0.9259259259259259]

ml_metrics_calculator_version: 1




Utility capture from DF_QPE/5dad...
(captured: $7.8e-01/1.5e+07, approximately 5.2e-06%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success DF_QPE (5dad...)
Task failed DF_QPE (5dad...)


Solver DF_QPE (5dad...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)



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: 8b4756f5-fc22-4c14-9b33-f11ba48eb72b

creation_timestamp: 2025-01-23T16:28:43.200733+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 82

number_of_problem_instances_solved: 8

number_of_tasks: 230

number_of_tasks_attempted: 230

number_of_tasks_solved: 72

number_of_tasks_solved_within_run_time_limit: 230

number_of_tasks_solved_within_accuracy_threshold: 72

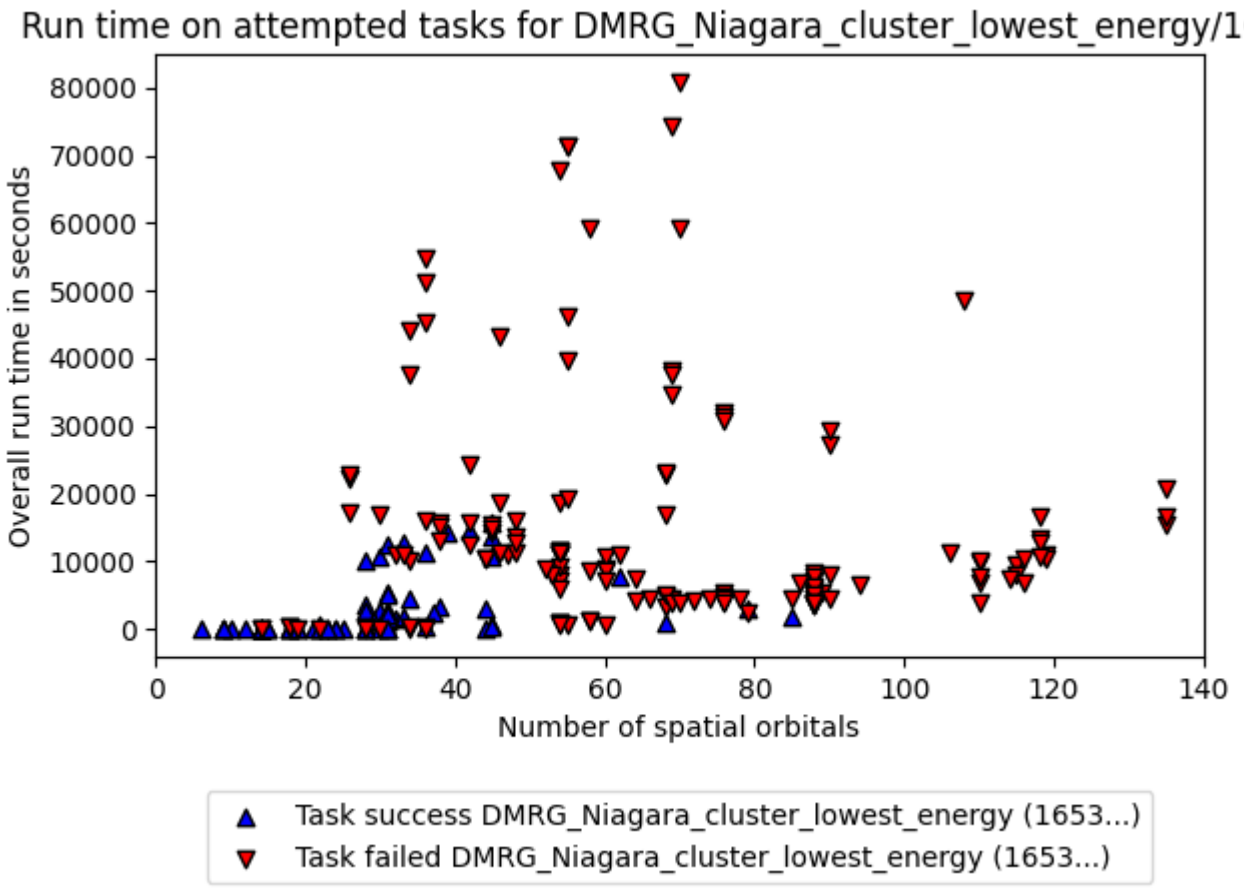
max_run_time_of_attempted_tasks: 80820.729907066

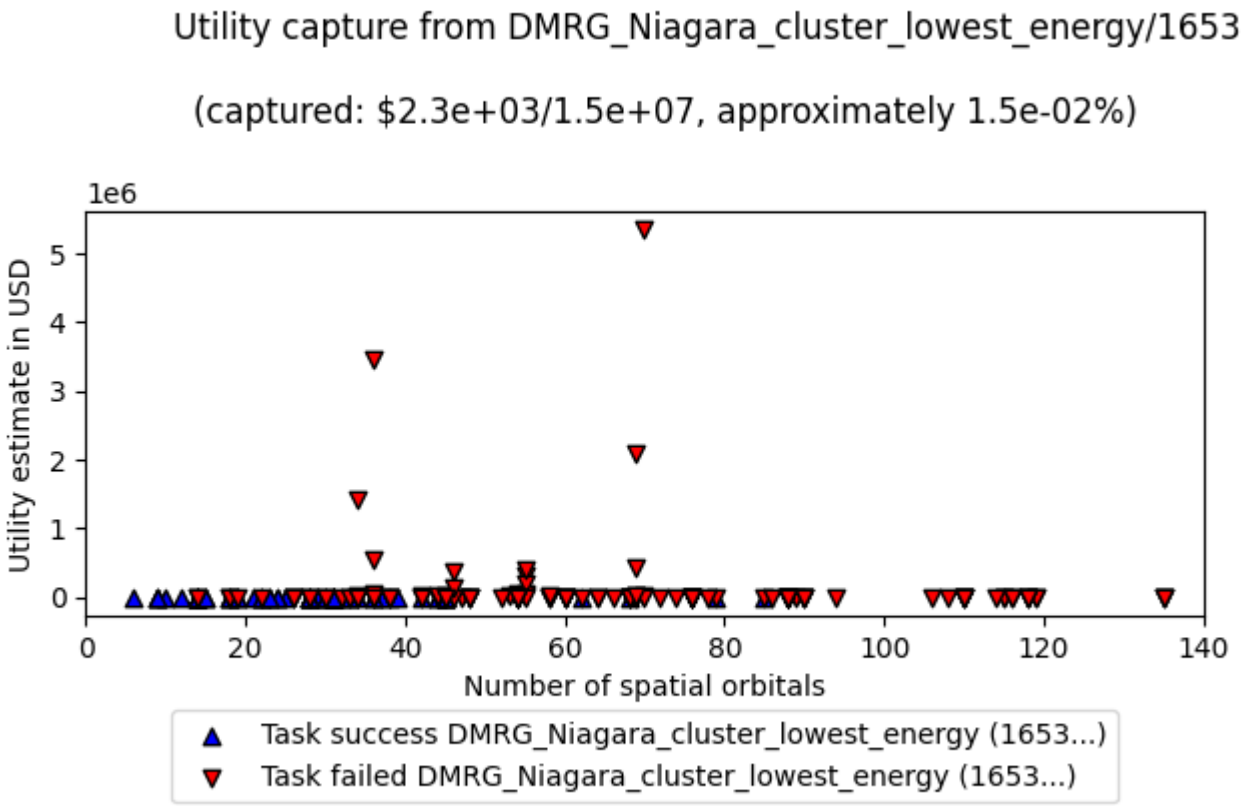
sum_of_run_time_of_attempted_tasks: 2456481.4481055504

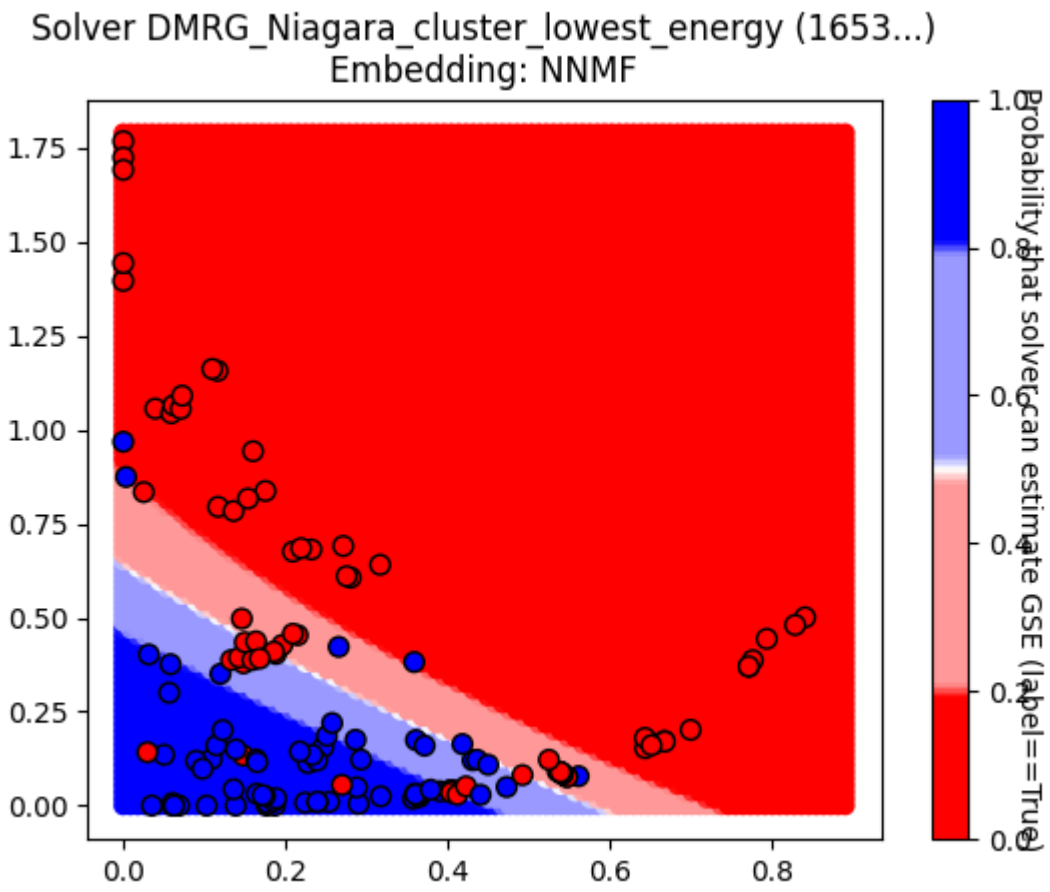
solvability_ratio: 0.1179

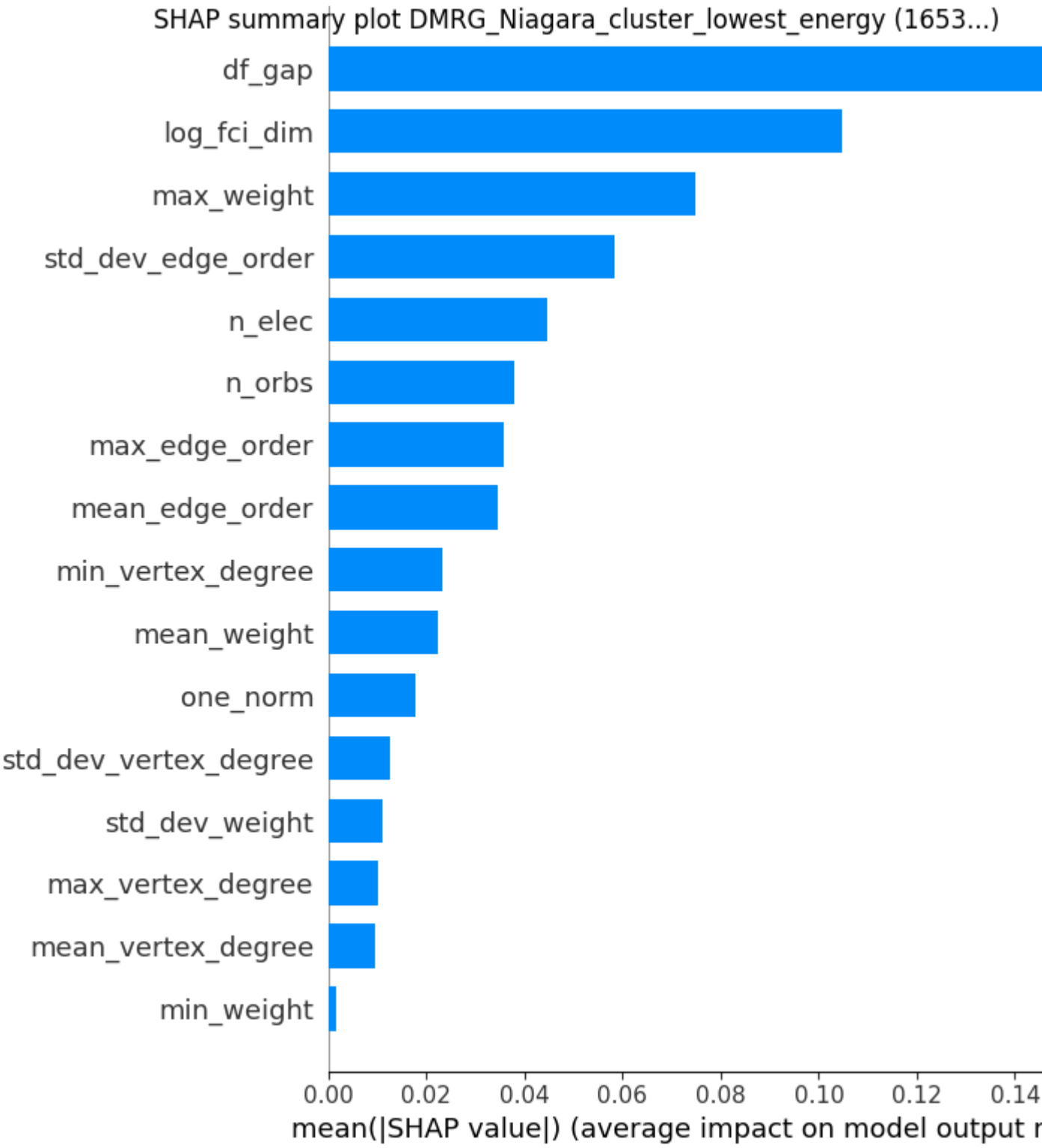
f1_score: [0.8955223880597015, 0.9014084507042254]

ml_metrics_calculator_version: 1


Run time on attempted tasks for DMRG_Niagara_cluster_lowest_energy/16
Overall run time in seconds
80000
70000
60000
50000
40000
30000
20000
10000
0
0
20
40
60
80
100
120
140
Number of spatial orbitals
Task success DMRG_Niagara_cluster_lowest_energy (1653...)
Task failed DMRG_Niagara_cluster_lowest_energy (1653...)


Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..
(captured: $2.3e+03/1.5e+07, approximately 1.5e-02%)
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...)


Solver DMRG_Niagara_cluster_lowest_energy (1653...)
Embedding: NNMF
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0.0
Probability that solver can estimate GSE (label==True)


SHAP summary plot DMRG_Niagara_cluster_lowest_energy (1653...)
df_gap
log_fci_dim
max_weight
std_dev_edge_order
n_elec
n_orbs
max_edge_order
mean_edge_order
min_vertex_degree
mean_weight
one_norm
std_dev_vertex_degree
std_dev_weight
max_vertex_degree
mean_vertex_degree
min_weight
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
mean(|SHAP value|) (average impact on model output