GSEE Benchmark Standard Report

Report based on data from 2025-01-16T19:10:17.205242+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: Thu Jan 16 11:55:29 2025

Latest creation time for a `performance_metrics.json` file: Thu Jan 16 14:12:17 2025

Latest creation time for a `solution.json` file: Thu Jan 16 14:04:59 2025

Problem Instance Summary Statistics

number of `problem_instances`: 82

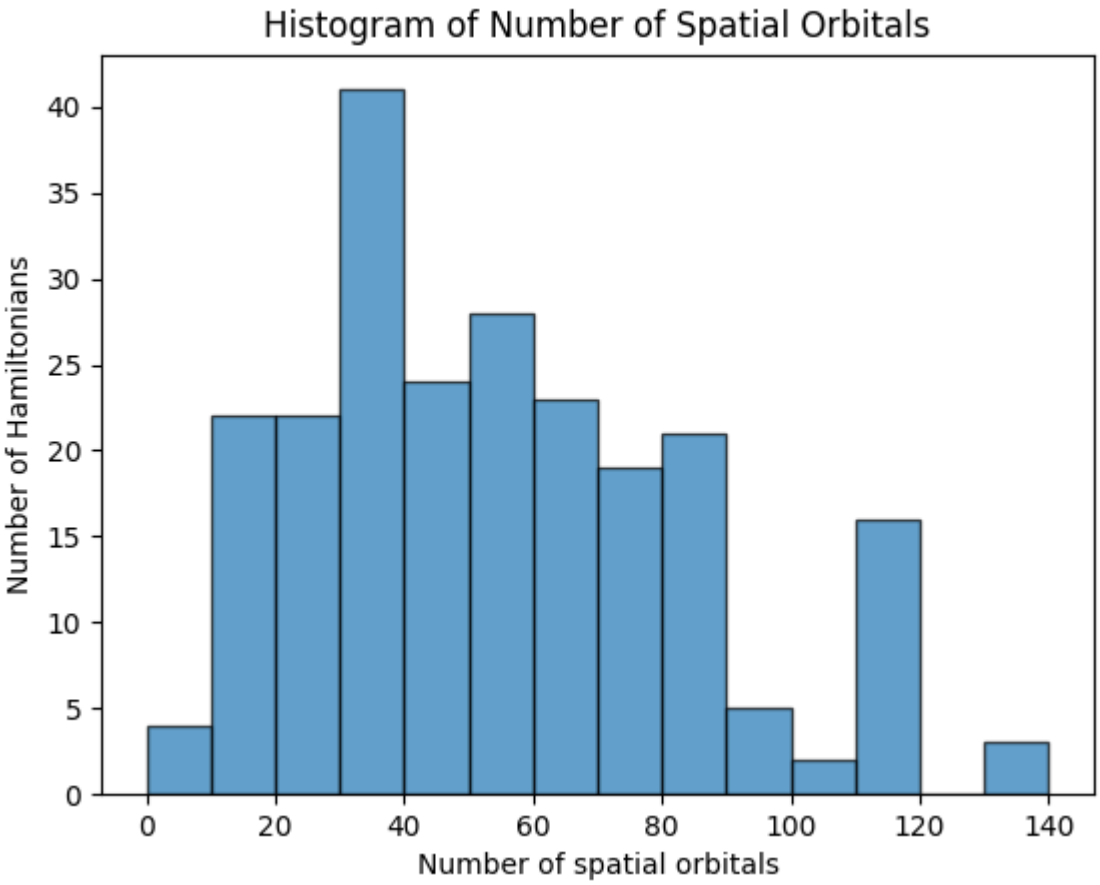
`problem_instance.json` with the most tasks: 16 (mo_n2_pincer/8a3787cc-d3d0-42a8-d9a9-7de2aed45208)

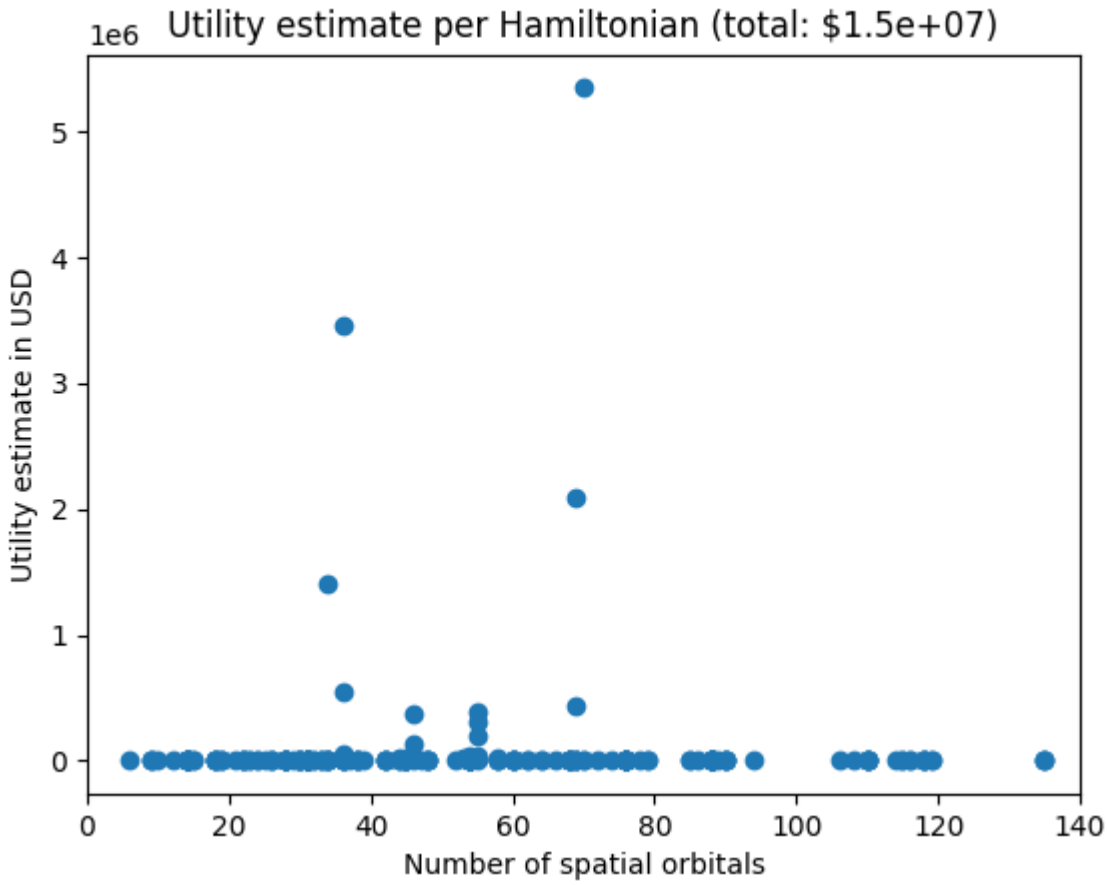
number of Hamiltonians (i.e., tasks): 230

minimum number of orbitals: 6

median number of orbitals: 53.5

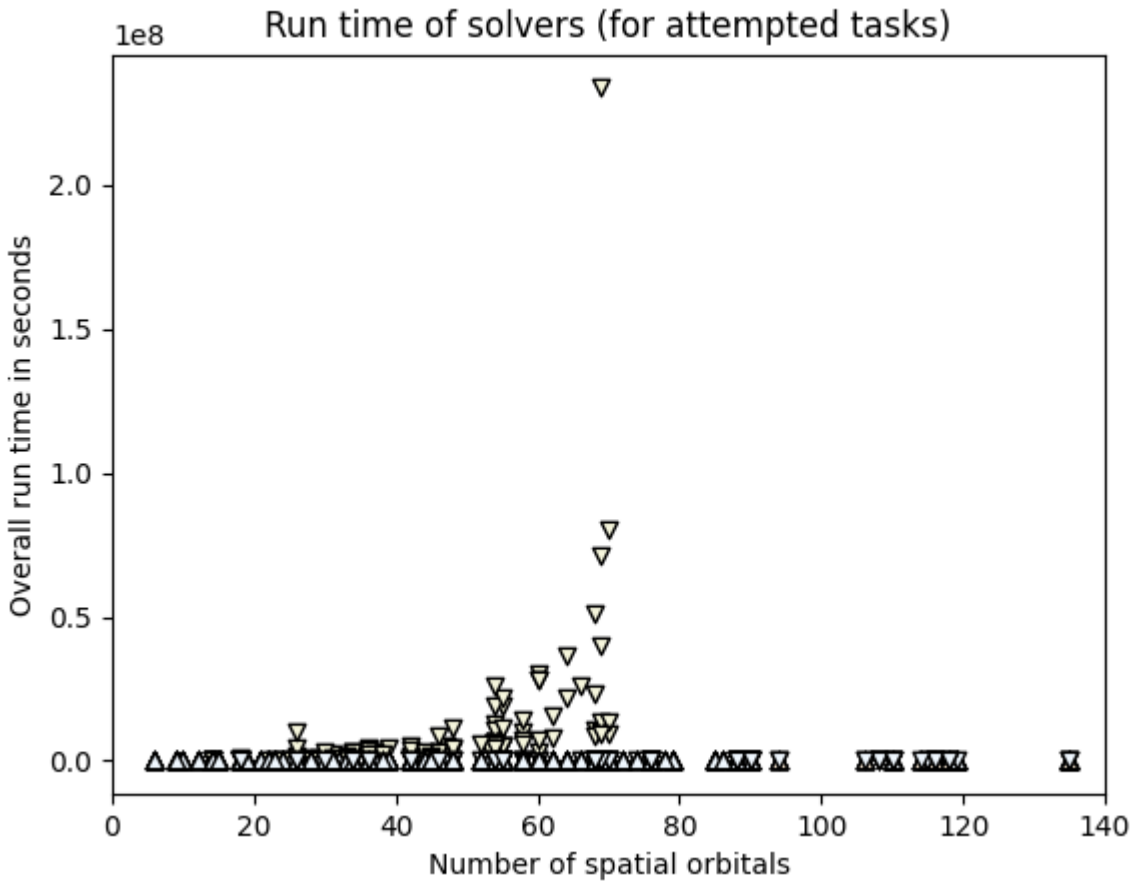
maximum number of orbitals: 135

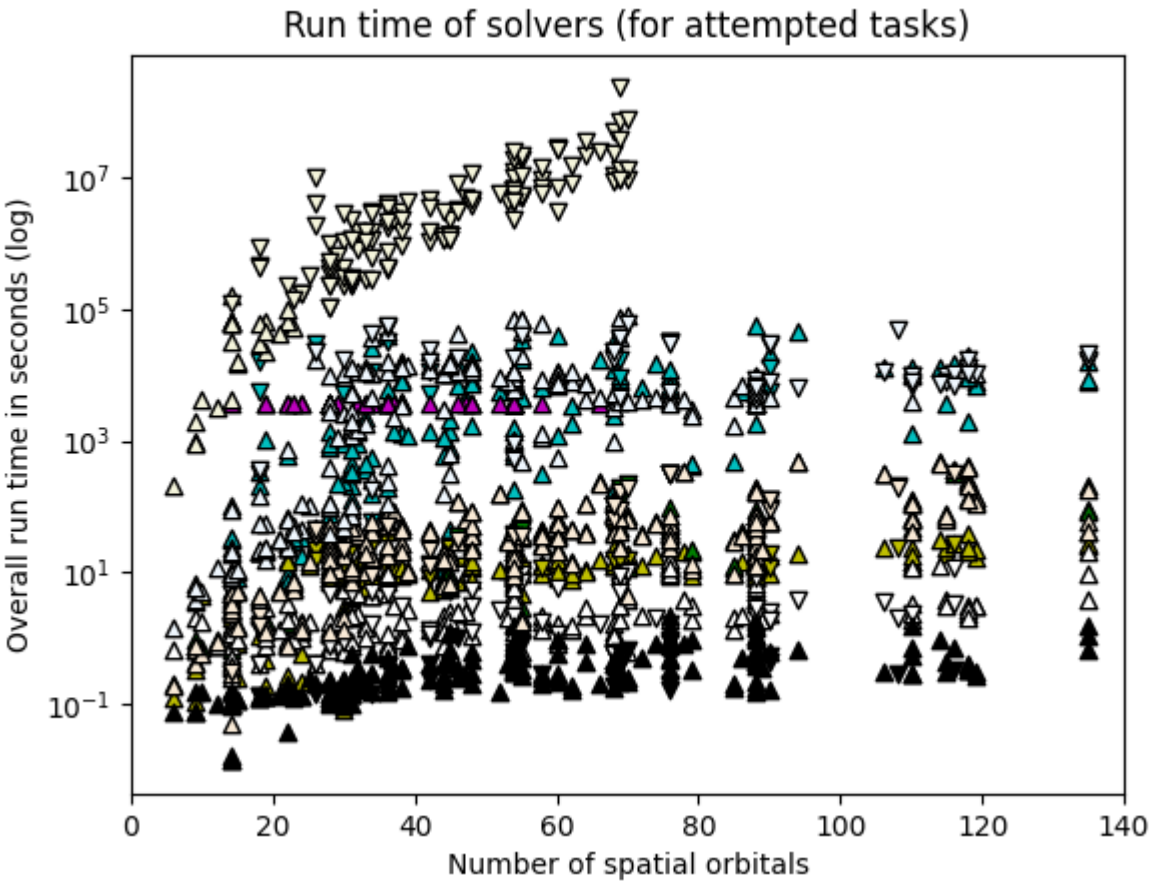

Histogram of Number of Spatial Orbitals
Number of Hamiltonians
Number of spatial orbitals
0
5
10
15
20
25
30
35
40
0
20
40
60
80
100
120
140



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: 5ab06b82-39c0-41e1-9612-02744f194e25

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 41

number_of_problem_instances_solved: 41

number_of_tasks: 230

number_of_tasks_attempted: 162

number_of_tasks_solved: 149

number_of_tasks_solved_within_run_time_limit: 162

number_of_tasks_solved_within_accuracy_threshold: 149

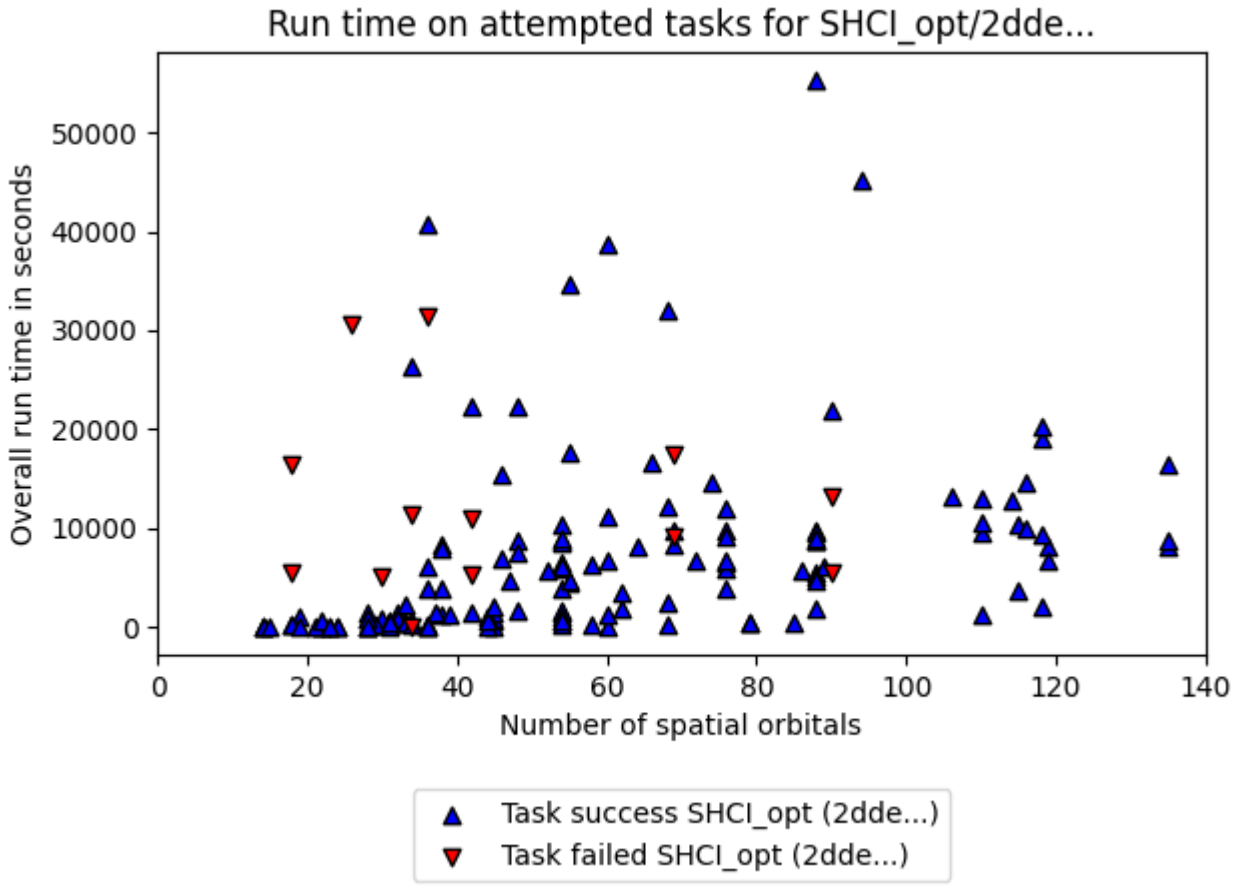
max_run_time_of_attempted_tasks: 55299.387

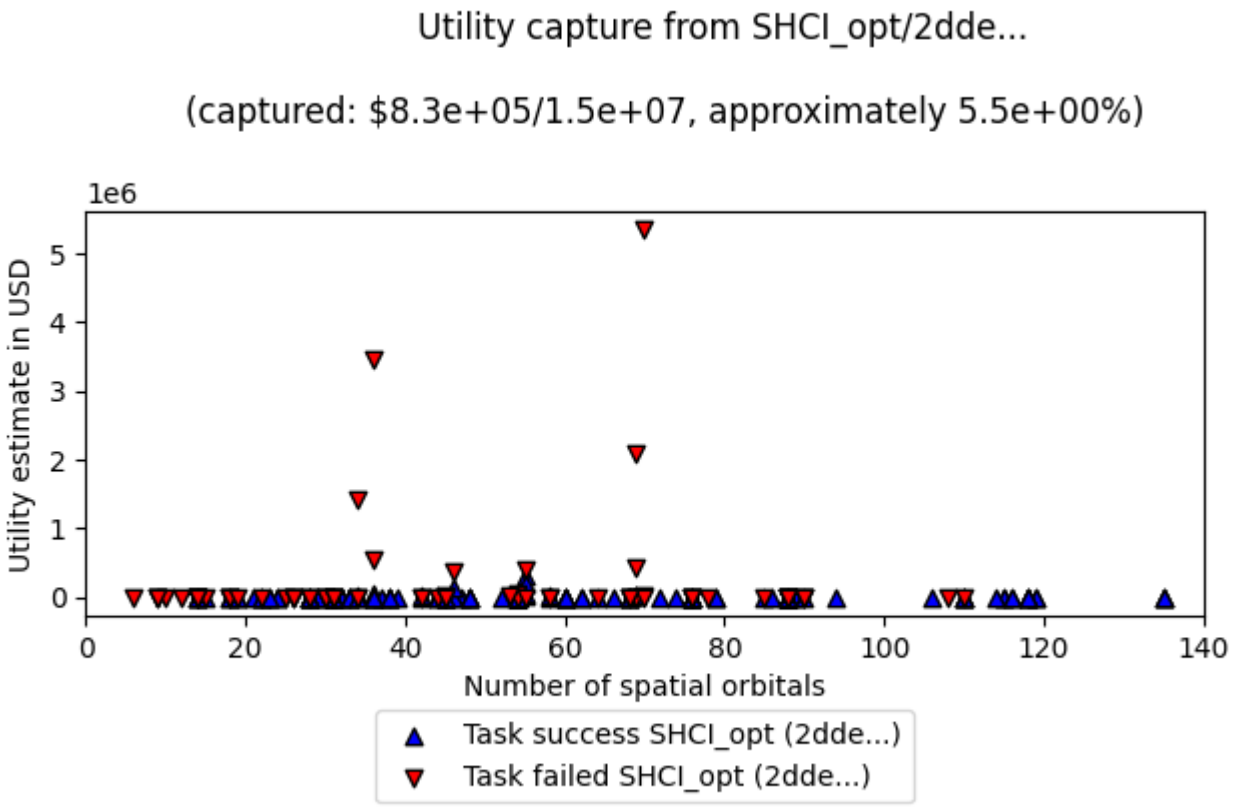
sum_of_run_time_of_attempted_tasks: 1138067.4269999997

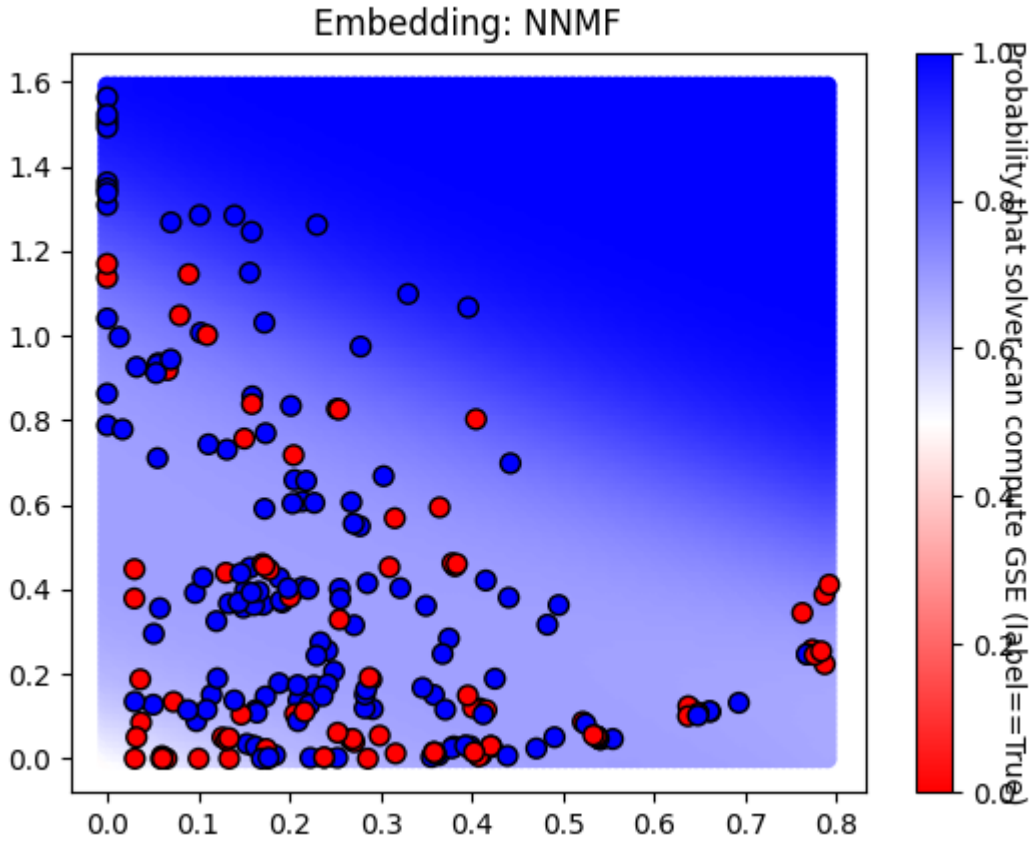
solvability_ratio: 0.9998

f1_score: [0.5691056910569106, 0.8427299703264095]

ml_metrics_calculator_version: 1




Utility capture from SHCI_opt/2dde...
(captured: $8.3e+05/1.5e+07, approximately 5.5e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success SHCI_opt (2dde...)
Task failed SHCI_opt (2dde...)



SHAP summary plot

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: 4437d609-d148-434f-98ce-661069b852df

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 4

number_of_problem_instances_solved: 4

number_of_tasks: 230

number_of_tasks_attempted: 53

number_of_tasks_solved: 53

number_of_tasks_solved_within_run_time_limit: 53

number_of_tasks_solved_within_accuracy_threshold: 53

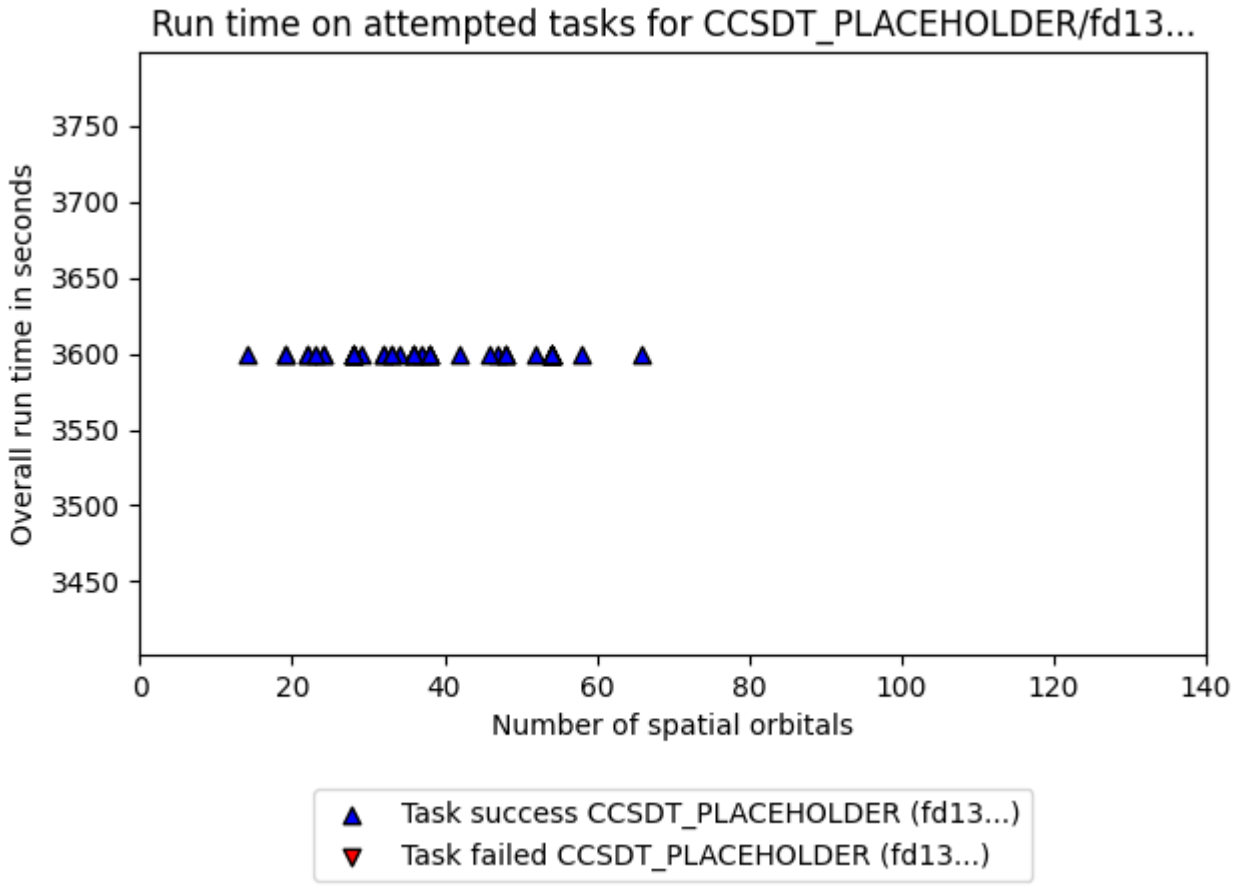
max_run_time_of_attempted_tasks: 3600.0

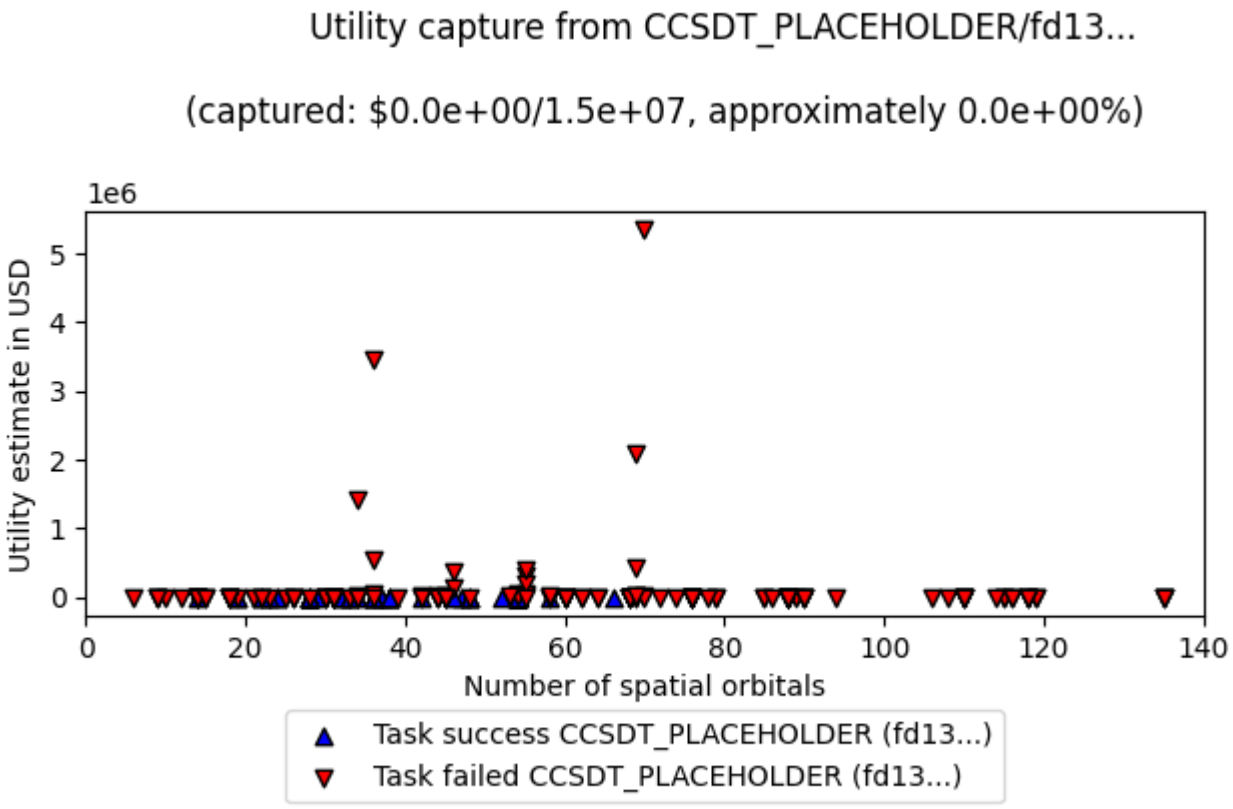
sum_of_run_time_of_attempted_tasks: 190800.0

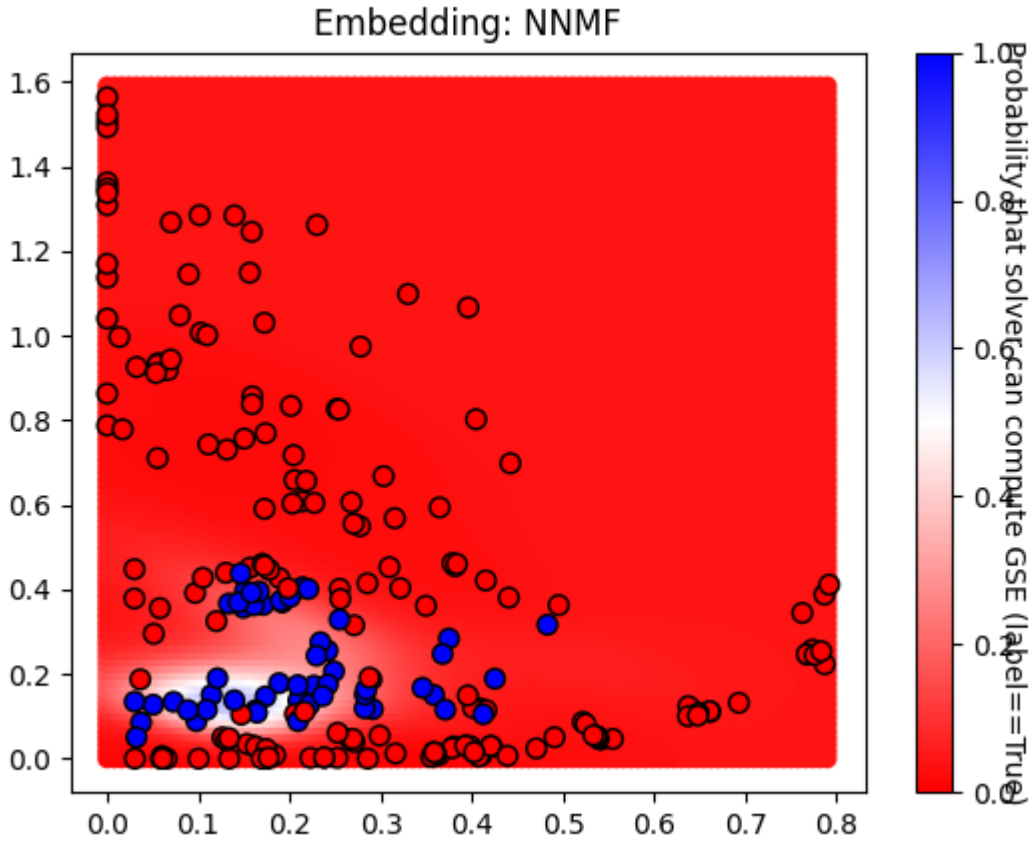
solvability_ratio: 0.0068

f1_score: [1.0, 1.0]

ml_metrics_calculator_version: 1




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...)



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: dcda23b6-0eb0-4da9-a605-b44aa85a6c69

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 82

number_of_problem_instances_solved: 69

number_of_tasks: 230

number_of_tasks_attempted: 230

number_of_tasks_solved: 193

number_of_tasks_solved_within_run_time_limit: 230

number_of_tasks_solved_within_accuracy_threshold: 193

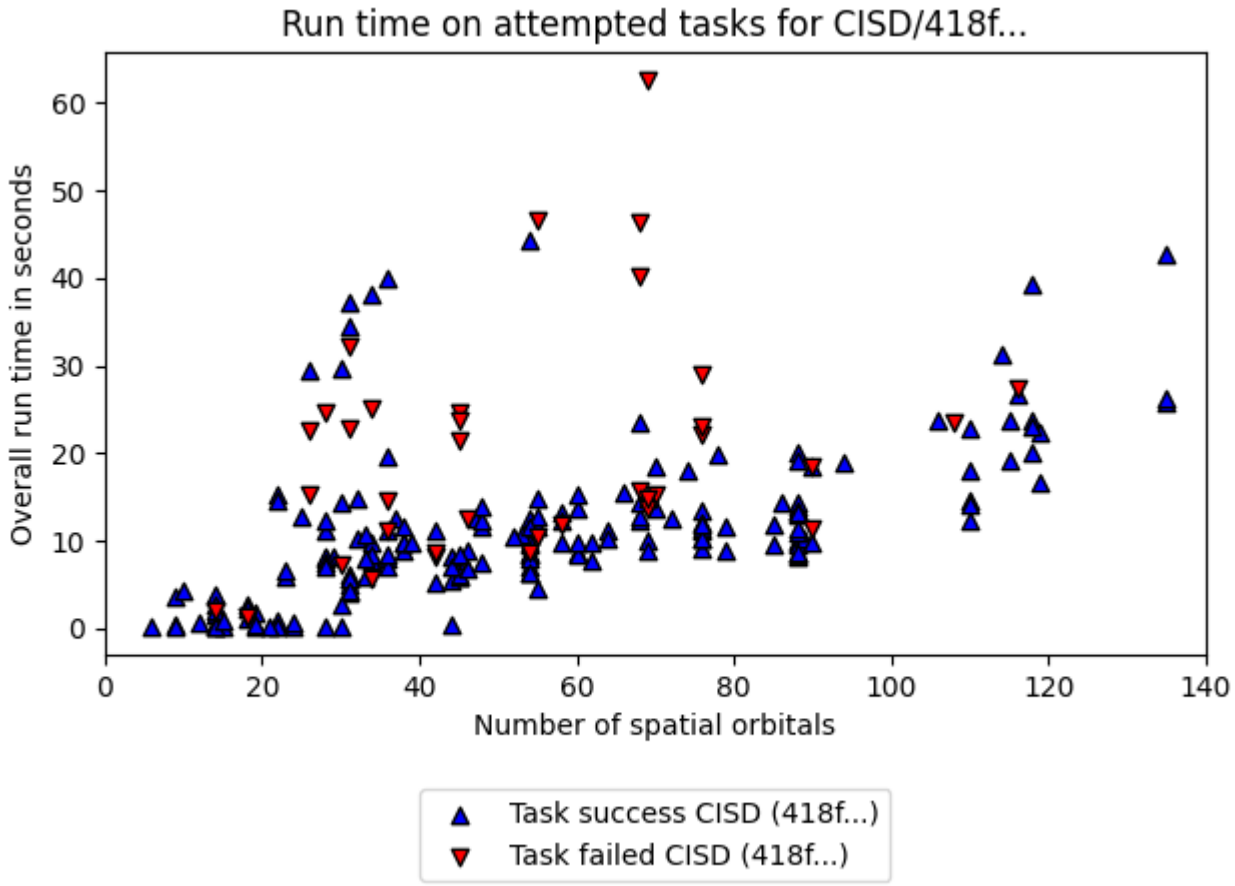
max_run_time_of_attempted_tasks: 62.58296537399292

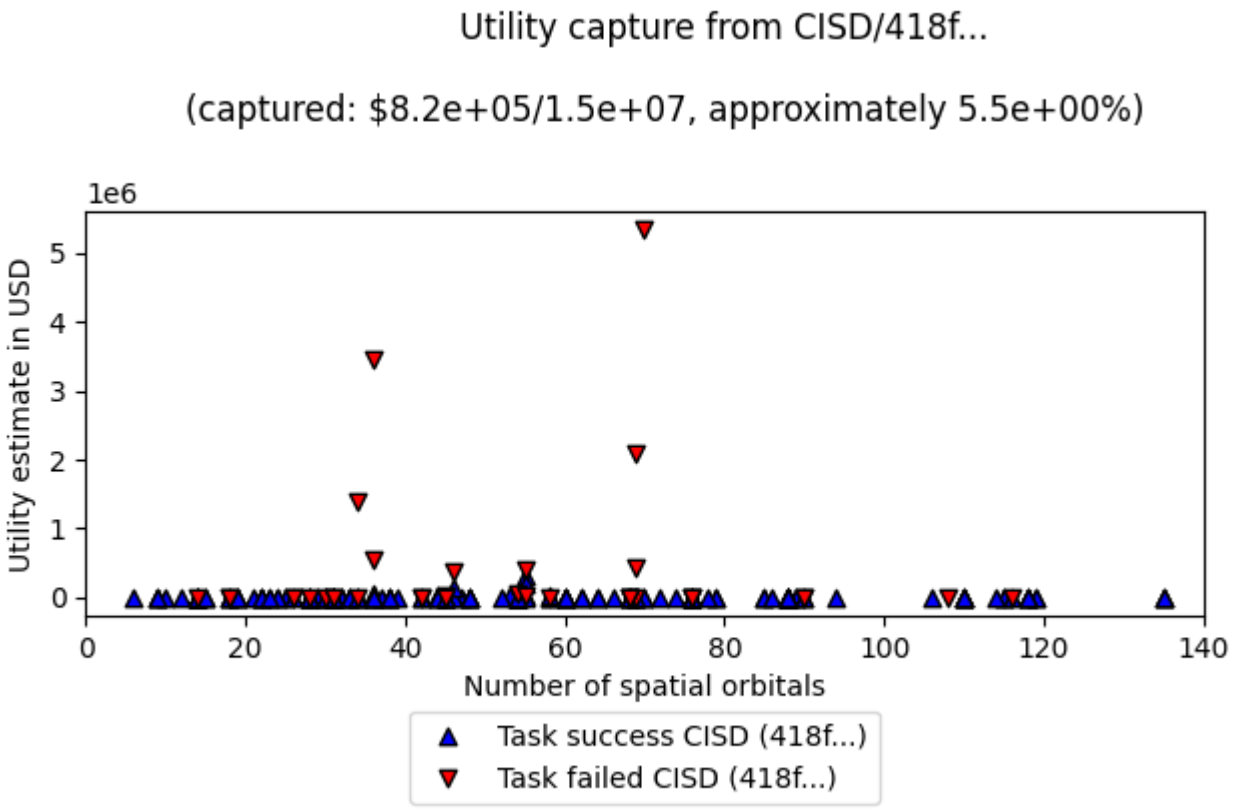
sum_of_run_time_of_attempted_tasks: 2895.8530027866364

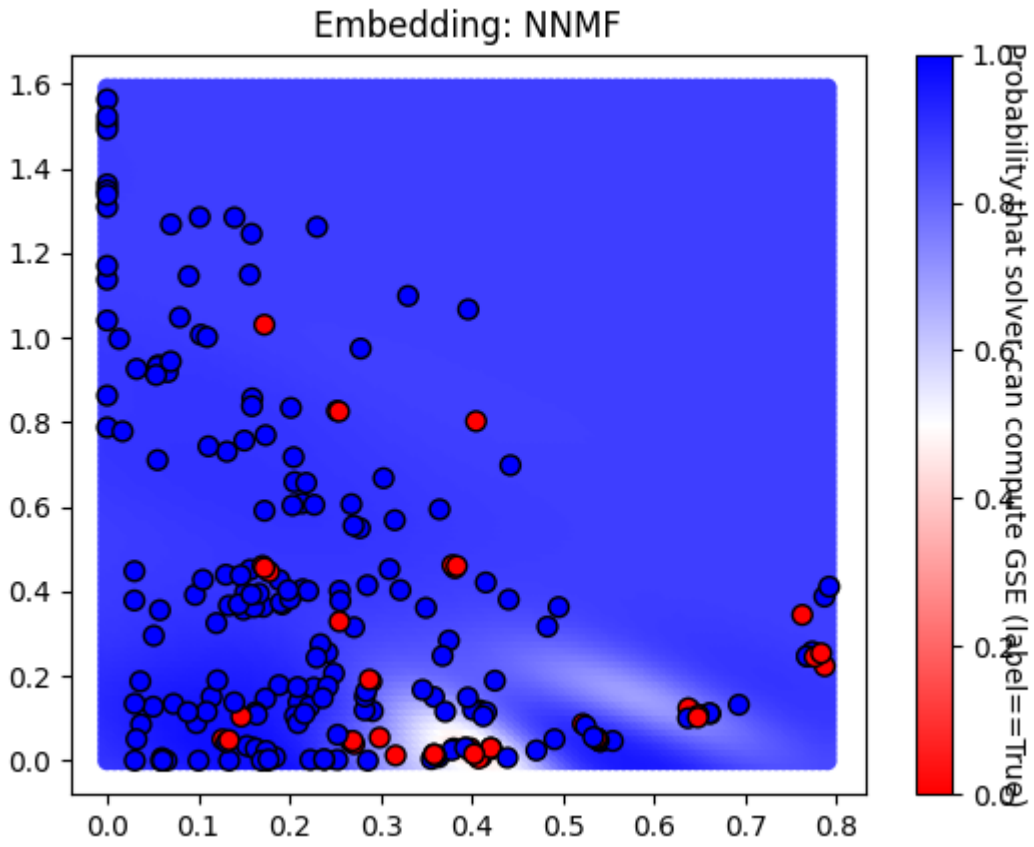
solvability_ratio: 0.9958

f1_score: [0.8131868131868132, 0.9539295392953929]

ml_metrics_calculator_version: 1




Utility capture from CISD/418f...
(captured: $8.2e+05/1.5e+07, approximately 5.5e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CISD (418f...)
Task failed CISD (418f...)



SHAP summary plot

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: 87854781-4b5b-46c5-b915-9b83ea8bc162

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 78

number_of_problem_instances_solved: 71

number_of_tasks: 230

number_of_tasks_attempted: 221

number_of_tasks_solved: 195

number_of_tasks_solved_within_run_time_limit: 221

number_of_tasks_solved_within_accuracy_threshold: 195

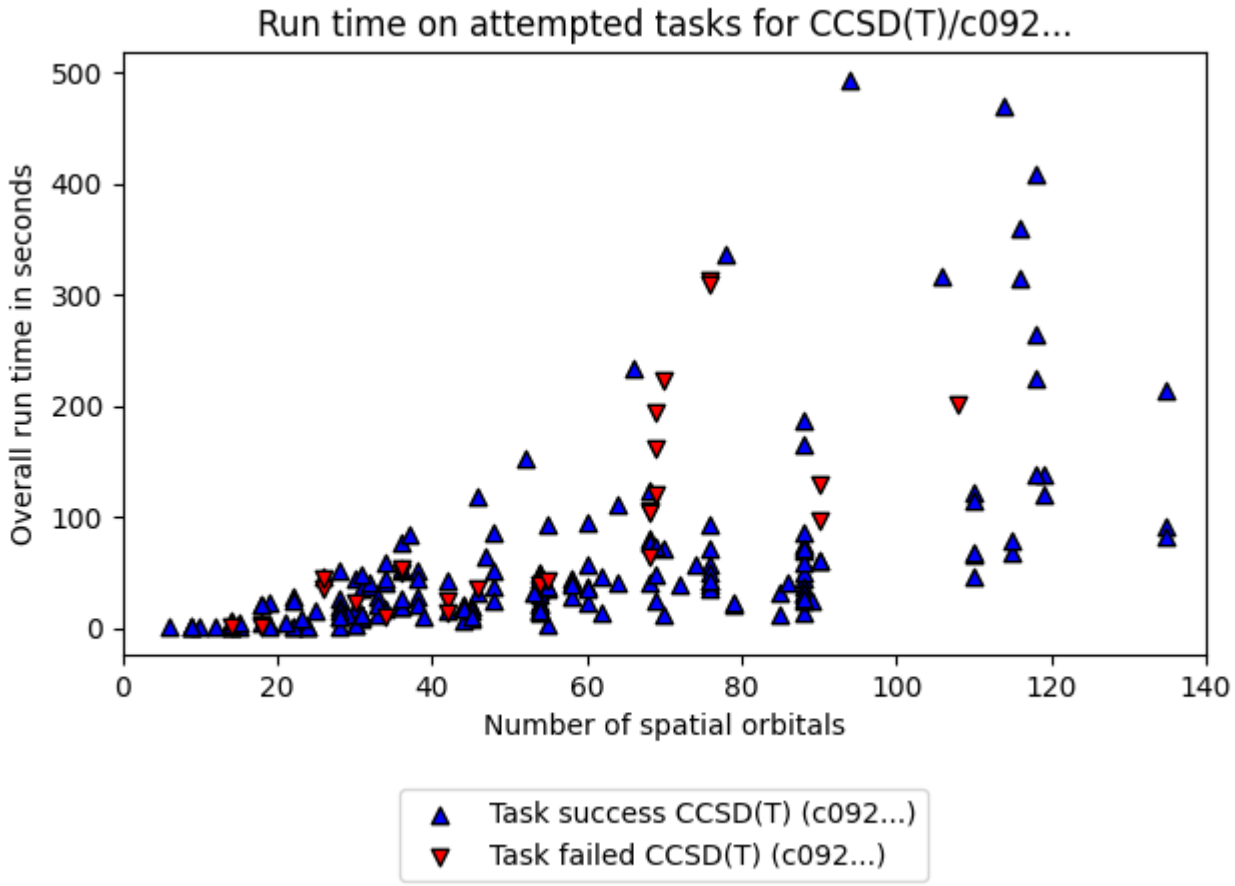
max_run_time_of_attempted_tasks: 493.4080808162689

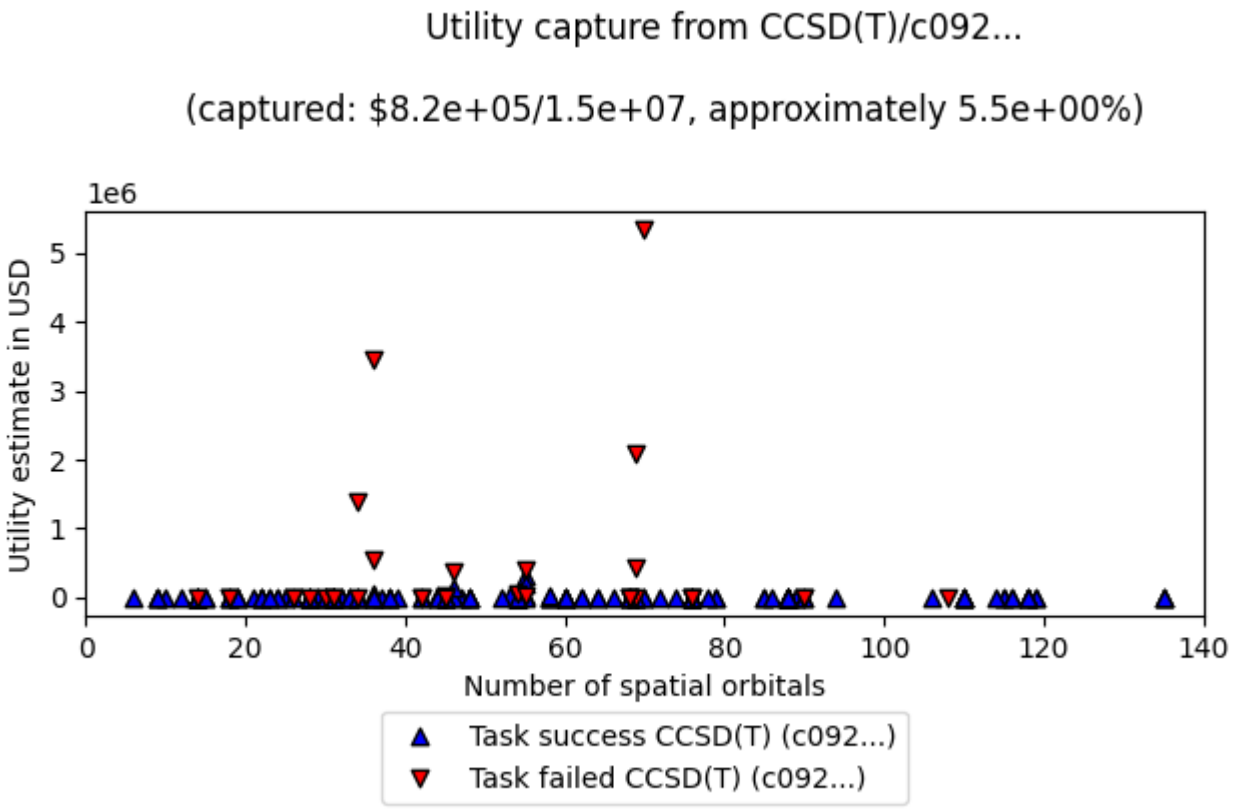
sum_of_run_time_of_attempted_tasks: 12968.4871737957

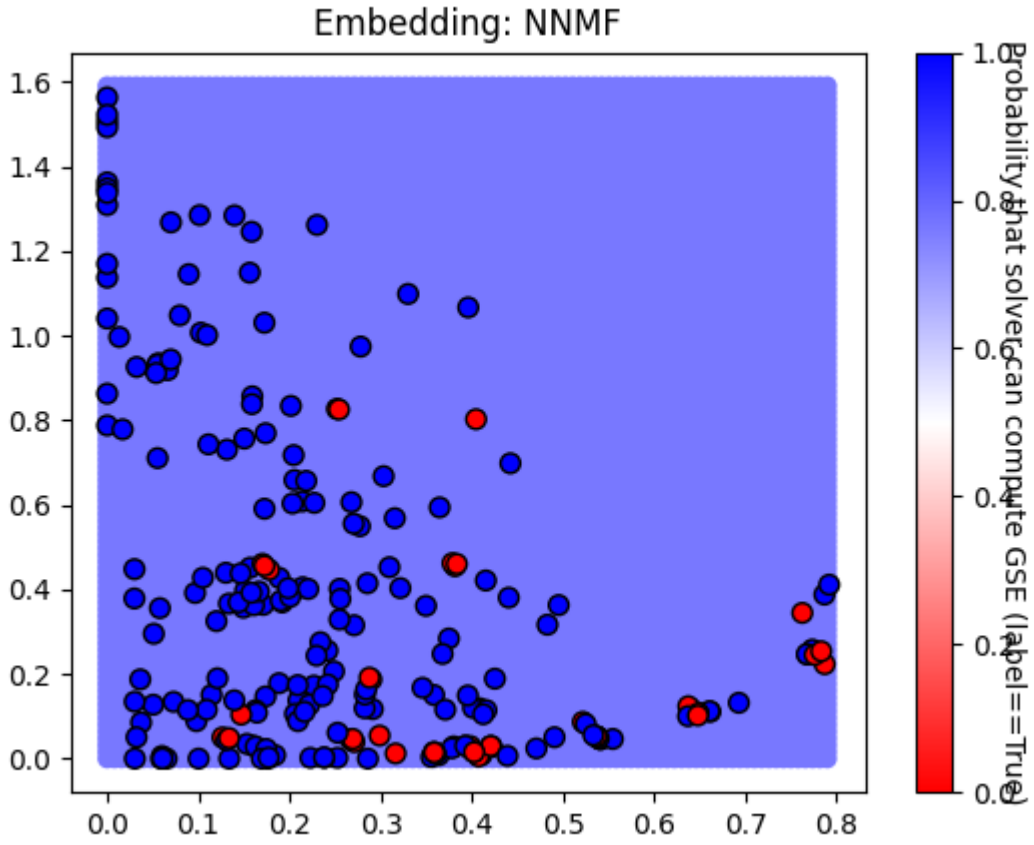
solvability_ratio: 1.0

f1_score: [0.0, 0.9176470588235294]

ml_metrics_calculator_version: 1




Utility capture from CCSD(T)/c092...
(captured: $8.2e+05/1.5e+07, approximately 5.5e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSD(T) (c092...)
Task failed CCSD(T) (c092...)



SHAP summary plot

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: f1a801ad-90cd-4c33-98d7-0db4033d37ee

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 82

number_of_problem_instances_solved: 56

number_of_tasks: 230

number_of_tasks_attempted: 230

number_of_tasks_solved: 174

number_of_tasks_solved_within_run_time_limit: 230

number_of_tasks_solved_within_accuracy_threshold: 174

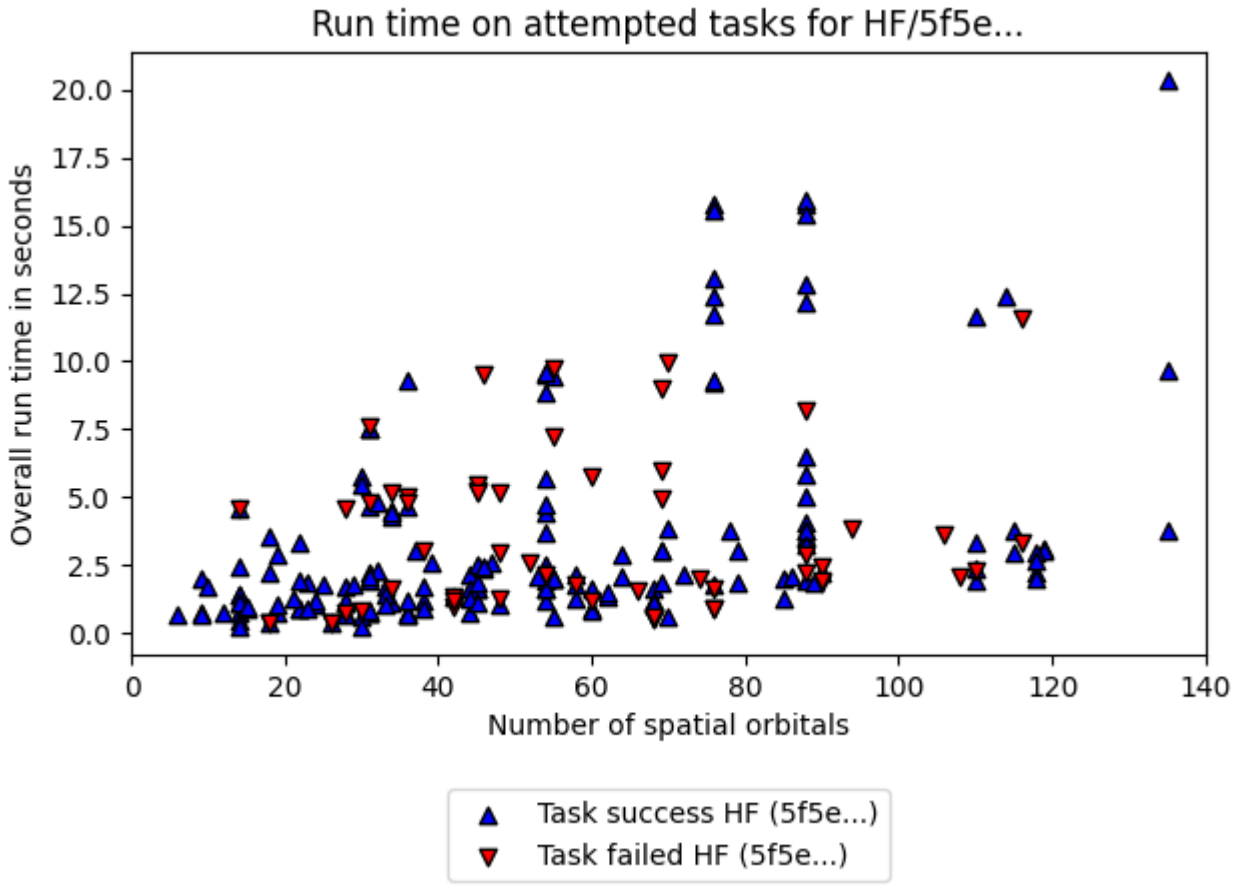
max_run_time_of_attempted_tasks: 20.338801622390747

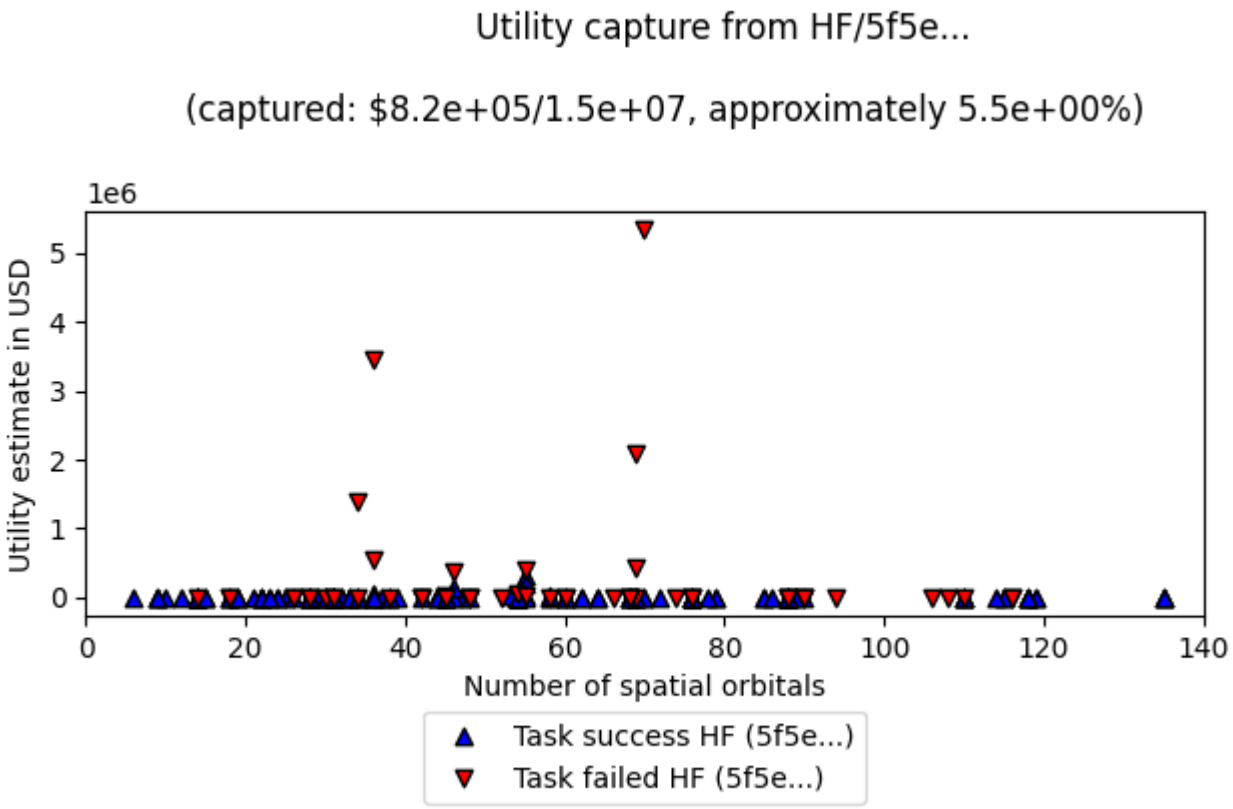
sum_of_run_time_of_attempted_tasks: 792.8028435707092

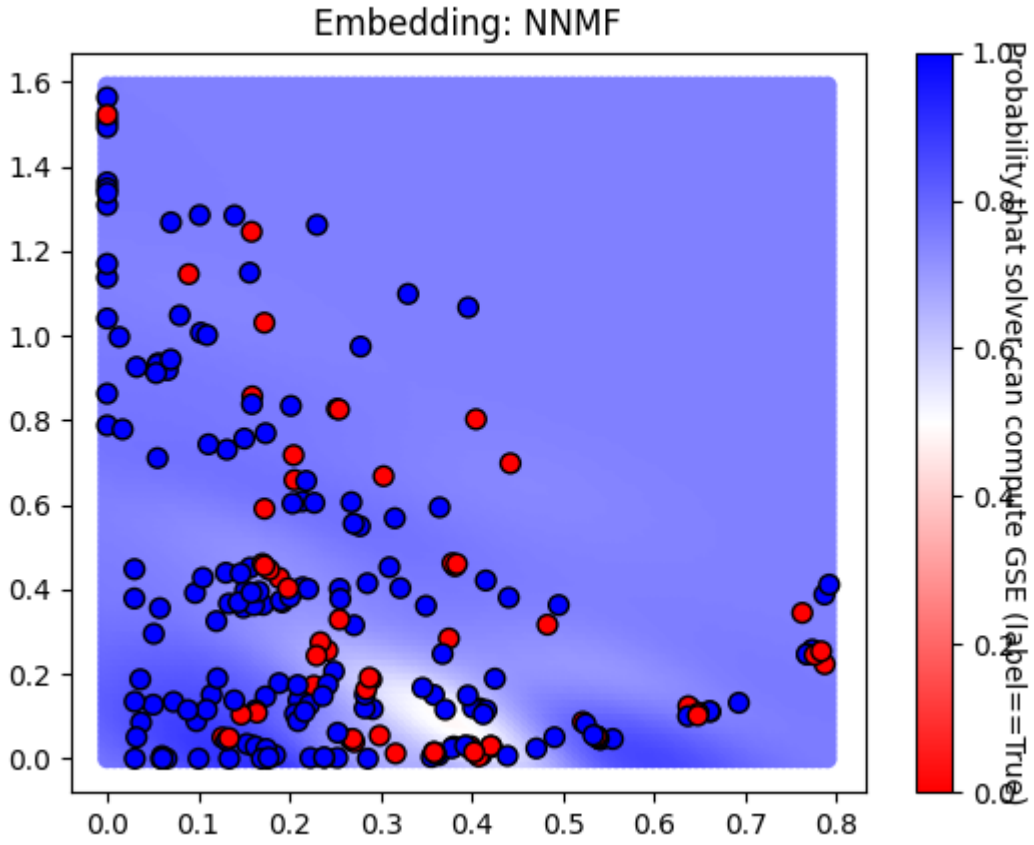
solvability_ratio: 0.9977

f1_score: [0.8888888888888888, 0.9580838323353293]

ml_metrics_calculator_version: 1




Utility capture from HF/5f5e...
(captured: $8.2e+05/1.5e+07, approximately 5.5e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success HF (5f5e...)
Task failed HF (5f5e...)



SHAP summary plot

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: 9289dadd-3c1e-46eb-8fdc-ececc06f5927

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 79

number_of_problem_instances_solved: 69

number_of_tasks: 230

number_of_tasks_attempted: 222

number_of_tasks_solved: 193

number_of_tasks_solved_within_run_time_limit: 222

number_of_tasks_solved_within_accuracy_threshold: 193

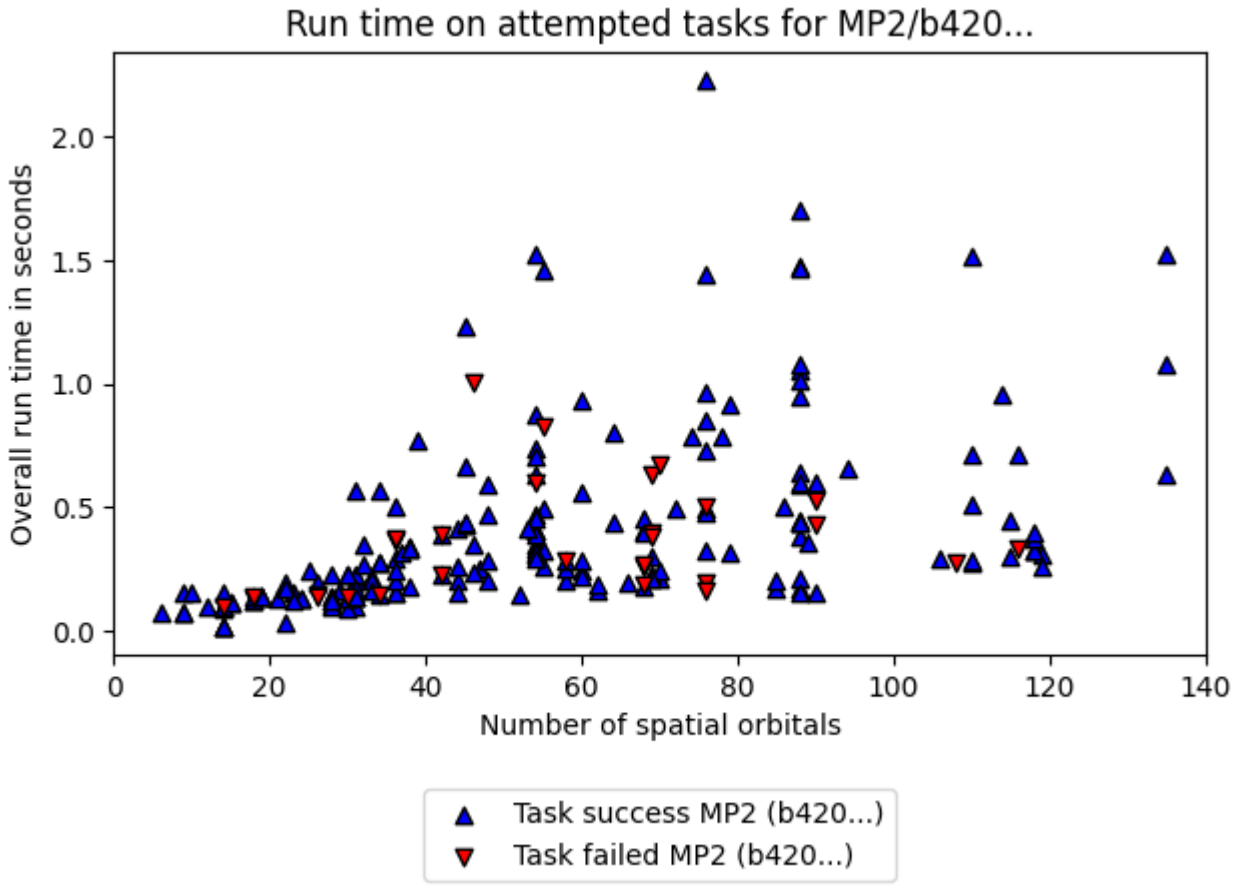
max_run_time_of_attempted_tasks: 2.230440139770508

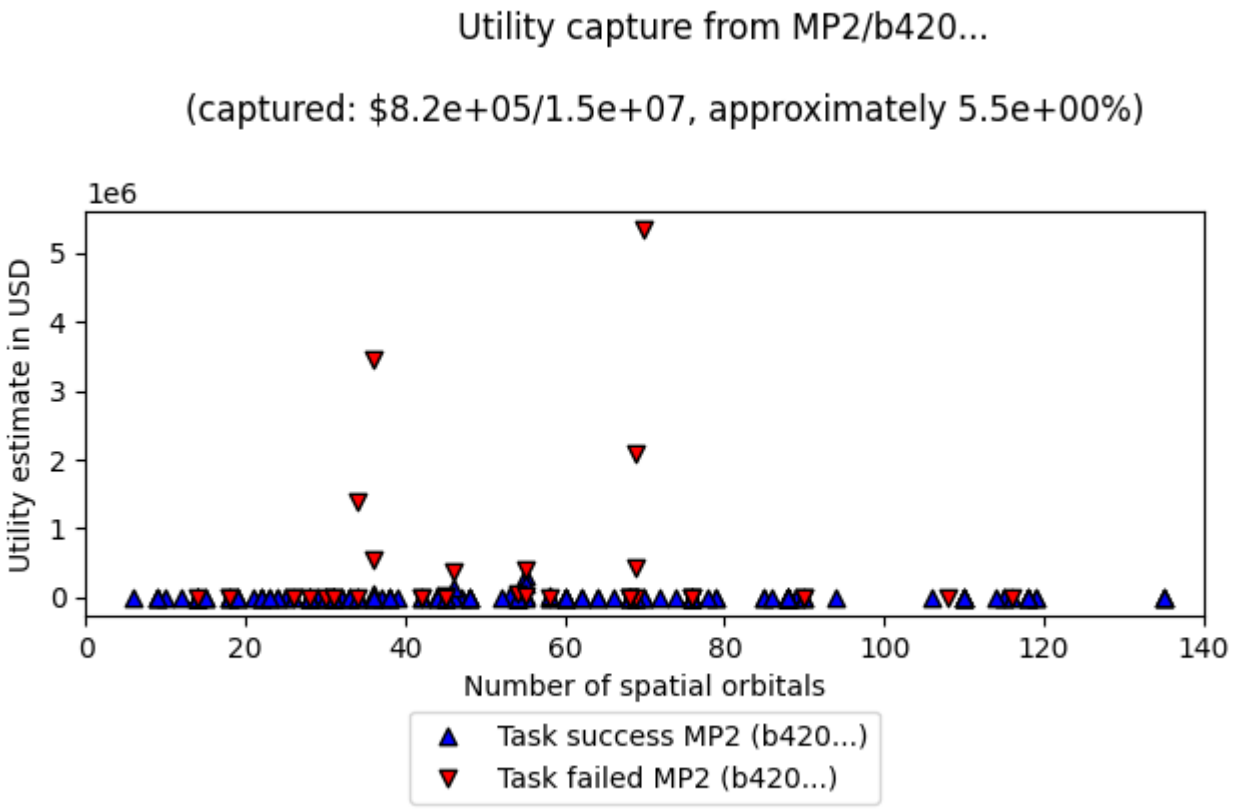
sum_of_run_time_of_attempted_tasks: 87.6544258594513

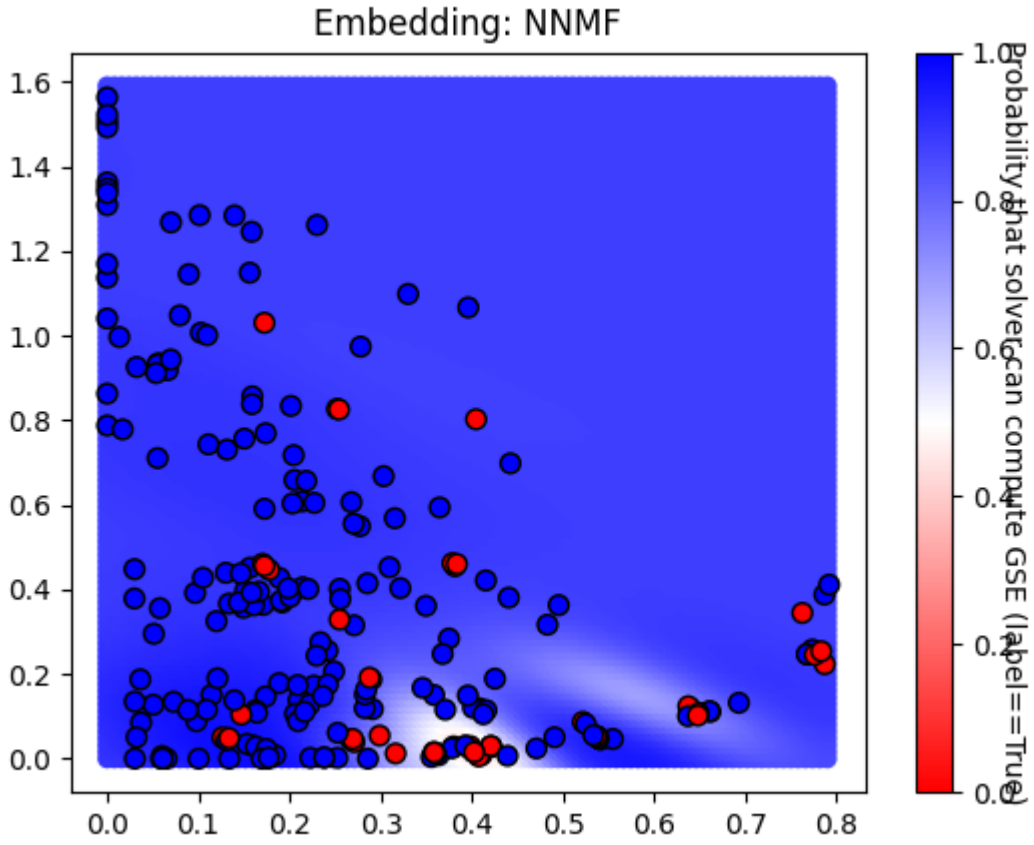
solvability_ratio: 0.9958

f1_score: [0.8131868131868132, 0.9539295392953929]

ml_metrics_calculator_version: 1




Utility capture from MP2/b420...
(captured: $8.2e+05/1.5e+07, approximately 5.5e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success MP2 (b420...)
Task failed MP2 (b420...)



SHAP summary plot

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: c4cbf554-6a23-4603-a65b-1e8902b4bedc

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 78

number_of_problem_instances_solved: 70

number_of_tasks: 230

number_of_tasks_attempted: 221

number_of_tasks_solved: 194

number_of_tasks_solved_within_run_time_limit: 221

number_of_tasks_solved_within_accuracy_threshold: 194

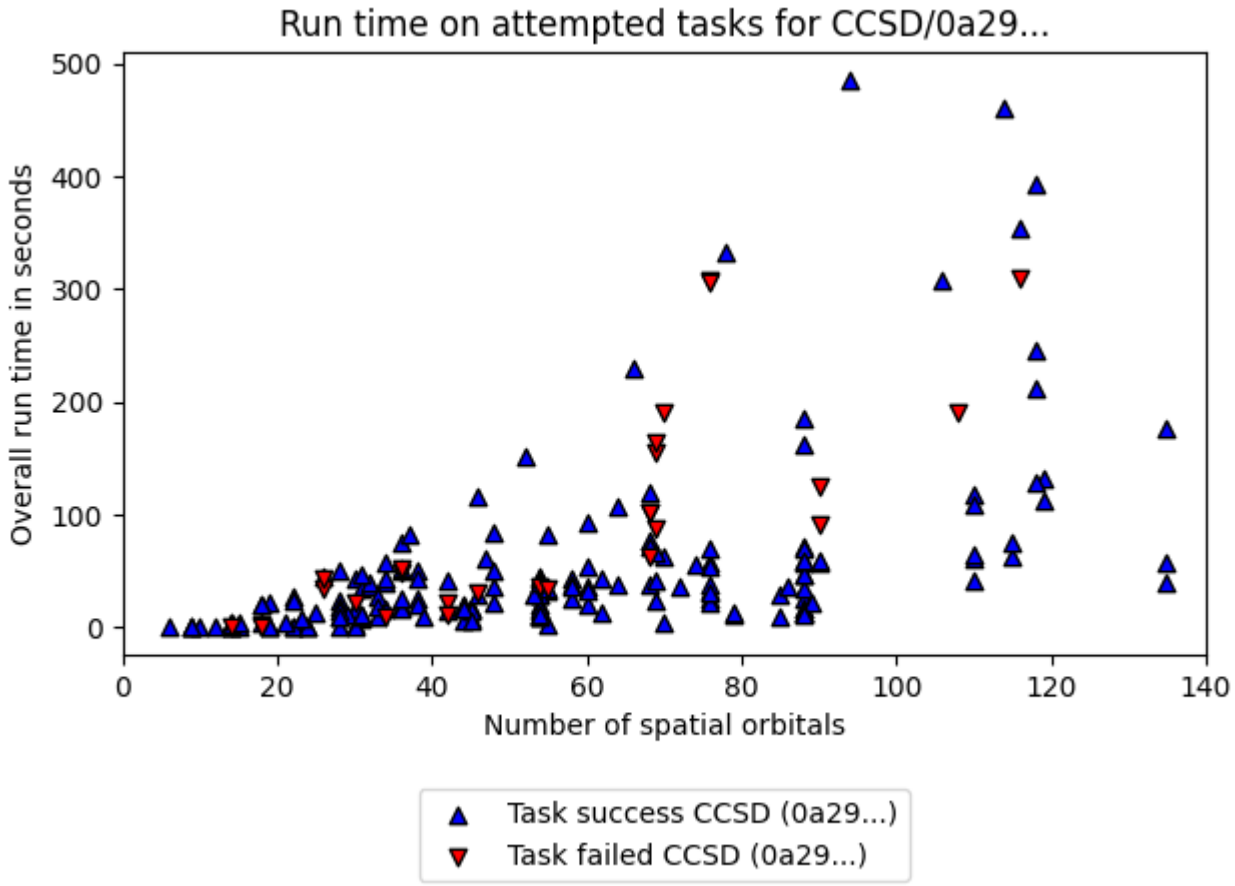
max_run_time_of_attempted_tasks: 485.1982181072235

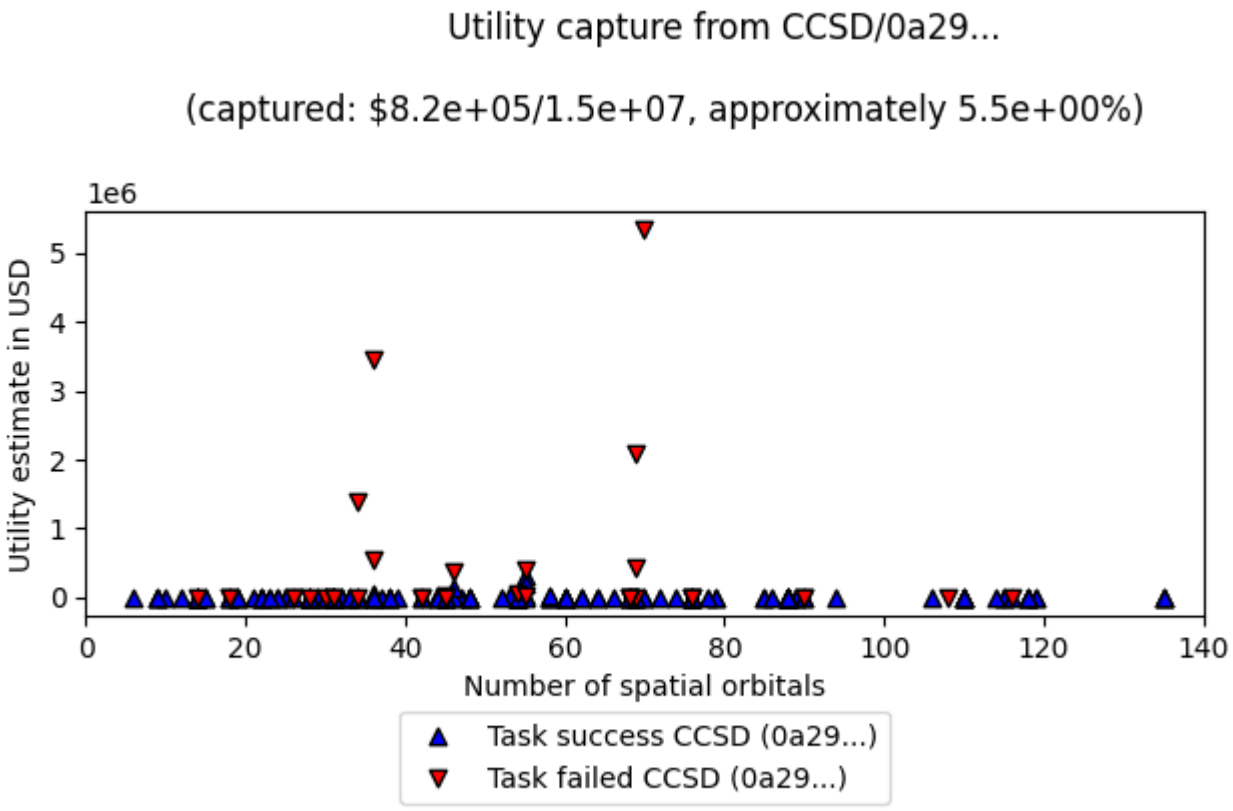
sum_of_run_time_of_attempted_tasks: 12029.76450586319

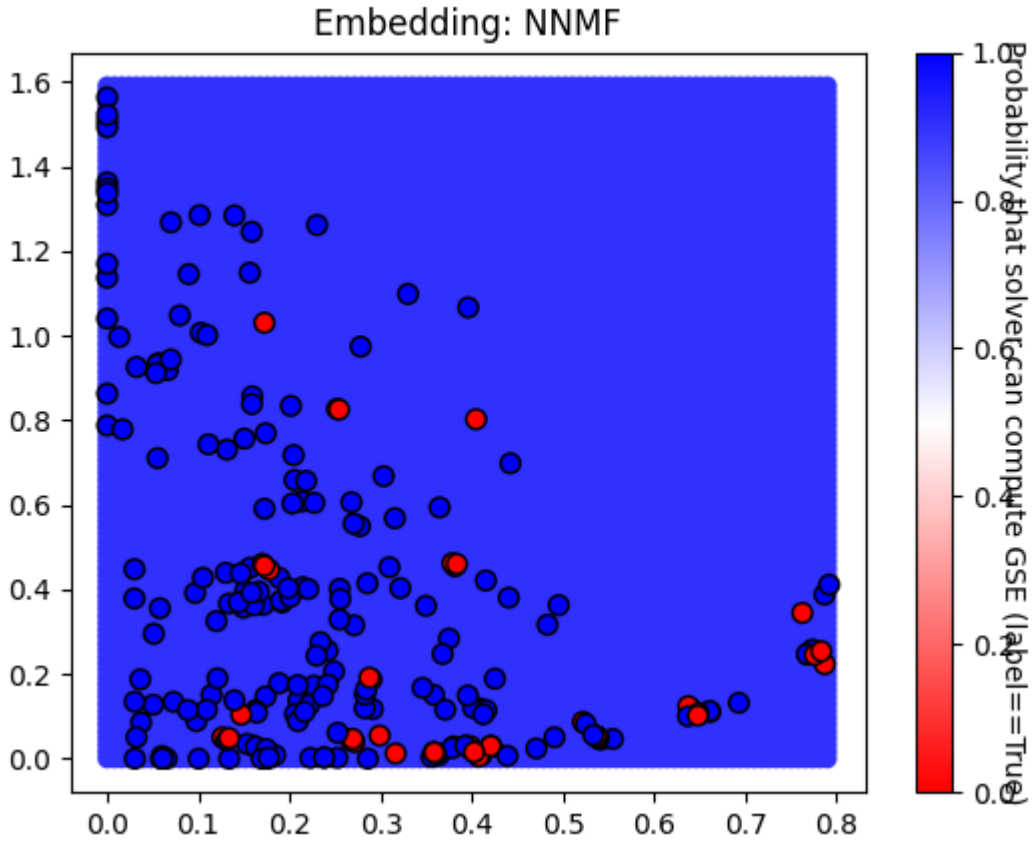
solvability_ratio: 1.0

f1_score: [0.2706766917293233, 0.0]

ml_metrics_calculator_version: 1




Utility capture from CCSD/0a29...
(captured: $8.2e+05/1.5e+07, approximately 5.5e+00%)
1e6
Utility estimate in USD
Number of spatial orbitals
Task success CCSD (0a29...)
Task failed CCSD (0a29...)



SHAP summary plot

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

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

solver_short_name:DF_QPE

compute_hardware_type:quantum_computer

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

software_details:[{'software_name': 'pyLIQTR', 'software_version': '1.2.1'}, {'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: 4230575a-1659-4082-a570-4edd43498b3a

creation_timestamp: 2025-01-16T19:10:17.205242+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

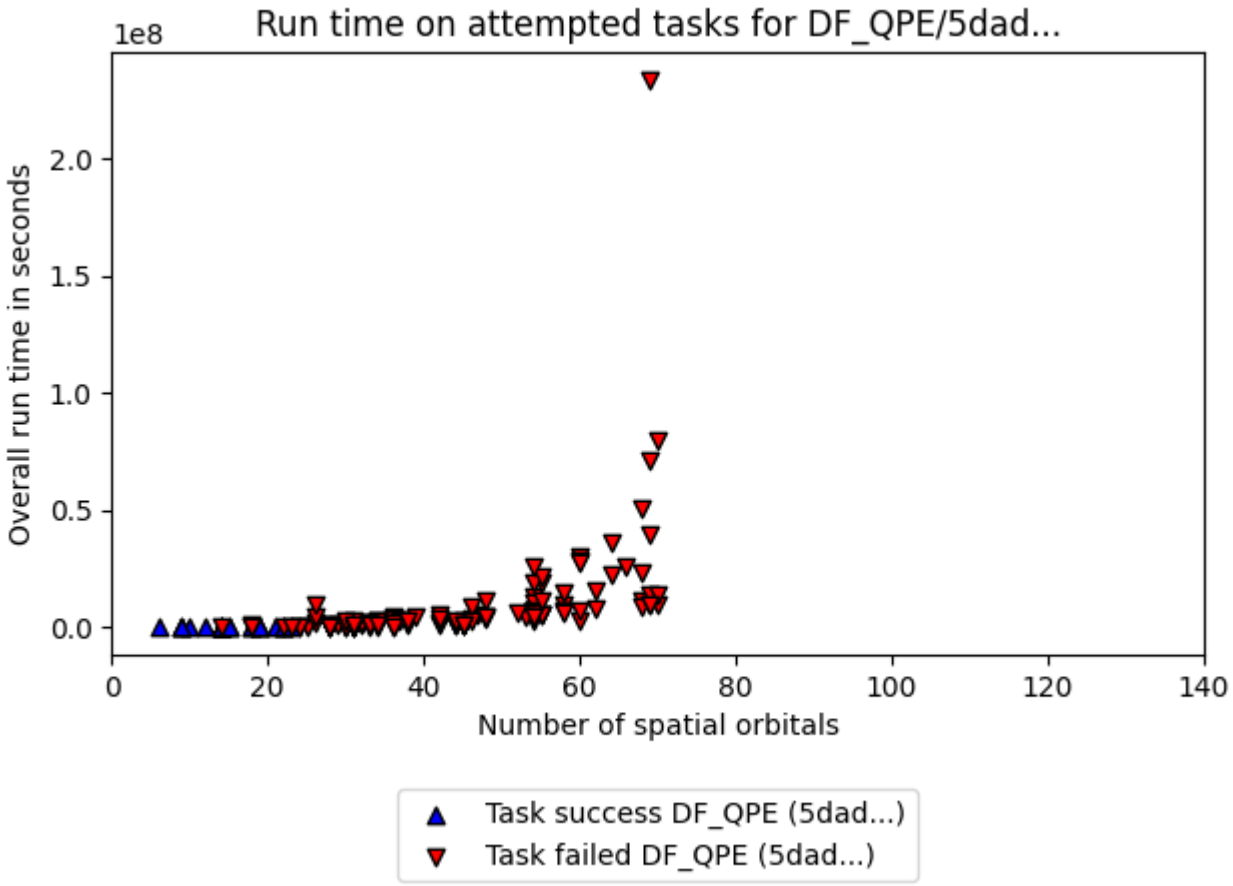
max_run_time_of_attempted_tasks: 233737829.40462503

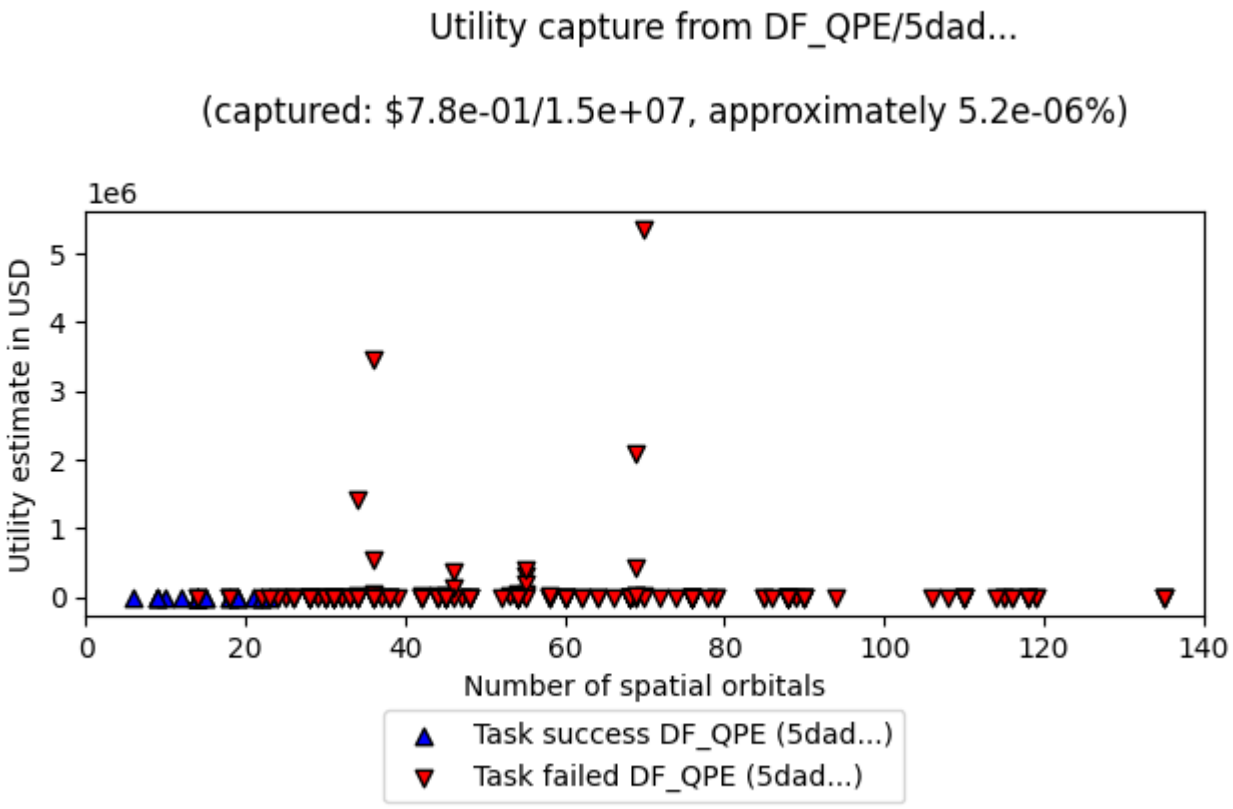
sum_of_run_time_of_attempted_tasks: 1180589418.3385448

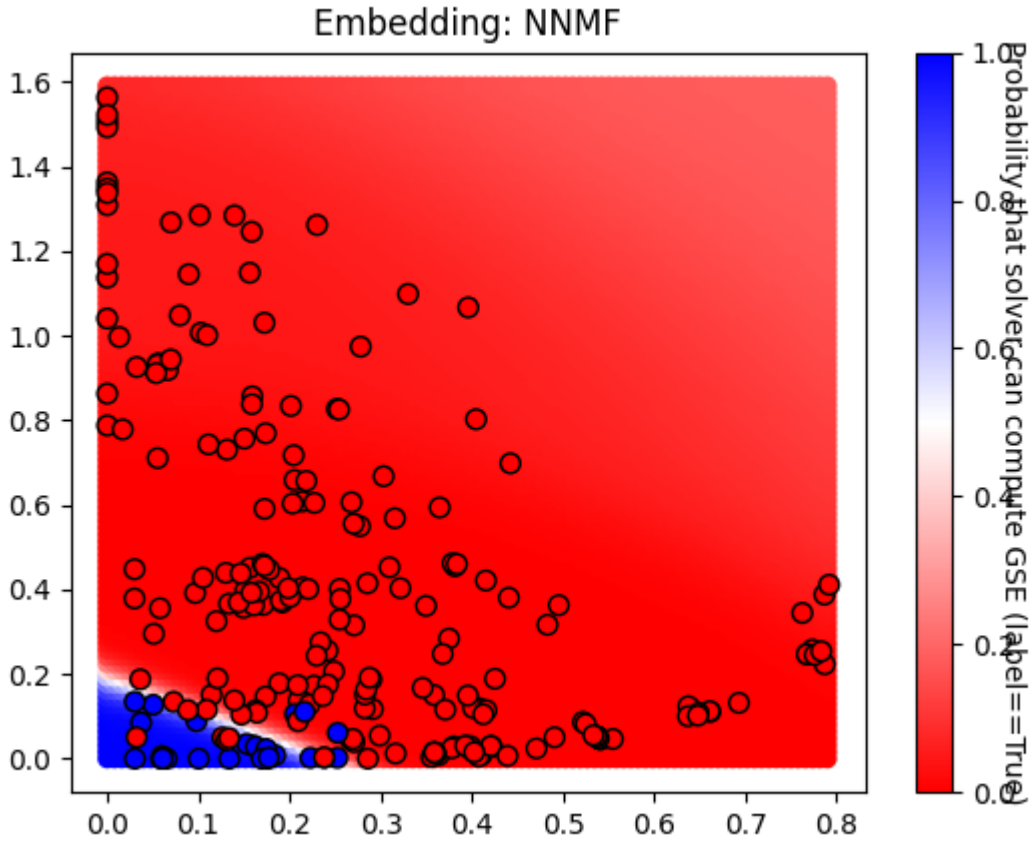
solvability_ratio: 0.0232

f1_score: [0.9950738916256158, 0.9629629629629629]

ml_metrics_calculator_version: 1


Run time on attempted tasks for DF_QPE/5dad...
1e8
Overall run time in seconds
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
Number of spatial orbitals
Task success DF_QPE (5dad...)
Task failed DF_QPE (5dad...)


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...)



SHAP summary plot

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: f70d1823-51a8-40d3-9652-e570ee63bf4d

creation_timestamp: 2025-01-16T19:10:17.205242+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 82

number_of_problem_instances_solved: 45

number_of_tasks: 230

number_of_tasks_attempted: 230

number_of_tasks_solved: 174

number_of_tasks_solved_within_run_time_limit: 230

number_of_tasks_solved_within_accuracy_threshold: 174

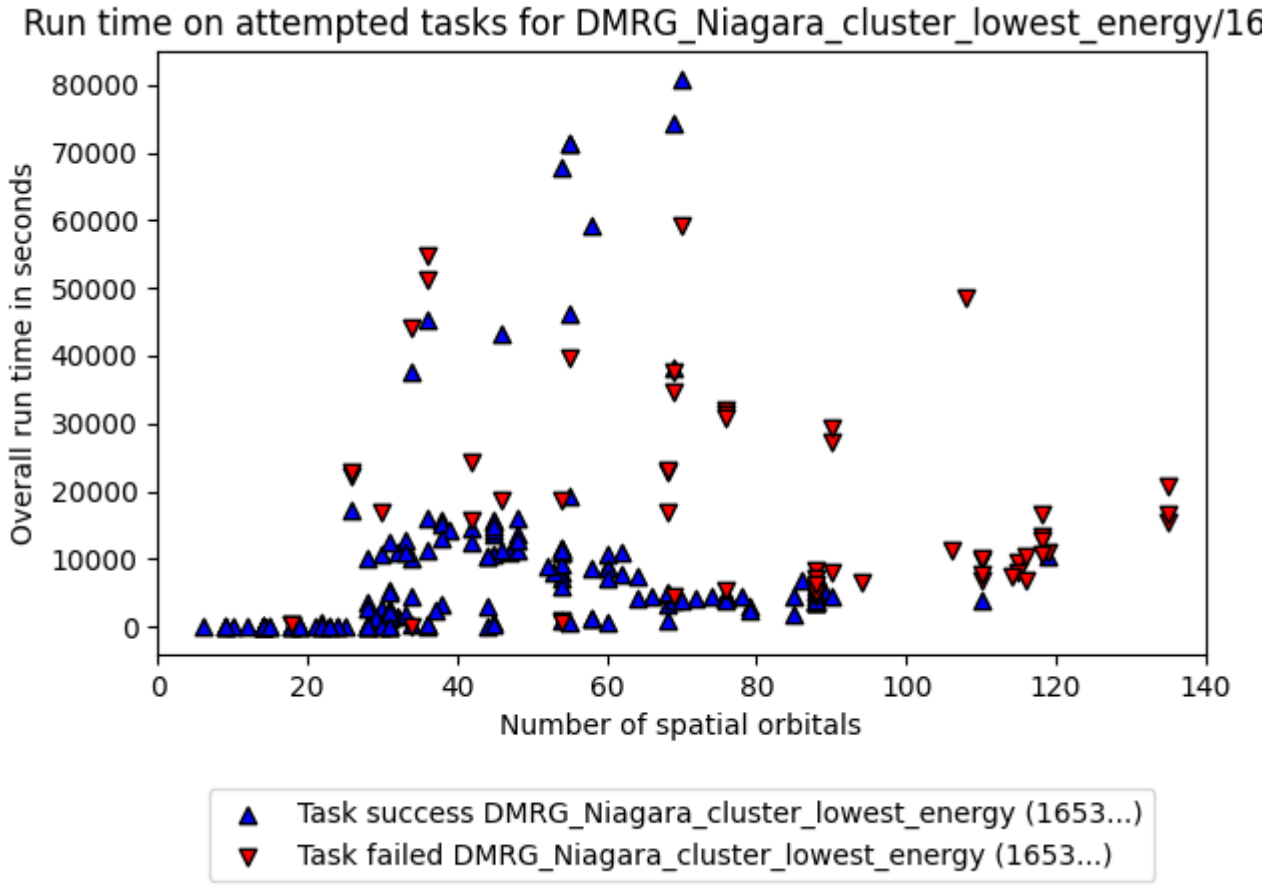
max_run_time_of_attempted_tasks: 80820.729907066

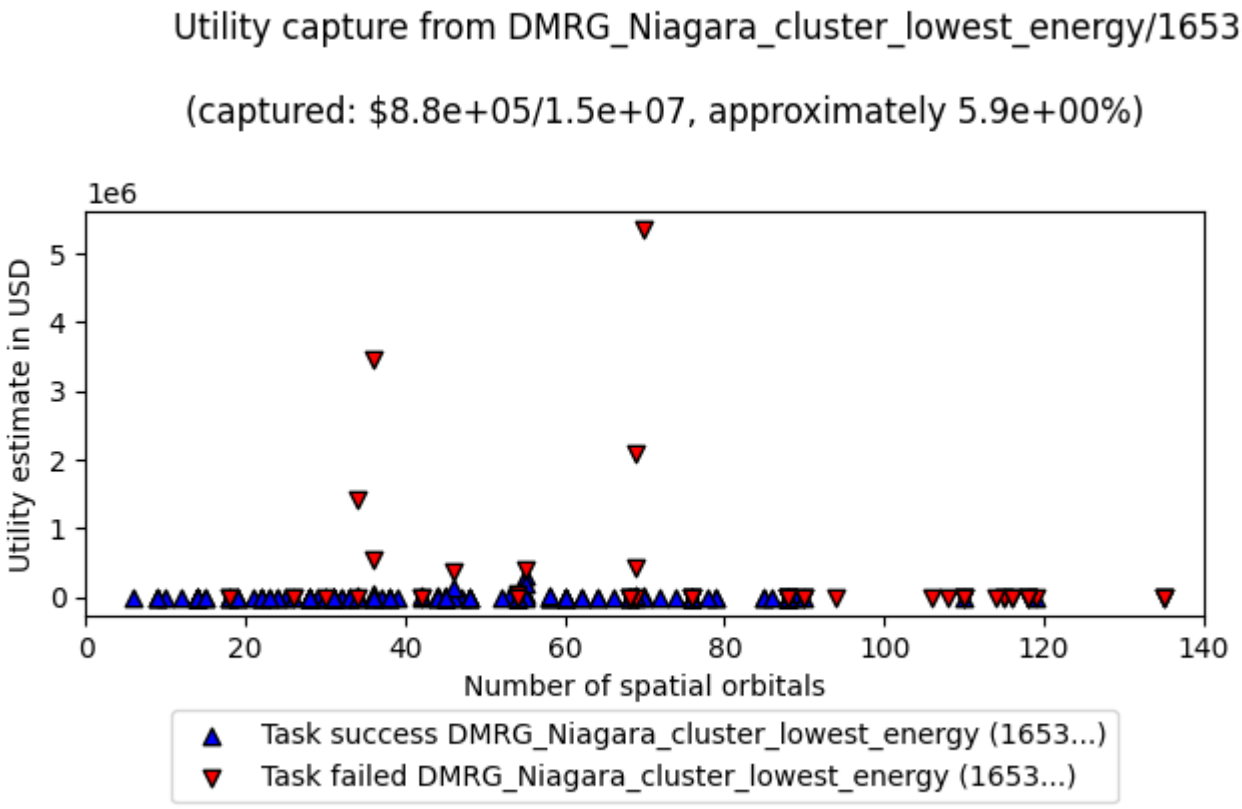
sum_of_run_time_of_attempted_tasks: 2456481.4481055504

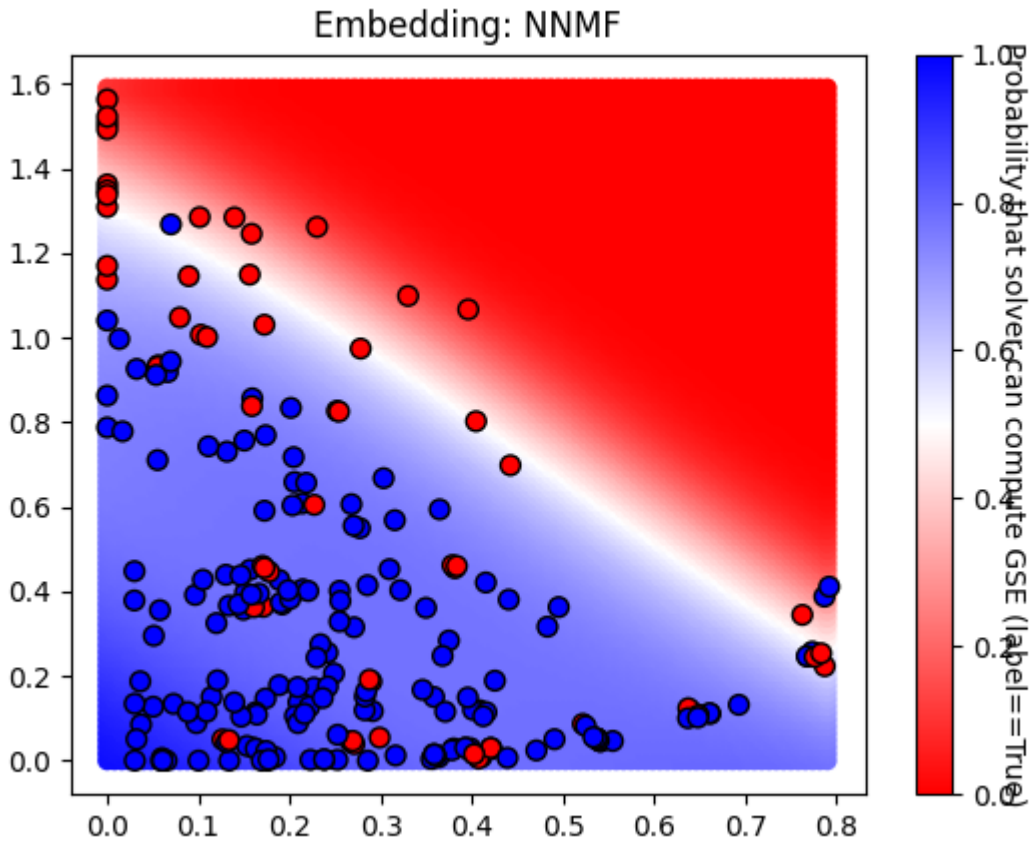
solvability_ratio: 0.5138

f1_score: [0.8545454545454545, 0.9542857142857143]

ml_metrics_calculator_version: 1




Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..
(captured: $8.8e+05/1.5e+07, approximately 5.9e+00%)
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...)



SHAP summary plot