GSEE Benchmark Standard Report

Report based on data from 2025-01-16T14:40:23.264140+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 08:13:11 2025

Latest creation time for a `performance_metrics.json` file: Thu Jan 16 09:41:20 2025

Latest creation time for a `solution.json` file: Thu Jan 16 08:27:31 2025

Problem Instance Summary Statistics
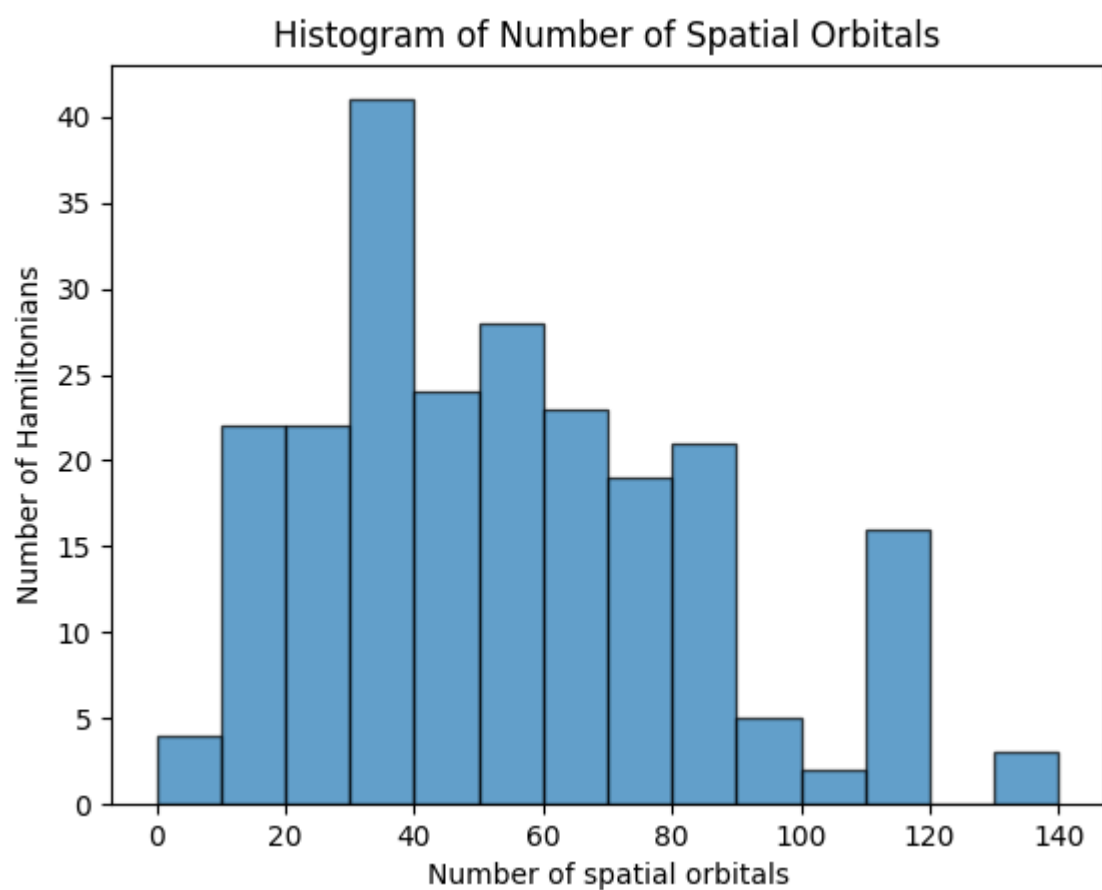
number of `problem_instances`: 82

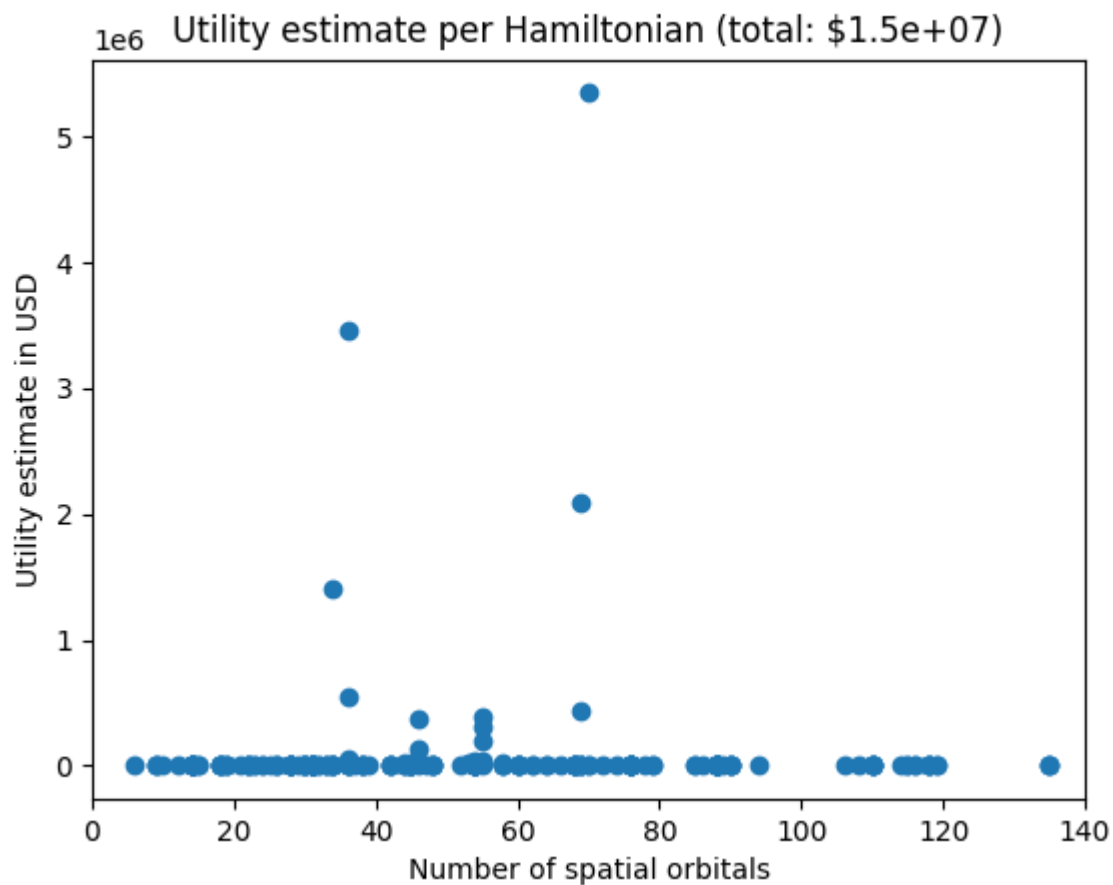`problem_instance.json` with the most tasks: 16 (mo_n2_pincer/8a3787cc-d3d0-42a8-d9a9-7de2aed45208)

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

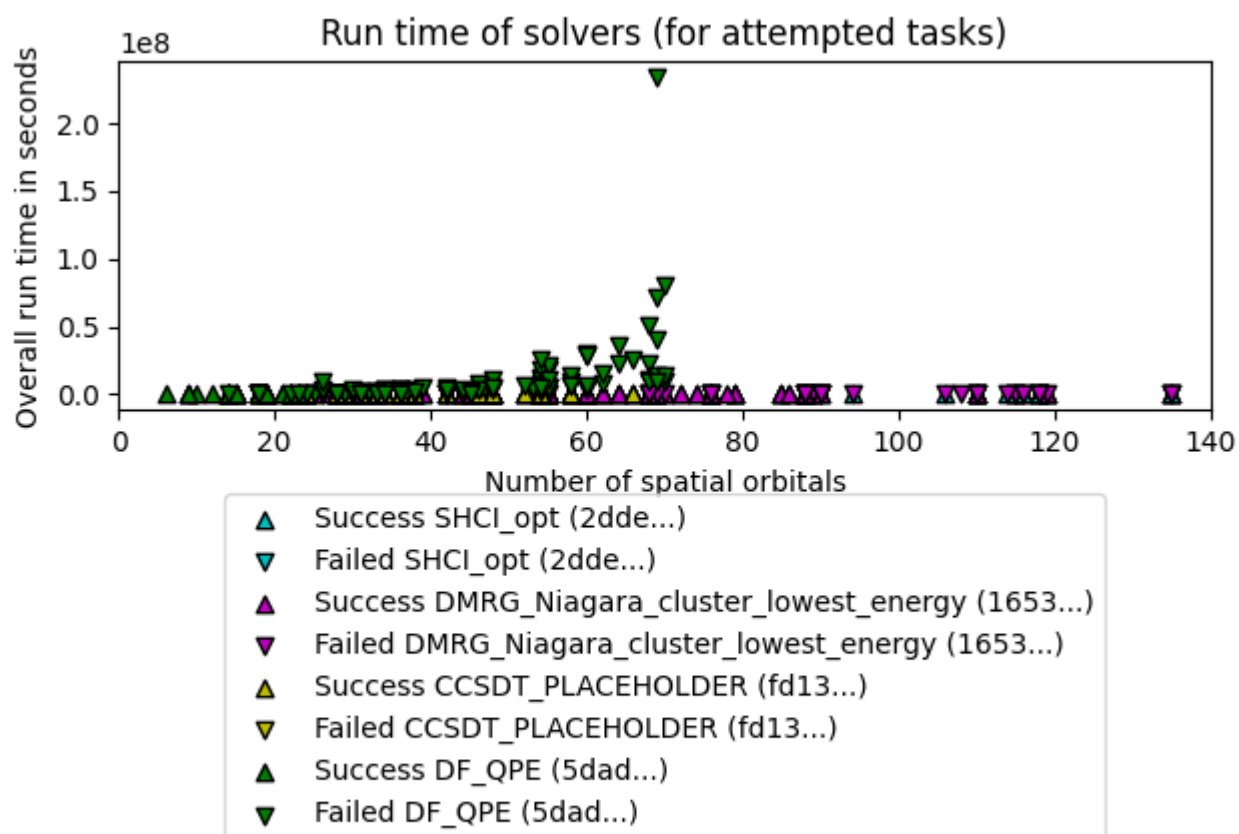minimum number of orbitals: 6

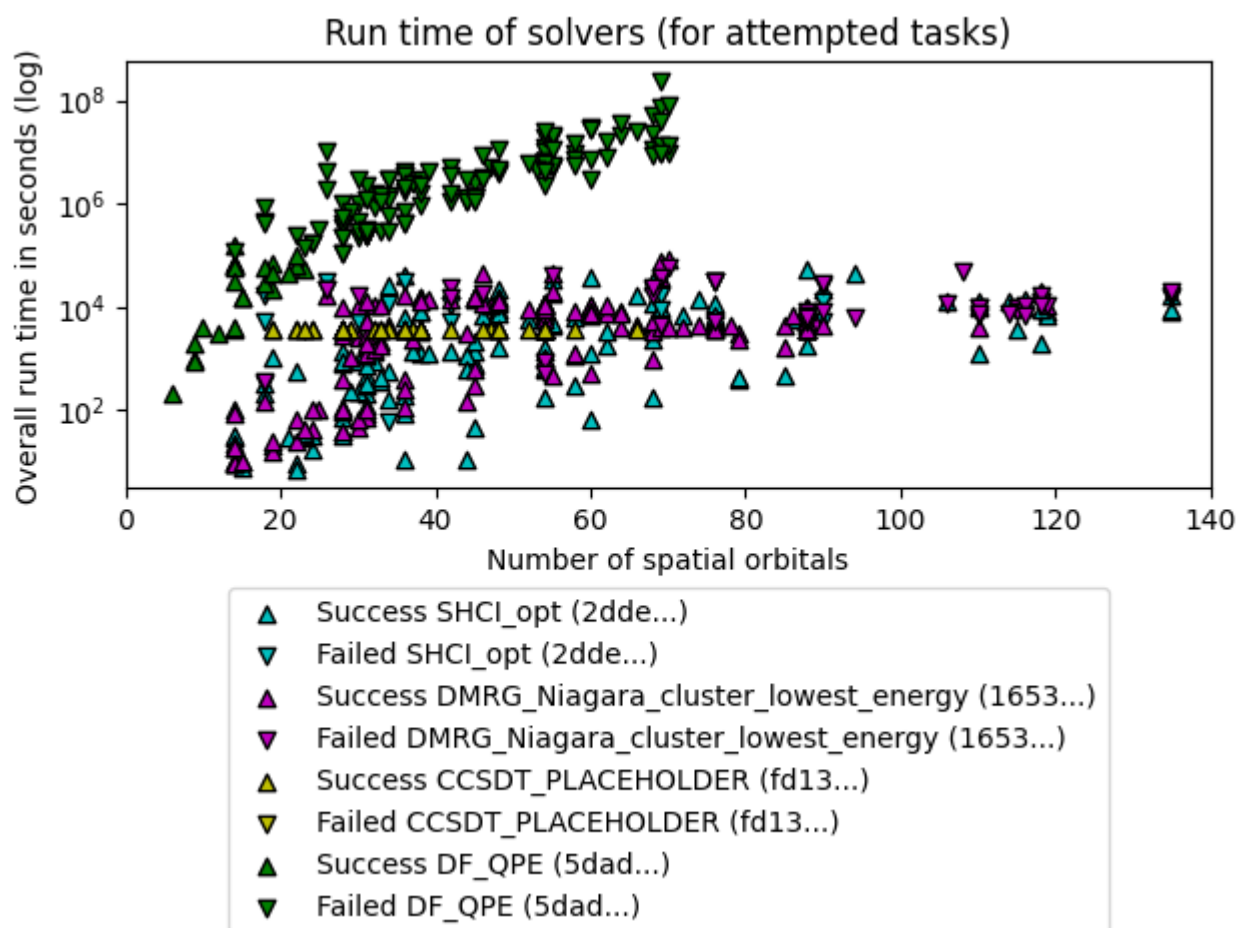median number of orbitals: 53.5

maximum number of orbitals: 135

Histogram of Number of Spatial Orbitals

Utility estimate per Hamiltonian (total: $1.5e+07)

Solver Summary Statistics

number of unique participating solvers: 4

Run time of solvers (for attempted tasks)

Legend:
- Success SHCI_opt (2dde...)
- Failed SHCI_opt (2dde...)
- Success DMRG_Niagara_cluster_lowest_energy (1653...)
- Failed DMRG_Niagara_cluster_lowest_energy (1653...)
- Success CCSDT_PLACEHOLDER (fd13...)
- Failed CCSDT_PLACEHOLDER (fd13...)
- Success DF_QPE (5dad...)
- Failed DF_QPE (5dad...)

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

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

solver_short_name:SHCI_opt

compute_hardware_type:classical_computer

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

algorithm_details:SHCI with optimized orbitals followed by SHCI+PT

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

performance_metrics_uuid: 5152b115-de8c-4ede-ad28-6a1e0b0d9203

creation_timestamp: 2025-01-16T14:40:23.264140+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
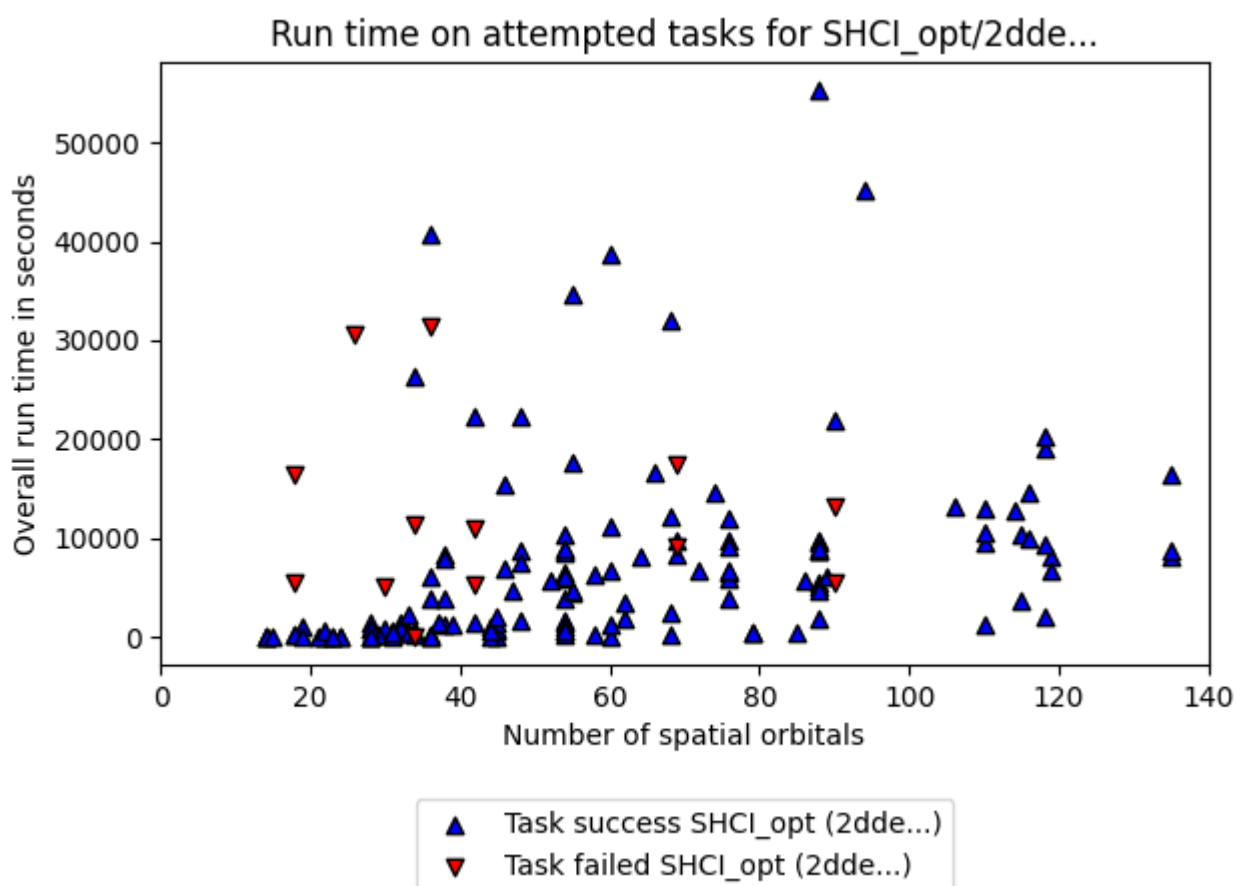
max_run_time_of_attempted_tasks: 55299.387

sum_of_run_time_of_attempted_tasks: 1138067.4269999997
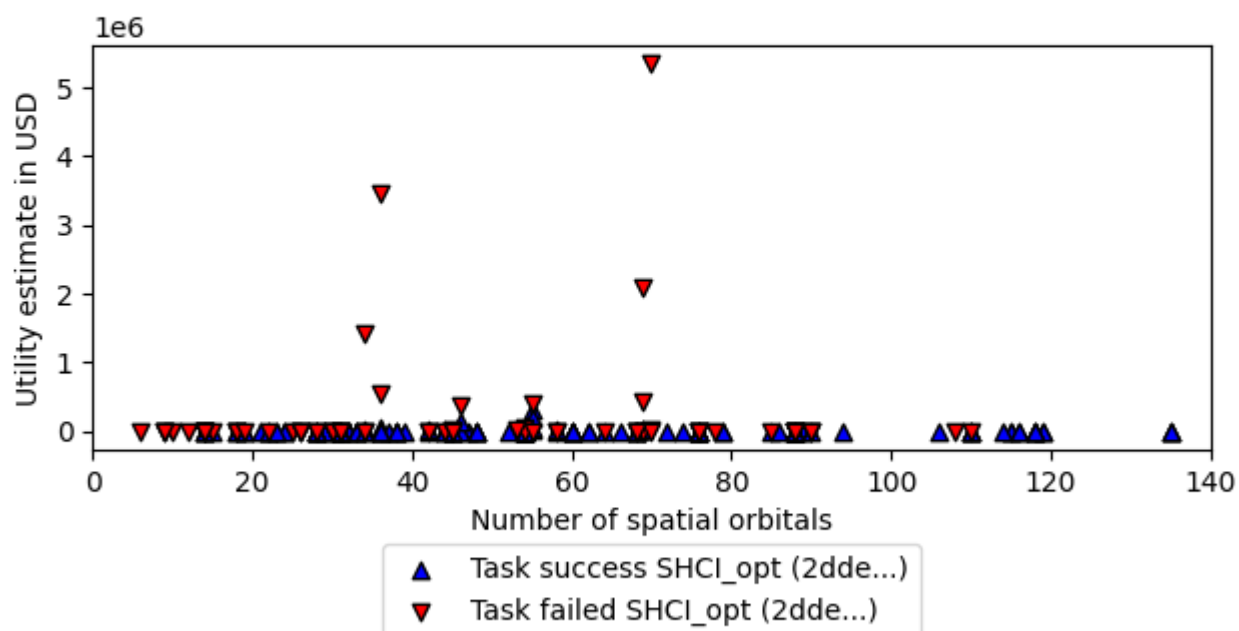
solvability_ratio: 0.9998
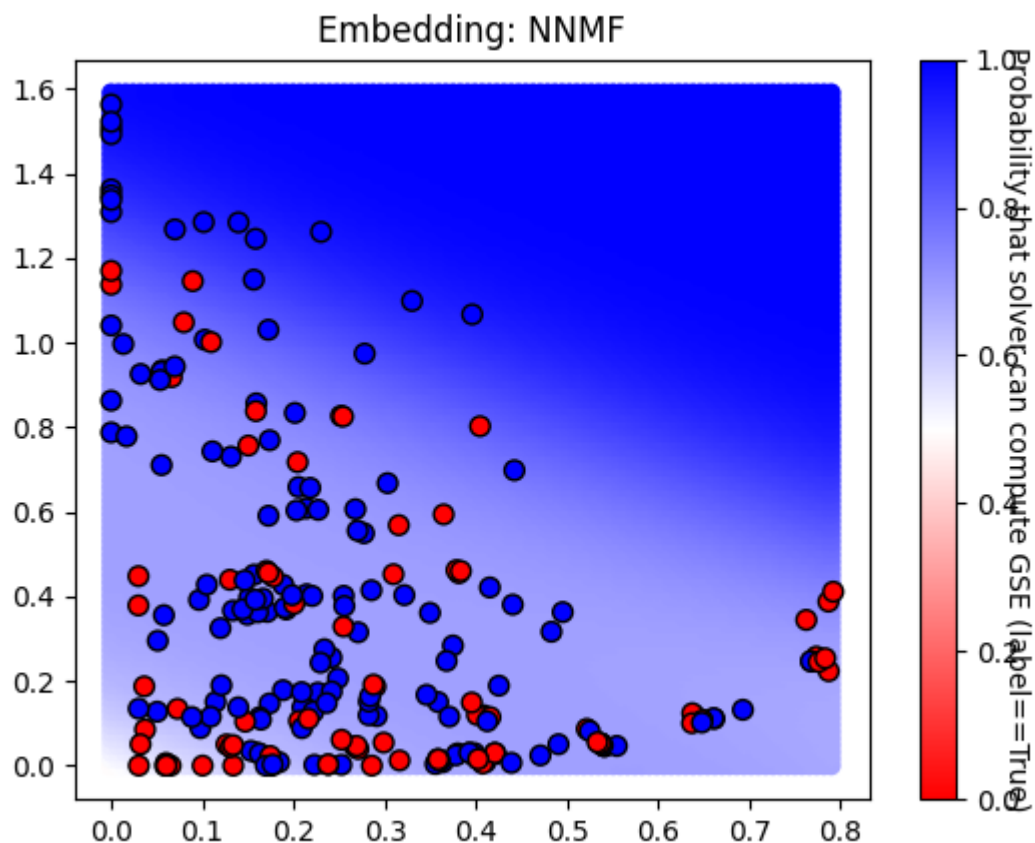
f1_score: [0.5691056910569106, 0.8427299703264095]

ml_metrics_calculator_version: 1

Run time on attempted tasks for SHCl_opt/2dde...

Utility capture from SHCl_opt/2dde...

(captured: $8.3e+05/1.5e+07, approximately 5.5e+00%)

Embedding: NNMF

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: c0016151-2581-4ef6-8531-a032ef34174a

creation_timestamp: 2025-01-16T14:40:23.264140+00:00

number_of_problem_instances: 82

number_of_problem_instances_attempted: 76

number_of_problem_instances_solved: 43

number_of_tasks: 230

number_of_tasks_attempted: 192

number_of_tasks_solved: 142

number_of_tasks_solved_within_run_time_limit: 192
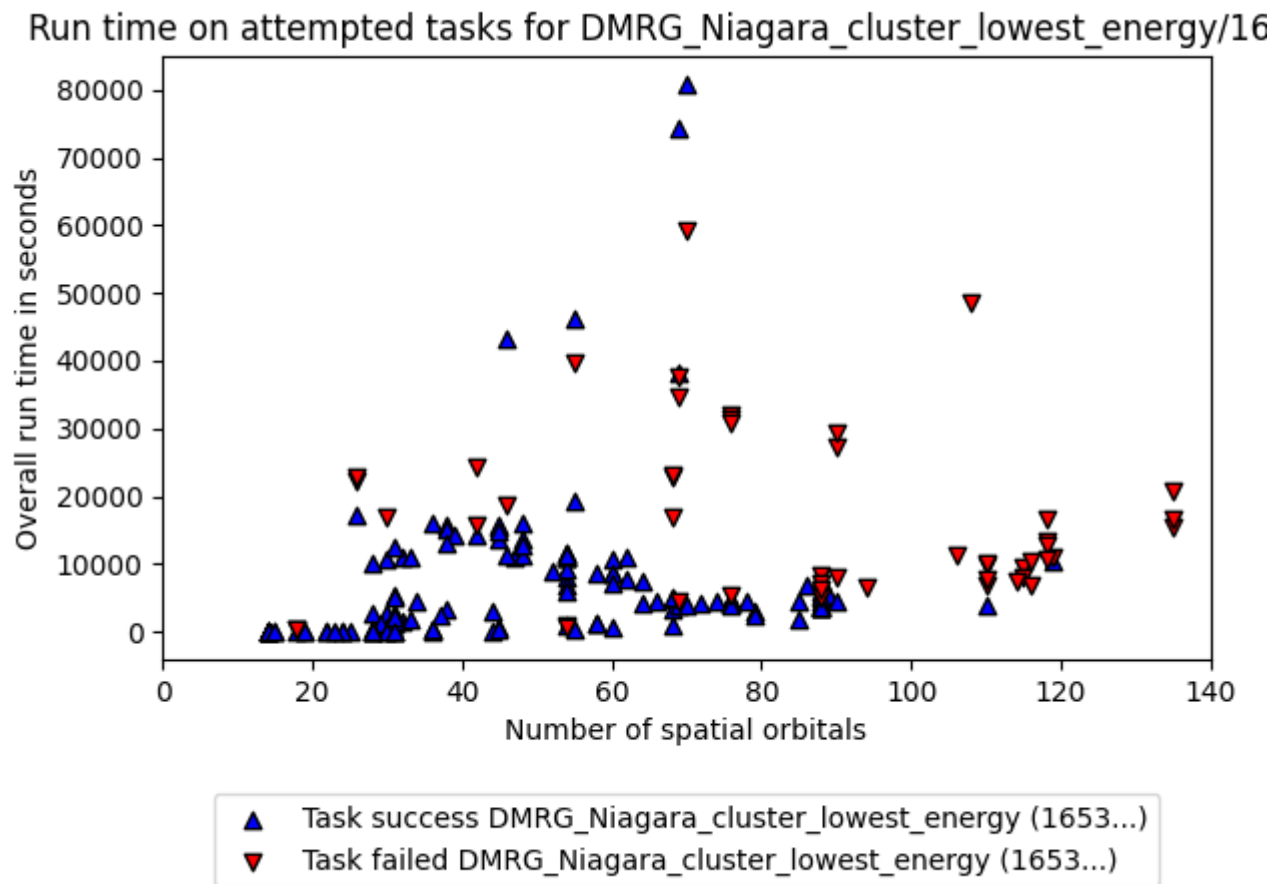
number_of_tasks_solved_within_accuracy_threshold: 142

max_run_time_of_attempted_tasks: 80820.729907066

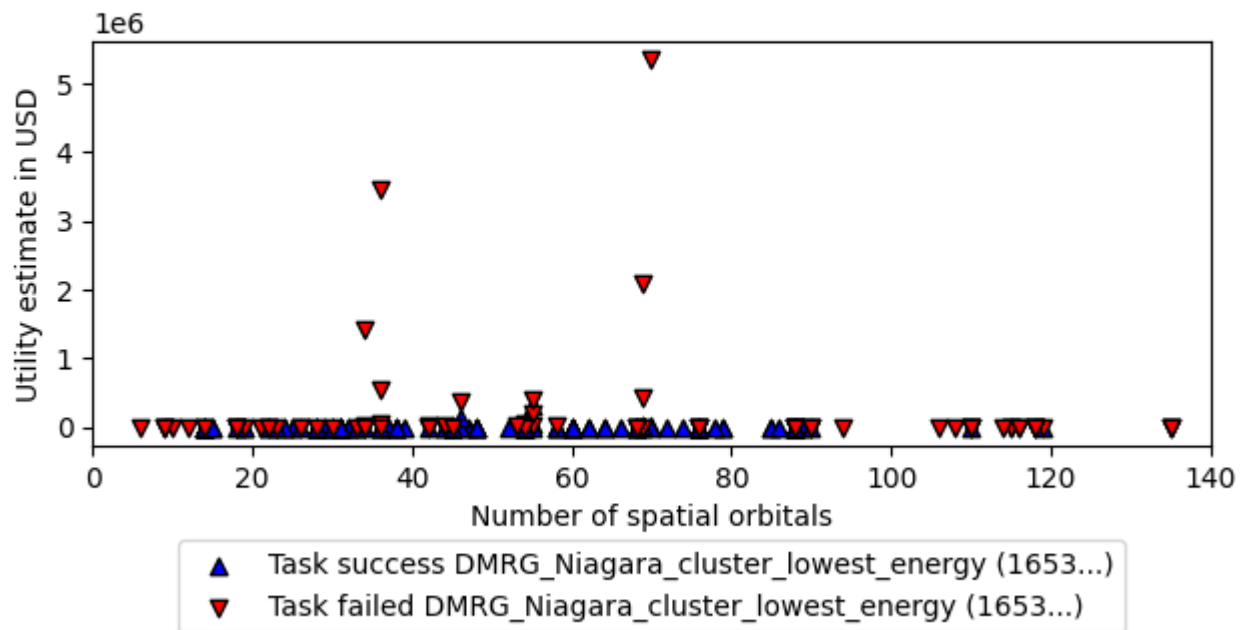sum_of_run_time_of_attempted_tasks: 1824772.0337238186

solvability_ratio: 0.3377

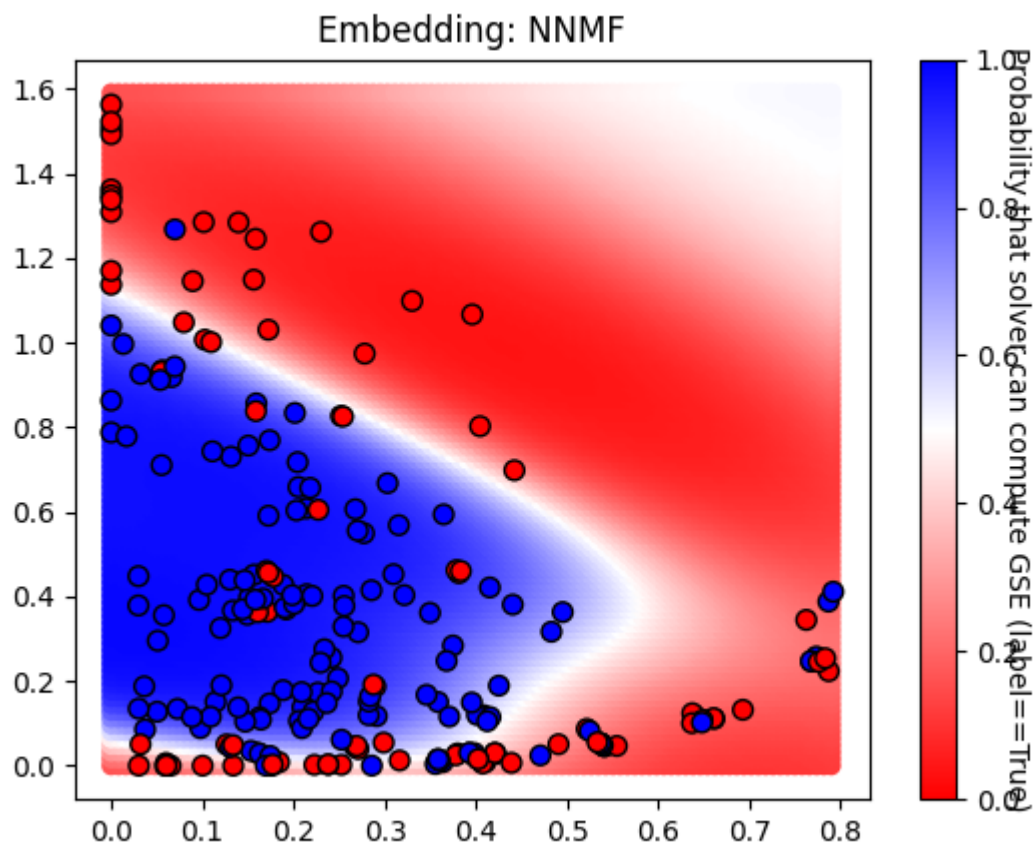f1_score: [0.865979381443299, 0.9022556390977443]

ml_metrics_calculator_version: 1

Run time on attempted tasks for DMRG_Niagara_cluster_lowest_energy/16

Utility capture from DMRG_Niagara_cluster_lowest_energy/1653..

(captured: $5.2e+05/1.5e+07, approximately 3.5e+00%)

Embedding: NNMF

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: 4271a06e-f531-4333-8477-b70c36c673fa

creation_timestamp: 2025-01-16T14:40:23.264140+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

Run time on attempted tasks for CCSDT_PLACEHOLDER/fd13...
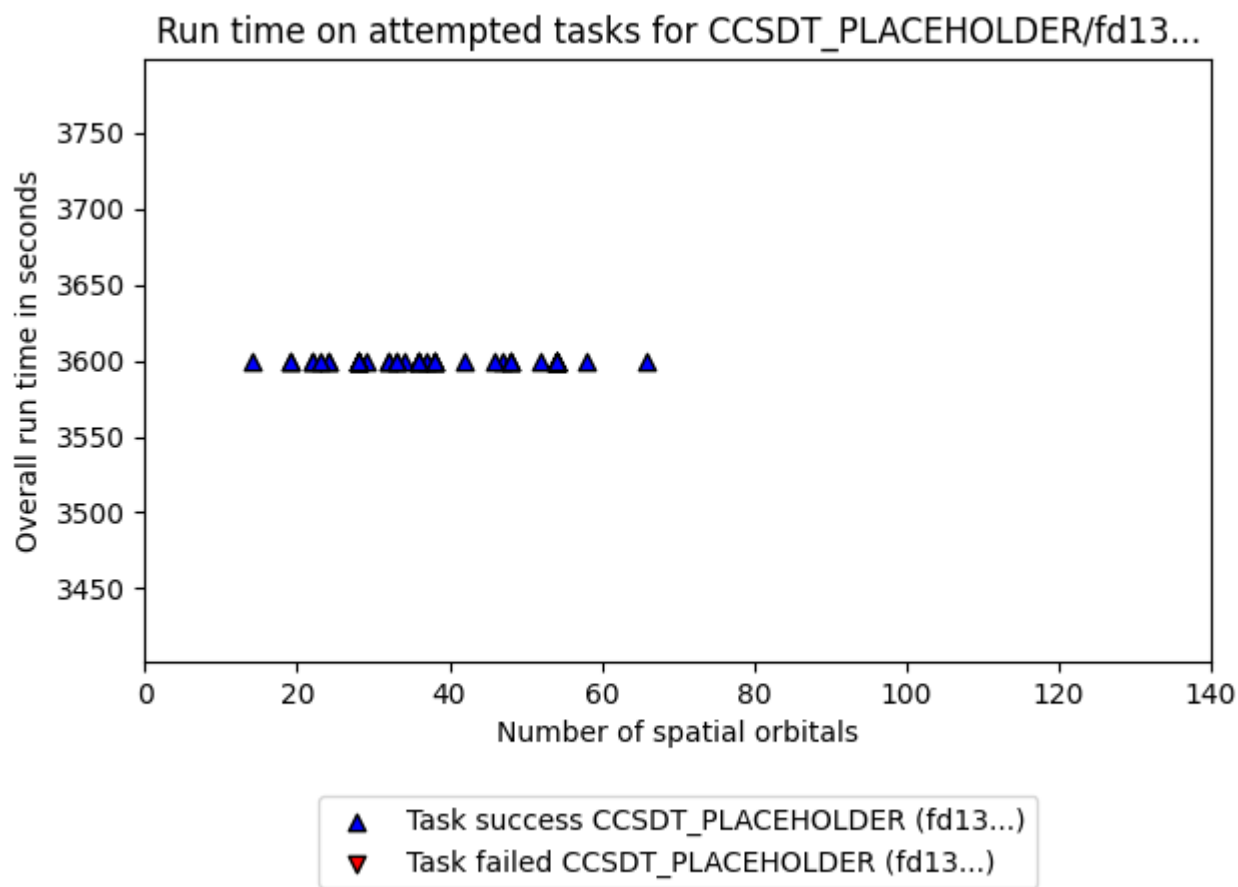
Utility capture from CCSDT_PLACEHOLDER/fd13...

(captured: $0.0e+00/1.5e+07, approximately 0.0e+00%)
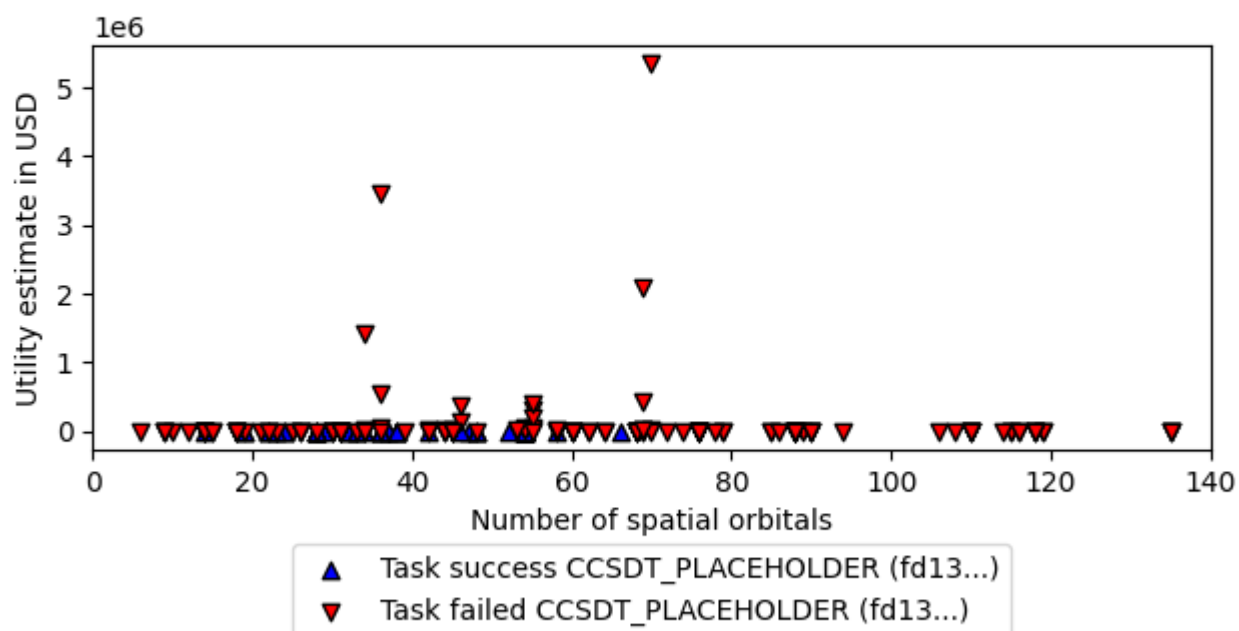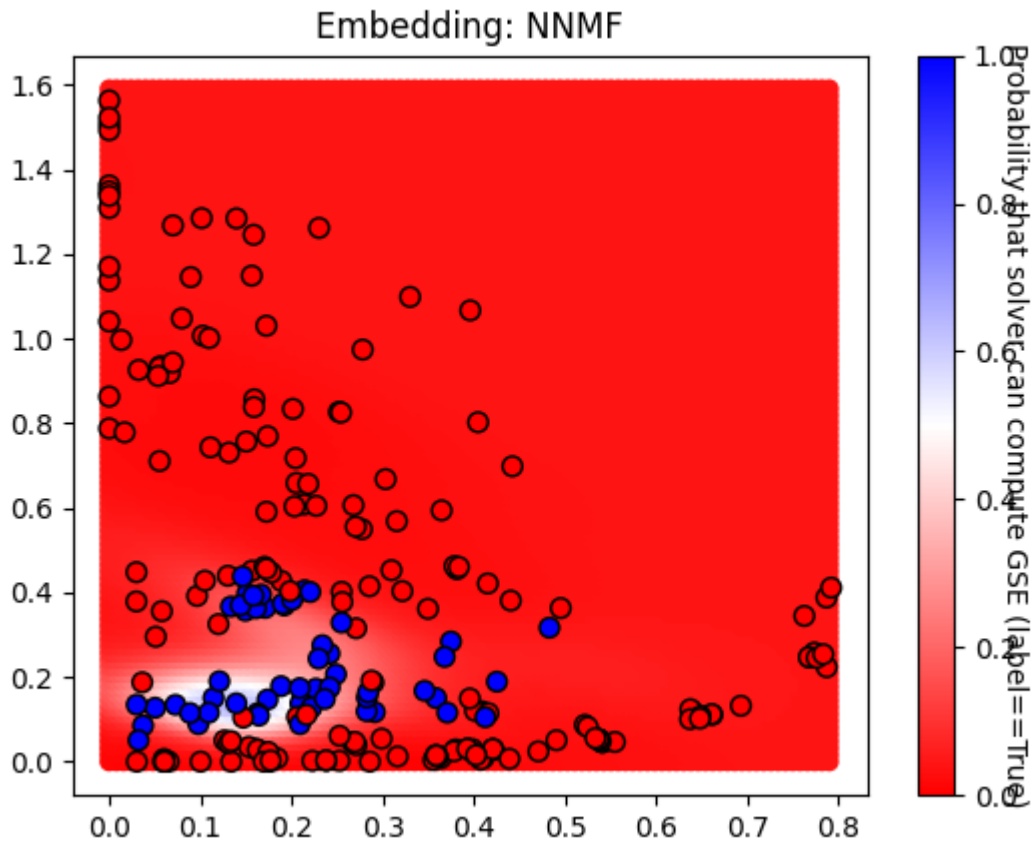
SHAP summary plot

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: 5c88eca6-6e53-4cb5-927a-9f7cd879f4b9

creation_timestamp: 2025-01-16T14:40:23.264140+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

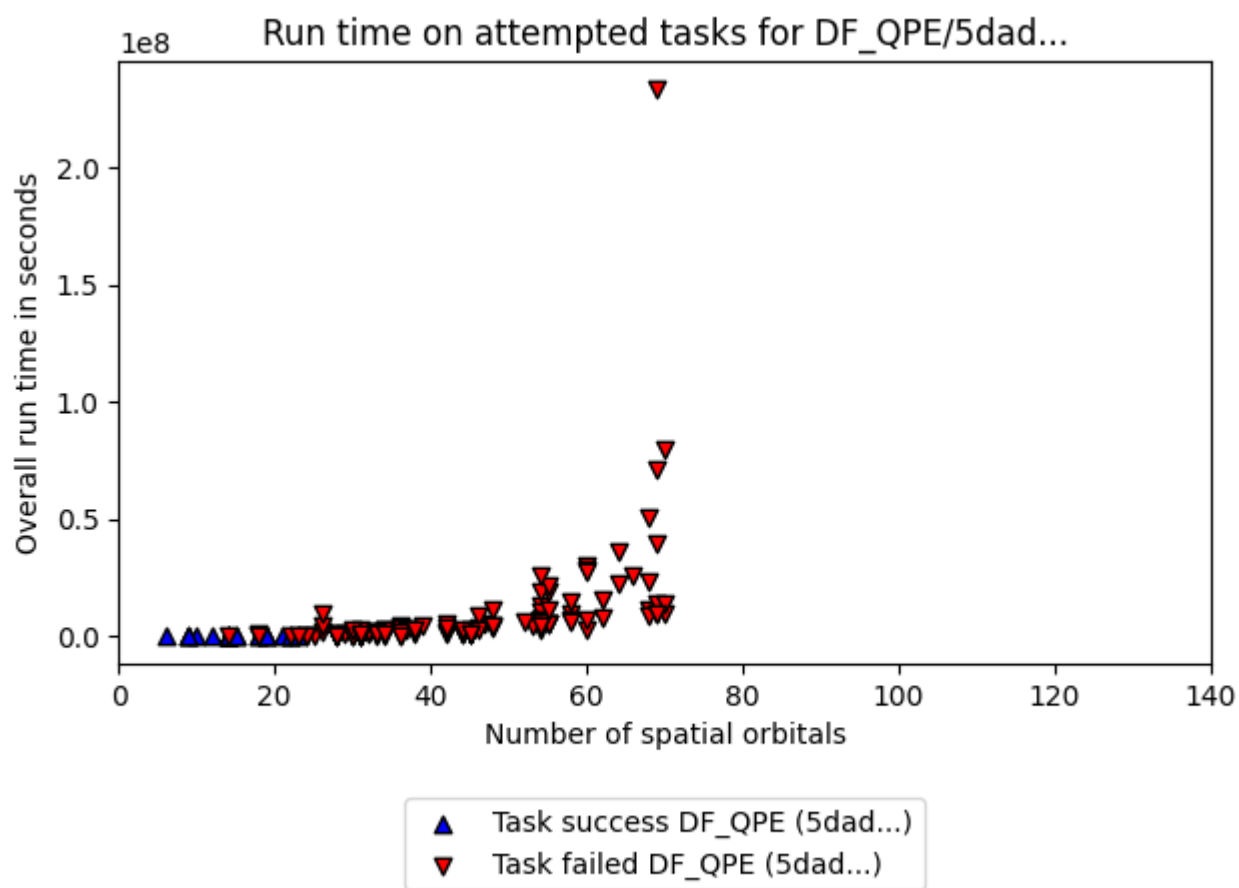number_of_tasks_solved_within_accuracy_threshold: 163

max_run_time_of_attempted_tasks: 233737829.40462503

sum_of_run_time_of_attempted_tasks: 1180589418.3385448
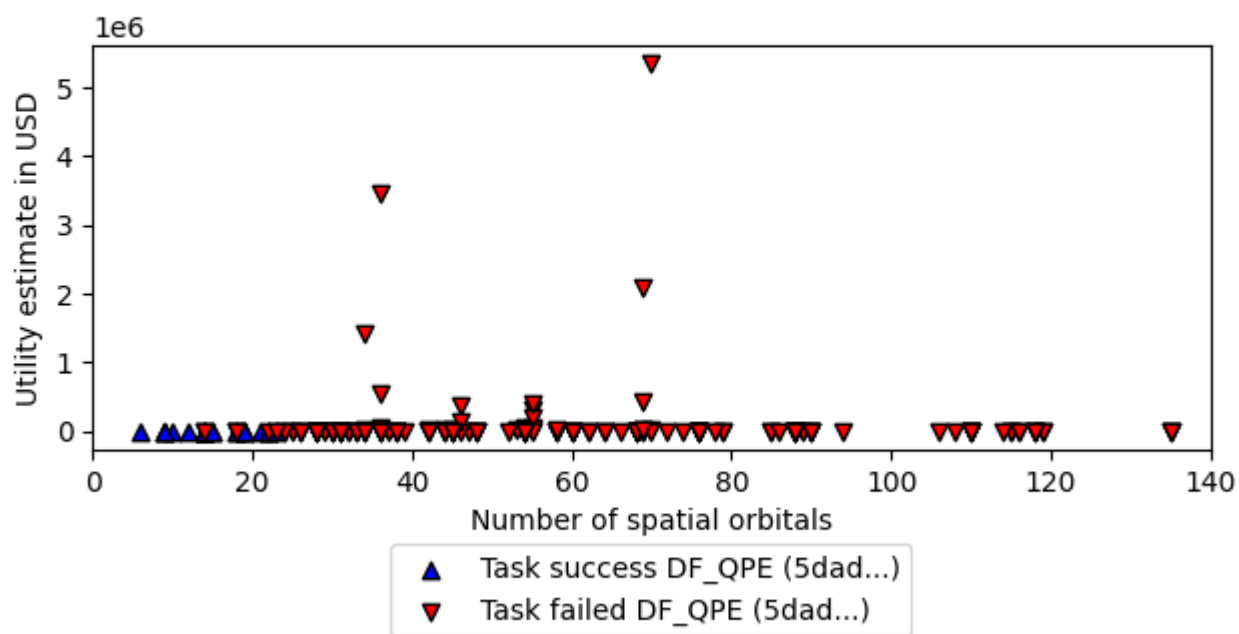
solvability_ratio: 0.0232

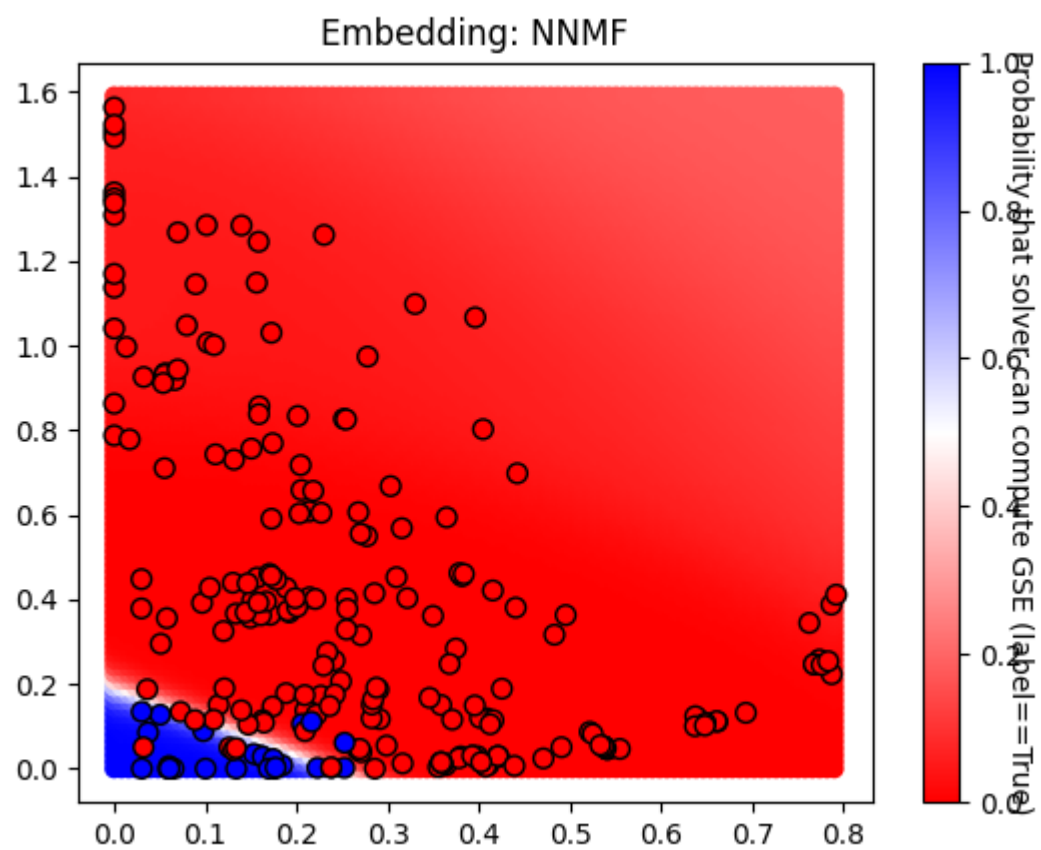f1_score: [0.9950738916256158, 0.96296296296296629]

ml_metrics_calculator_version: 1

Run time on attempted tasks for DF_QPE/5dad...

- ▲ 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%)

Embedding: NNMF

Probability that solver can compute GSE (label==True)

SHAP summary plot