

# GSEE Benchmark Standard Report

Report based on data from 2025-01-16T15:18:34.432203+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 10:20:39 2025

Latest creation time for a solution.json file: Thu Jan 16 10:13:00 2025

## Problem Instance Summary Statistics

number of problem\_instances: 82

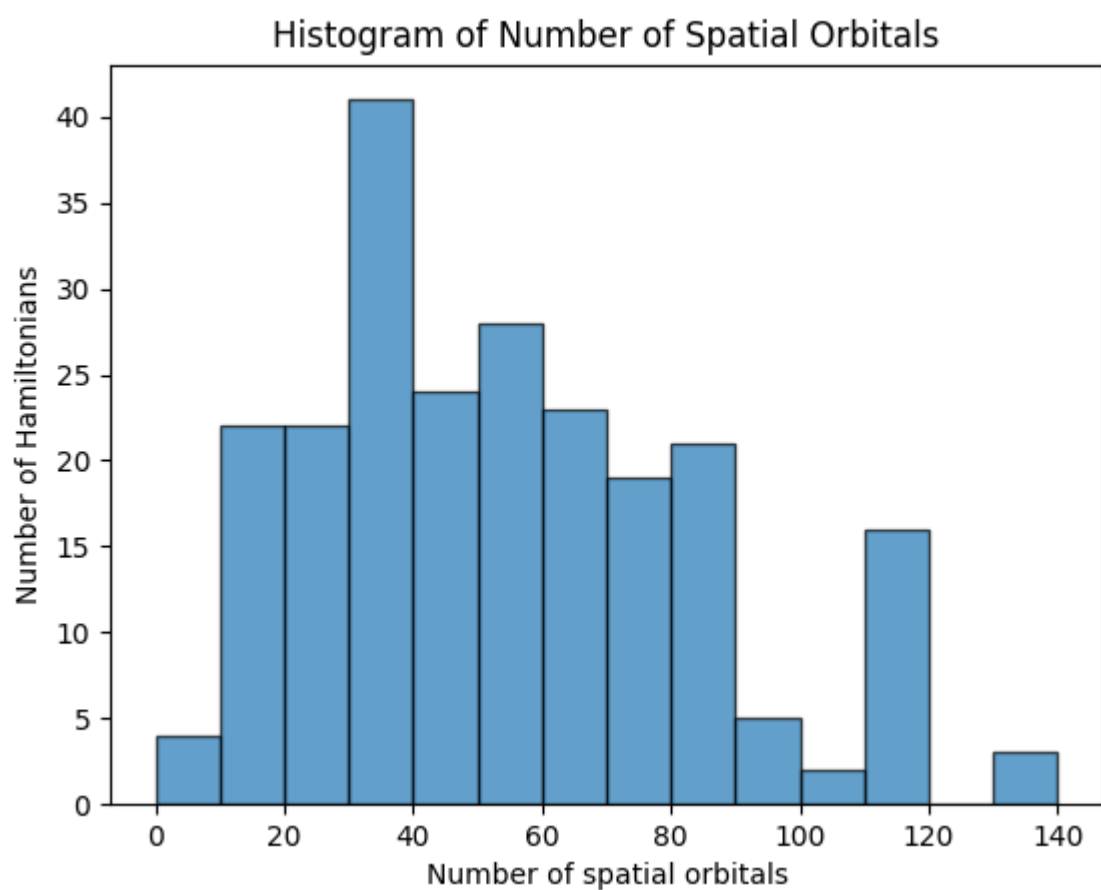
problem\_instance.json with the most tasks: 16 (mo\_n2\_pincer/8a3787cc-d3d0-42a8-d9a9-7de2aed45208)

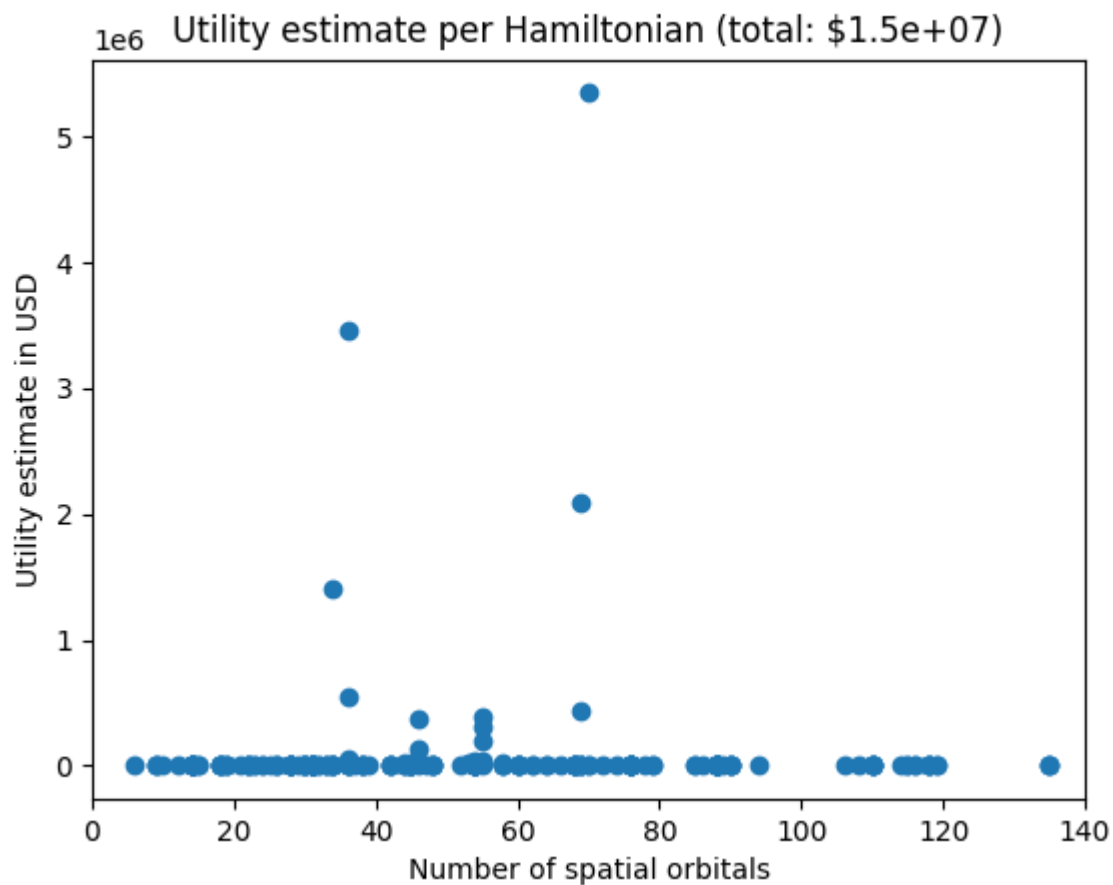
number of Hamiltonians (i.e., tasks): 230

minimum number of orbitals: 6

median number of orbitals: 53.5

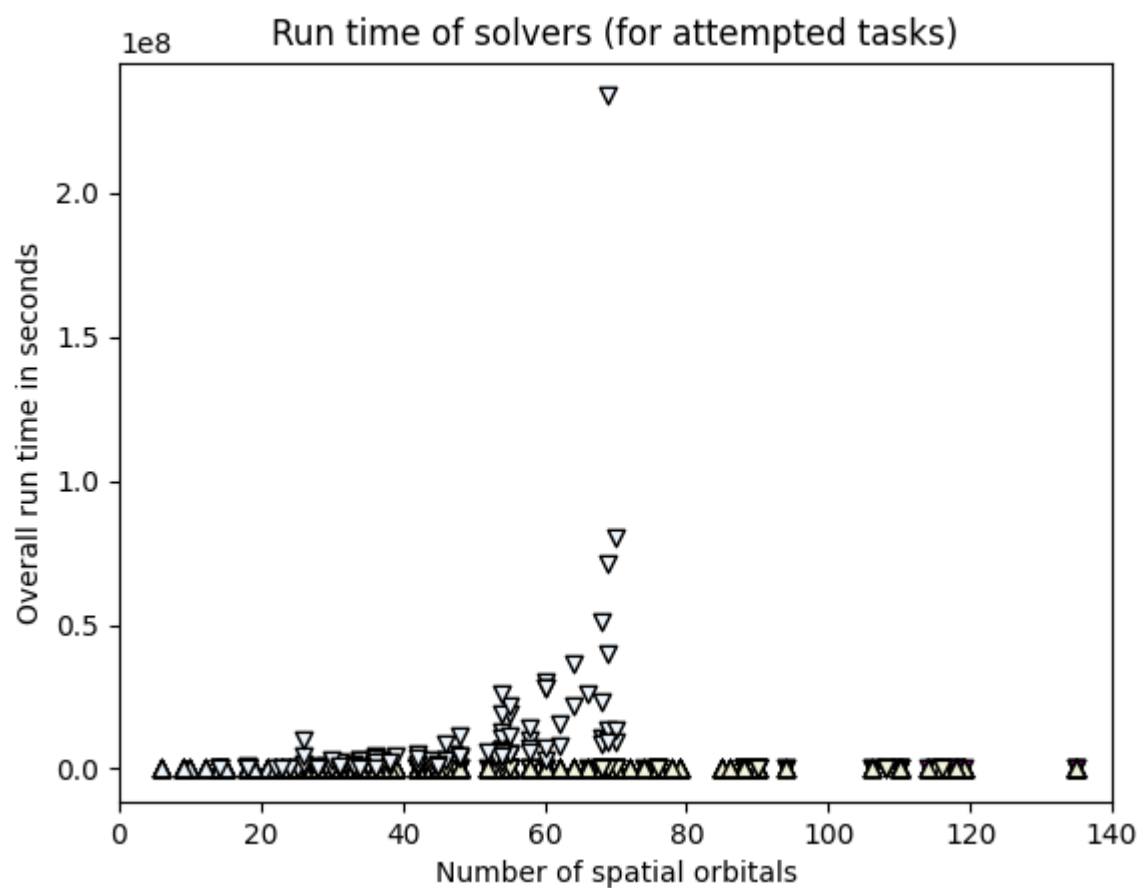
maximum number of orbitals: 135

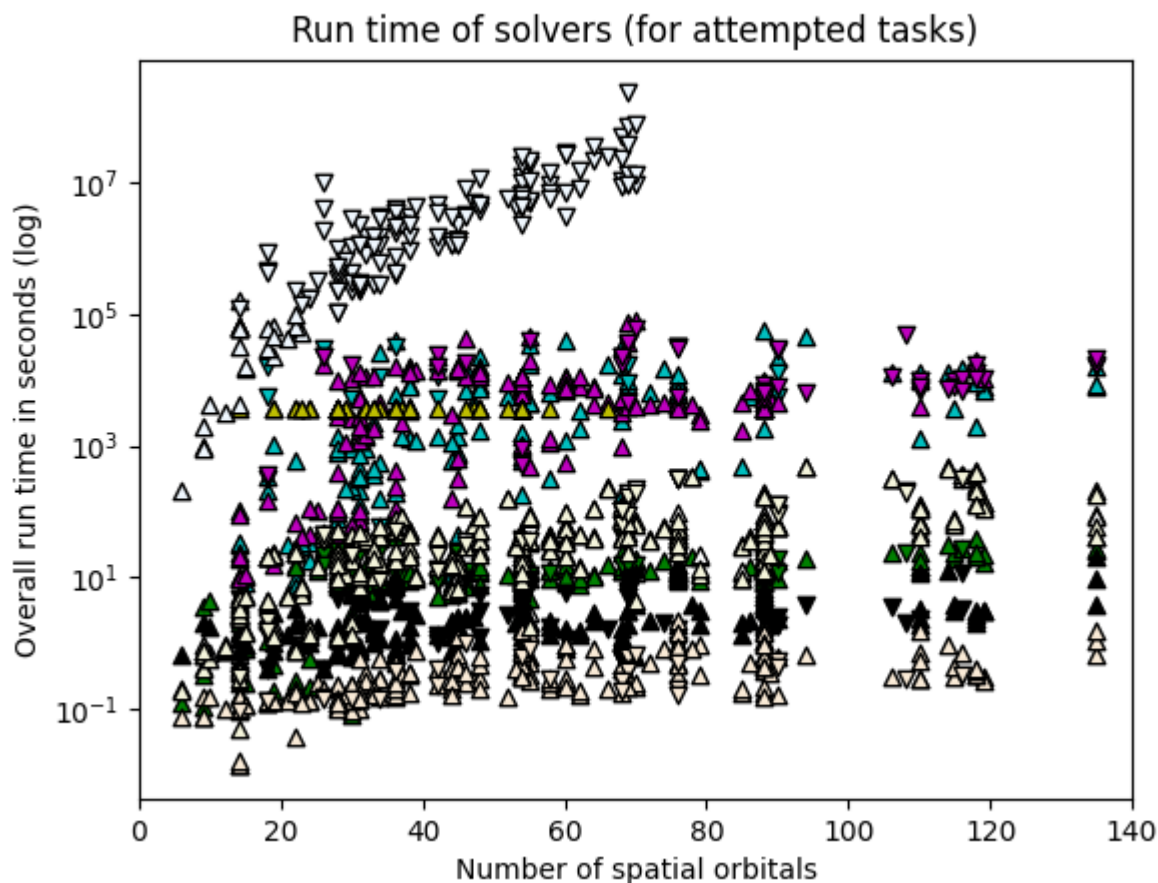




## Solver Summary Statistics

number of unique participating solvers: 9





## 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: a1f1169a-3107-40f9-b2ea-81395d34dd87

creation\_timestamp: 2025-01-16T15:18:34.432203+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

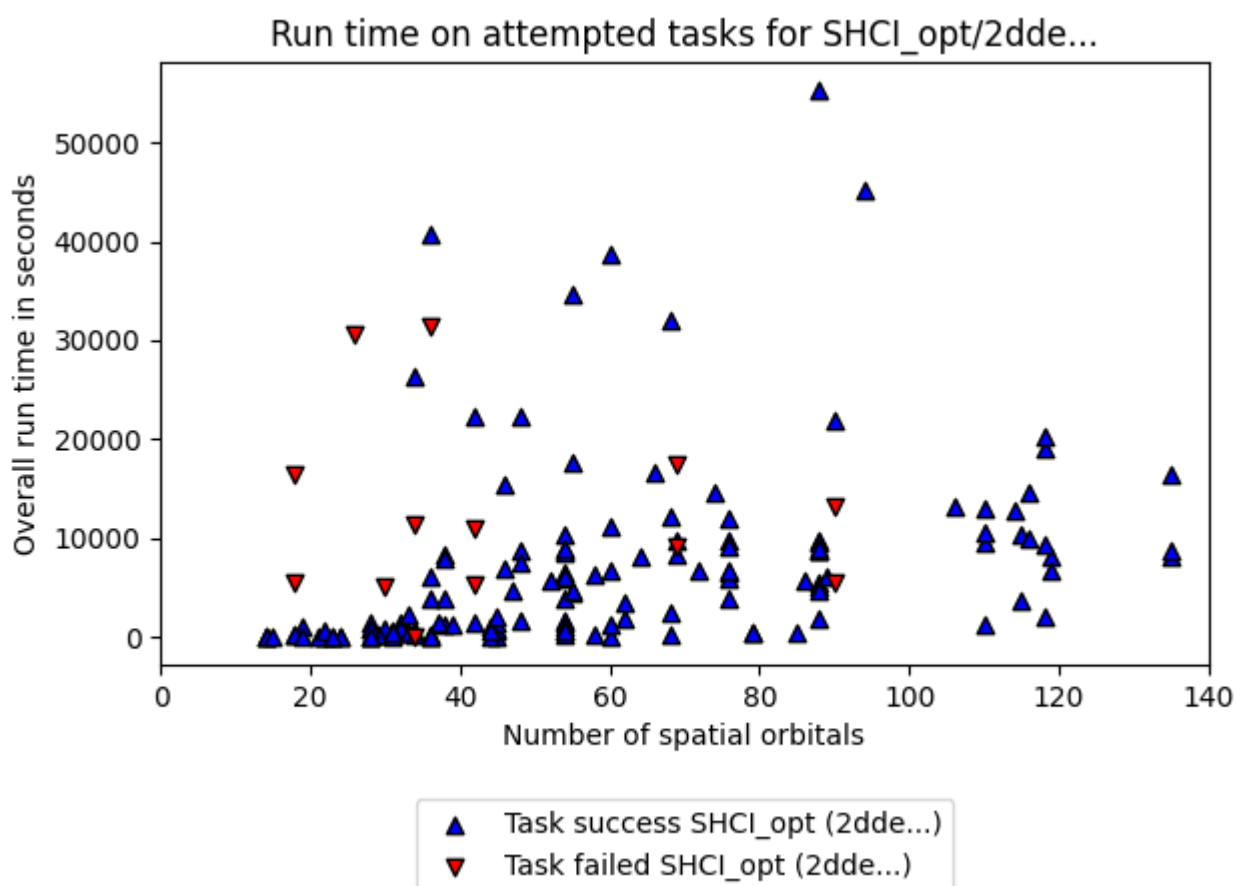
max\_run\_time\_of\_attempted\_tasks: 55299.387

sum\_of\_run\_time\_of\_attempted\_tasks: 1138067.4269999997

solvability\_ratio: 0.9998

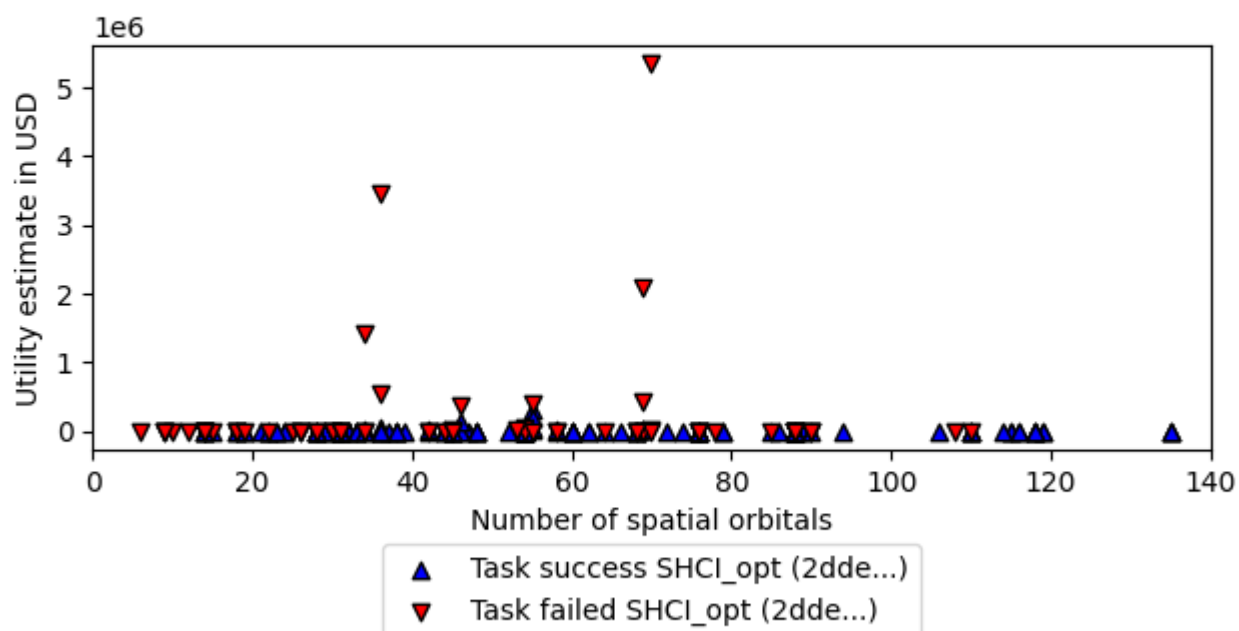
f1\_score: [0.5691056910569106, 0.8427299703264095]

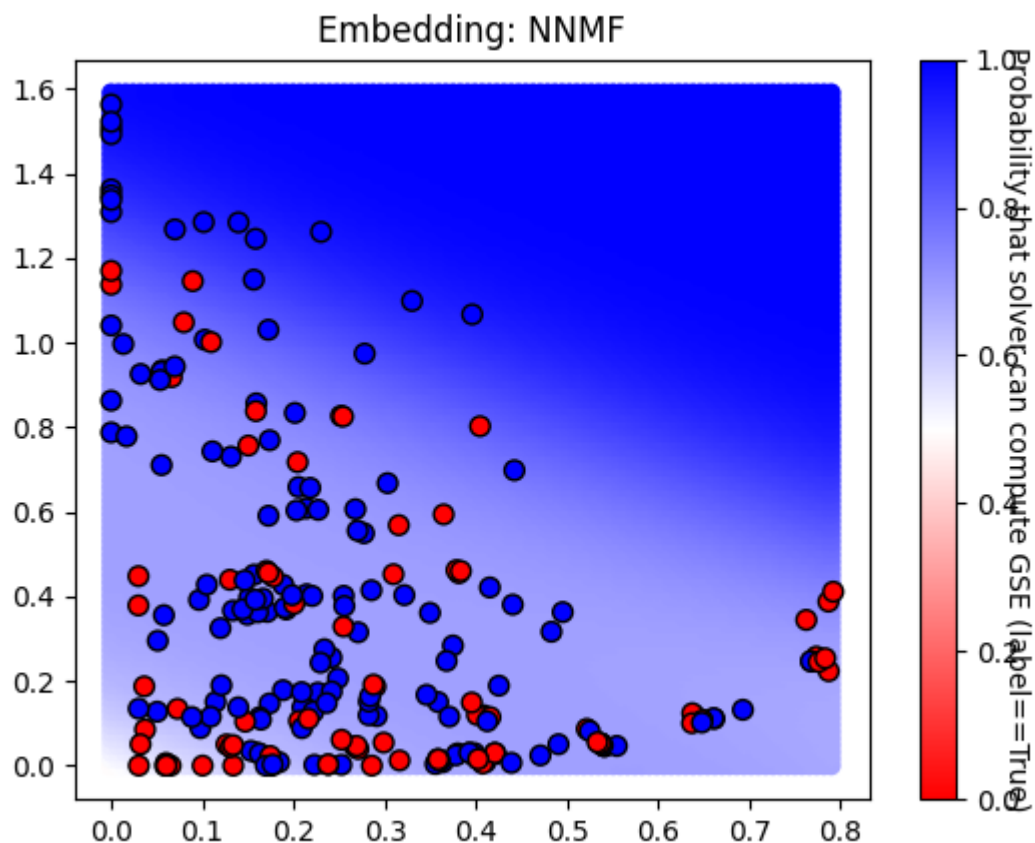
ml\_metrics\_calculator\_version: 1



# Utility capture from SHCI\_opt/2dde...

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





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: 78af3c47-7749-473f-97bf-d95cb682577b

creation\_timestamp: 2025-01-16T15:18:34.432203+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

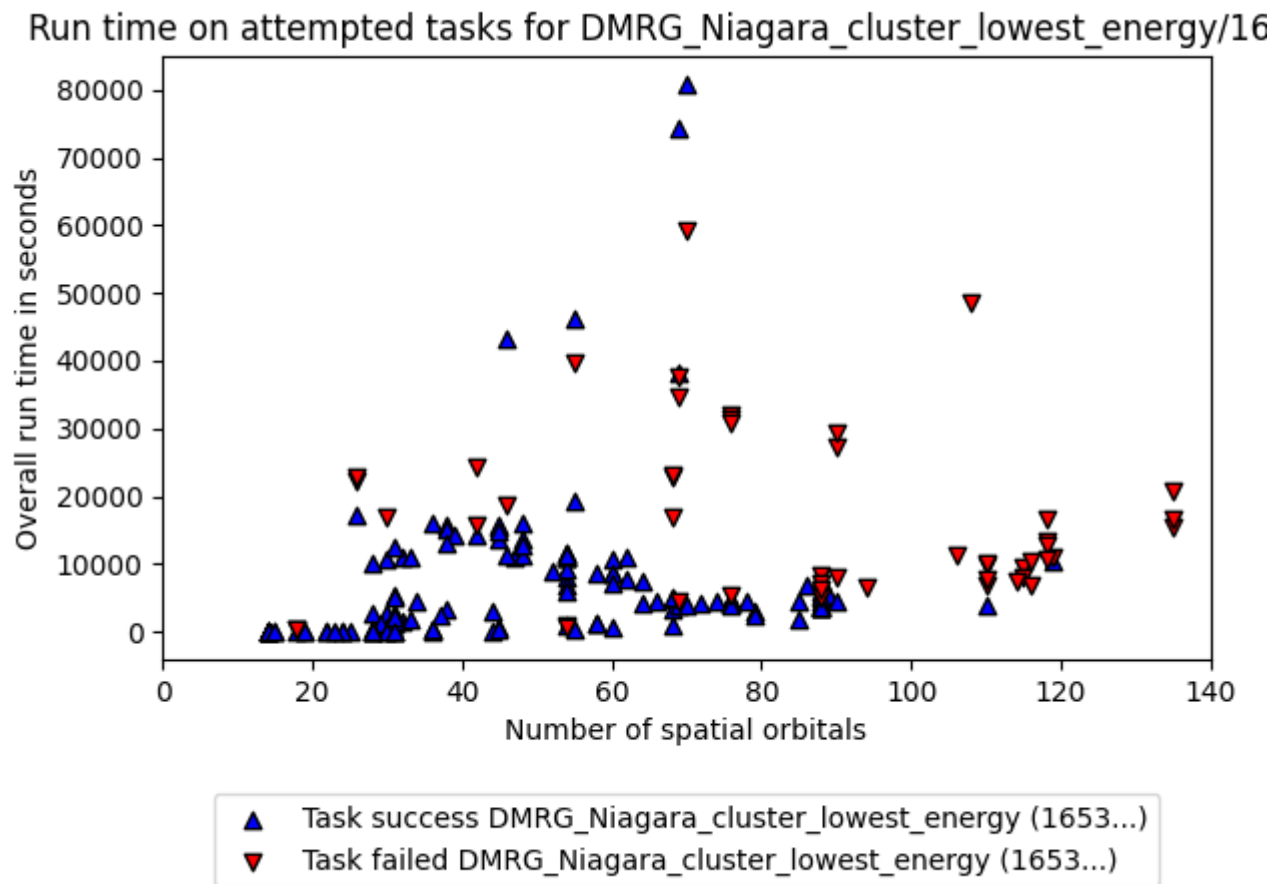
max\_run\_time\_of\_attempted\_tasks: 80820.729907066

sum\_of\_run\_time\_of\_attempted\_tasks: 1824772.0337238186

solvability\_ratio: 0.3377

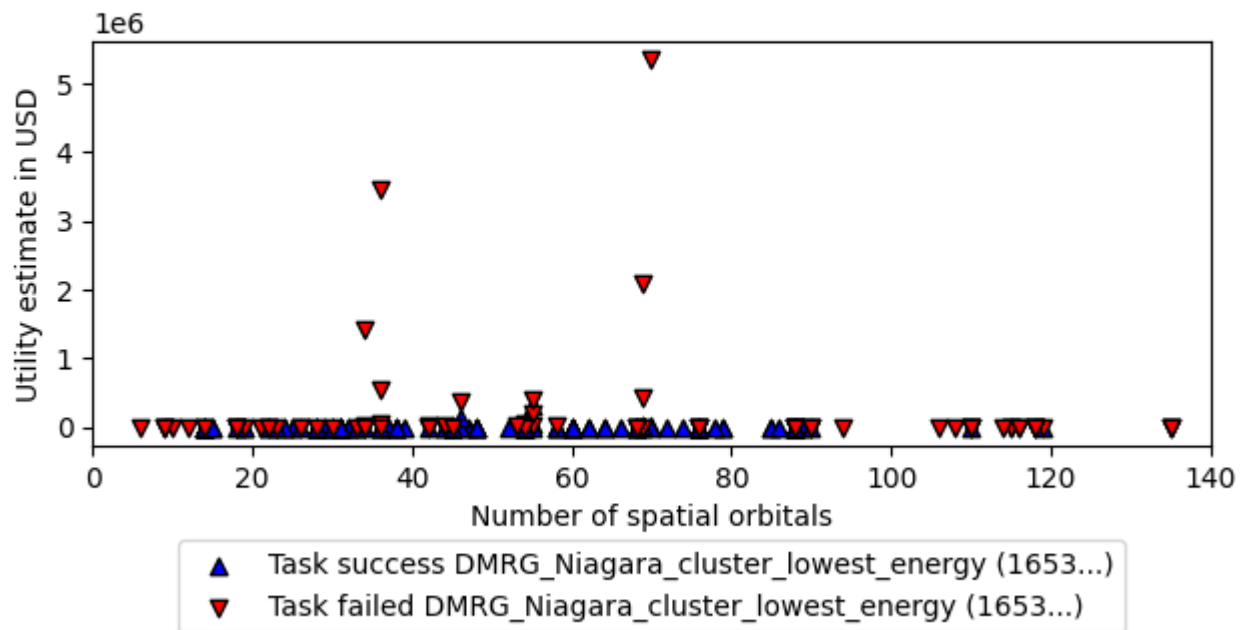
f1\_score: [0.865979381443299, 0.9022556390977443]

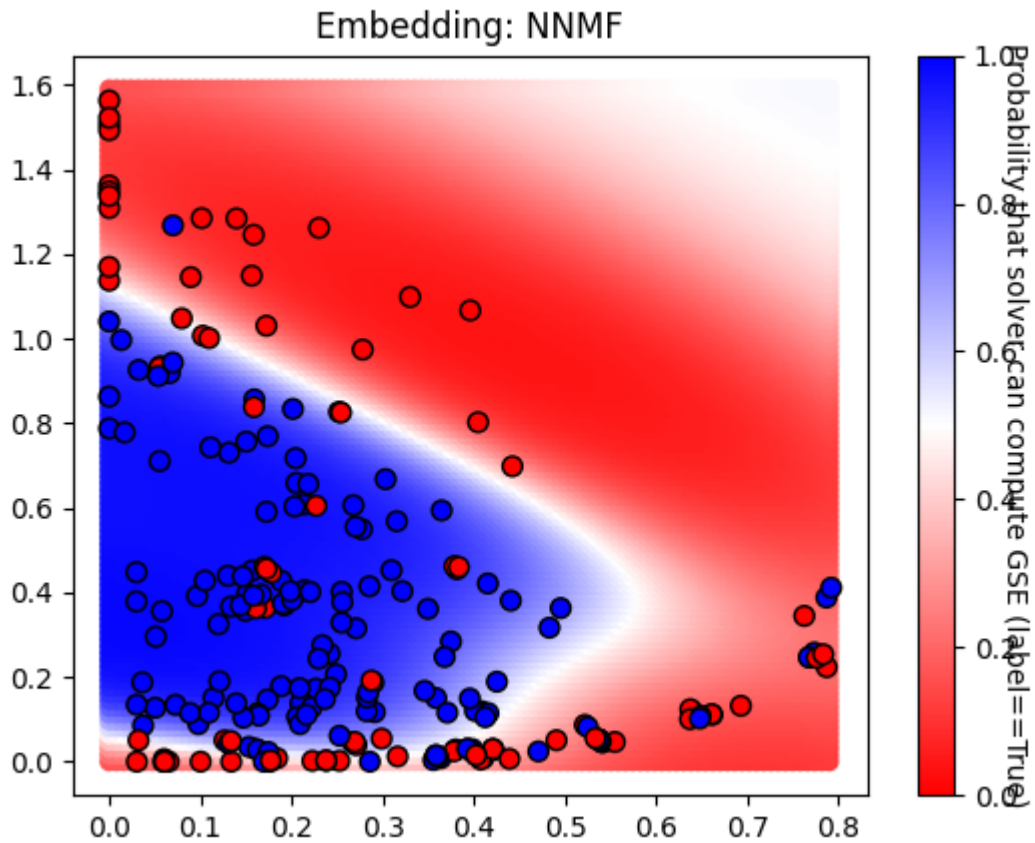
ml\_metrics\_calculator\_version: 1



Utility capture from DMRG\_Niagara\_cluster\_lowest\_energy/1653..

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





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

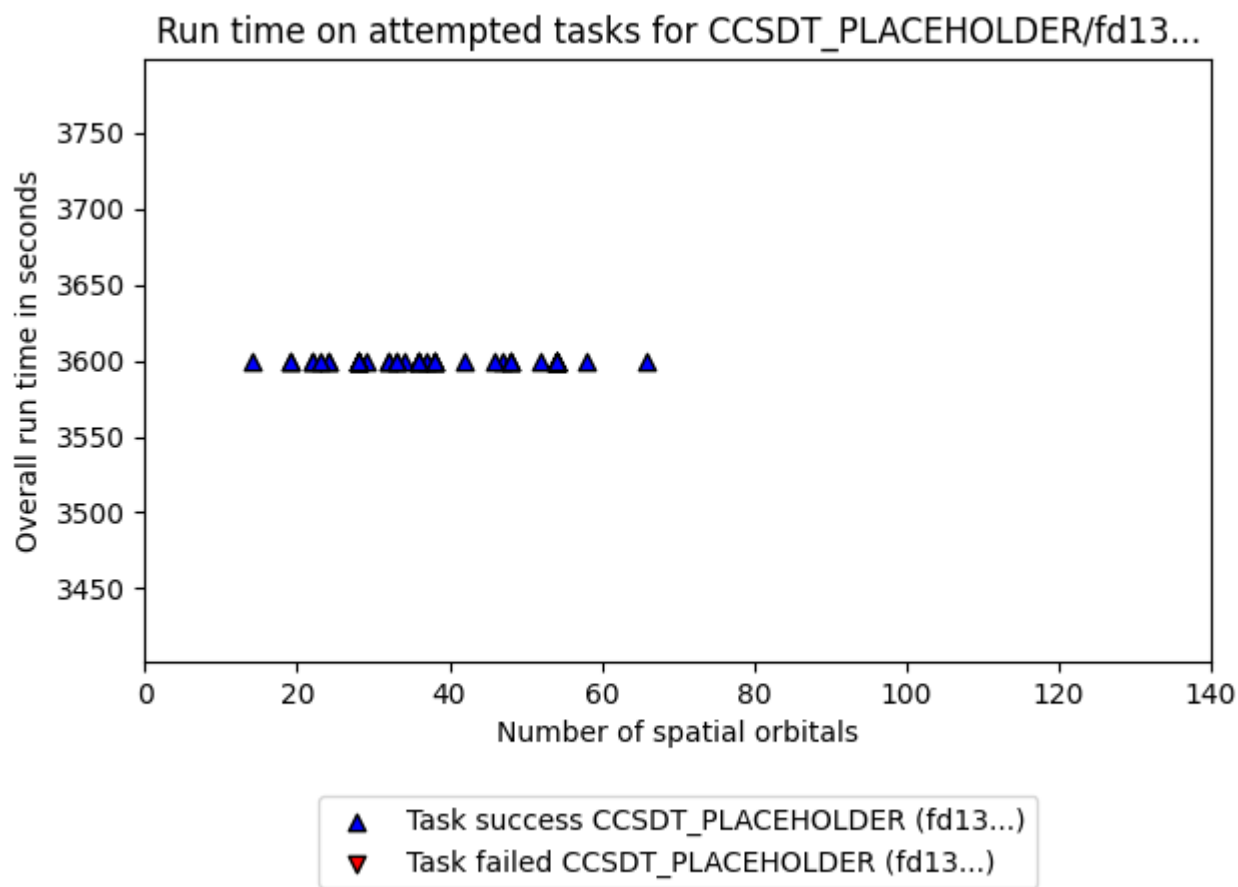
performance\_metrics\_uuid: 78854cab-8150-46b7-9bbf-c4a43e85c501

creation\_timestamp: 2025-01-16T15:18:34.432203+00:00

number\_of\_problem\_instances: 82

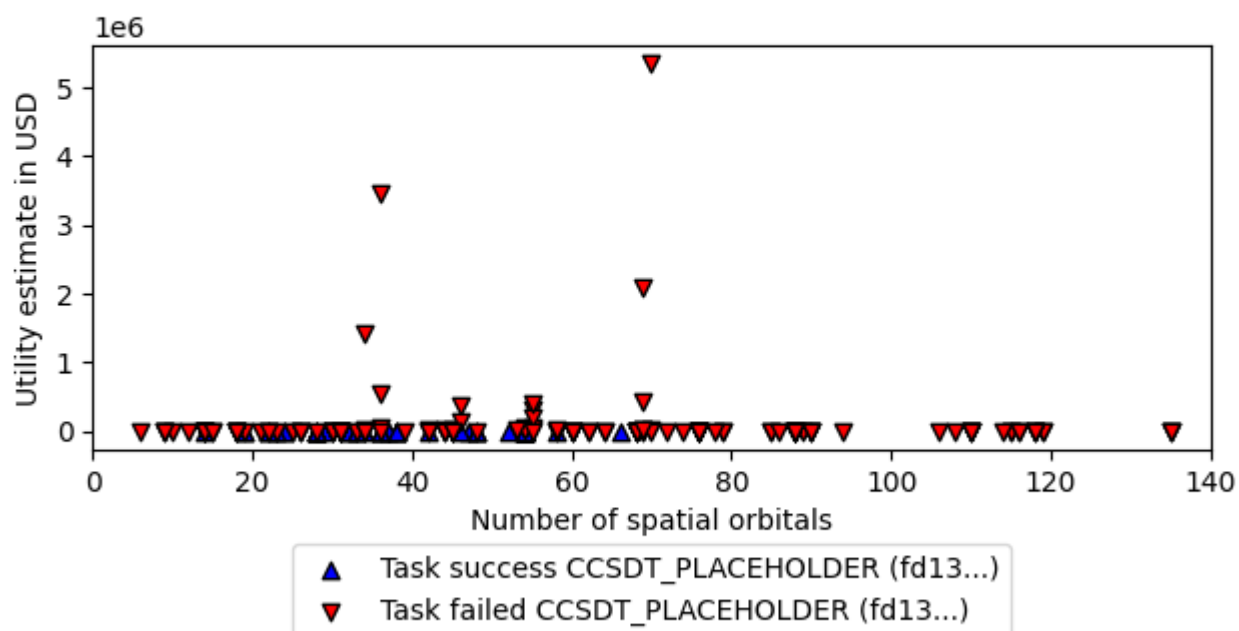
number\_of\_problem\_instances\_attempted: 4

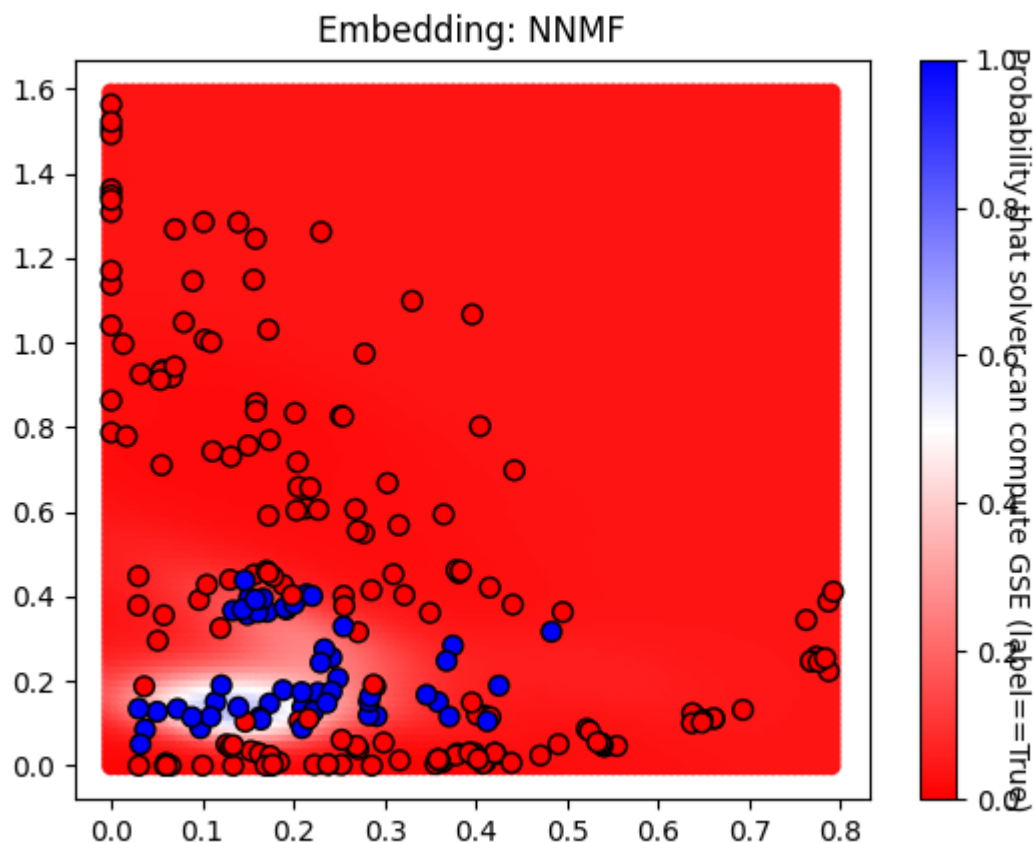
number\_of\_problem\_instances\_solved: 4  
number\_of\_tasks: 230  
number\_of\_tasks\_attempted: 53  
number\_of\_tasks\_solved: 53  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 53  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 53  
max\_run\_time\_of\_attempted\_tasks: 3600.0  
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%)





SHAP summary plot

## **Solver CISC, 418f060e-496b-4024-8d2d-9b1f8791e76d**

solver\_uuid:418f060e-496b-4024-8d2d-9b1f8791e76d

solver\_short\_name:CISC

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:CISC

software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: 9ba7b981-3ffe-470f-8a38-ff2f0694e6ac

creation\_timestamp: 2025-01-16T15:18:34.432203+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

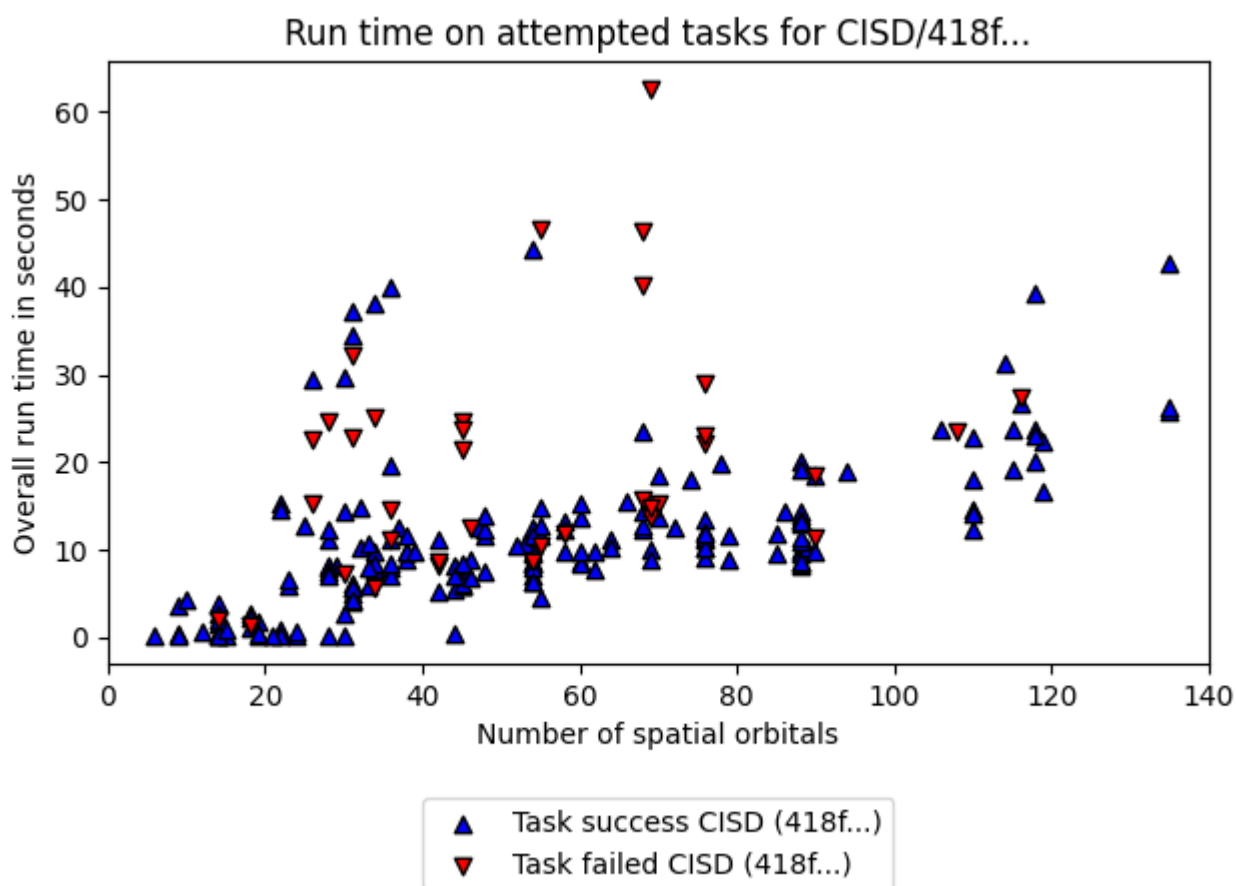
max\_run\_time\_of\_attempted\_tasks: 62.58296537399292

sum\_of\_run\_time\_of\_attempted\_tasks: 2895.8530027866364

solvability\_ratio: 0.9958

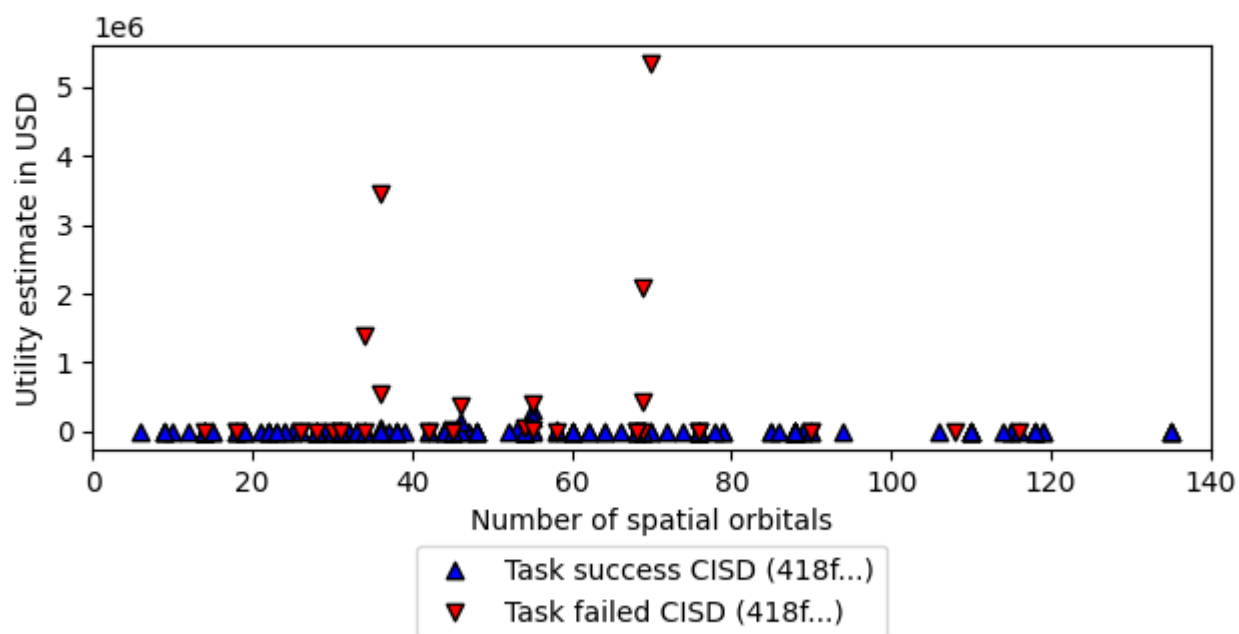
f1\_score: [0.8131868131868132, 0.9539295392953929]

ml\_metrics\_calculator\_version: 1

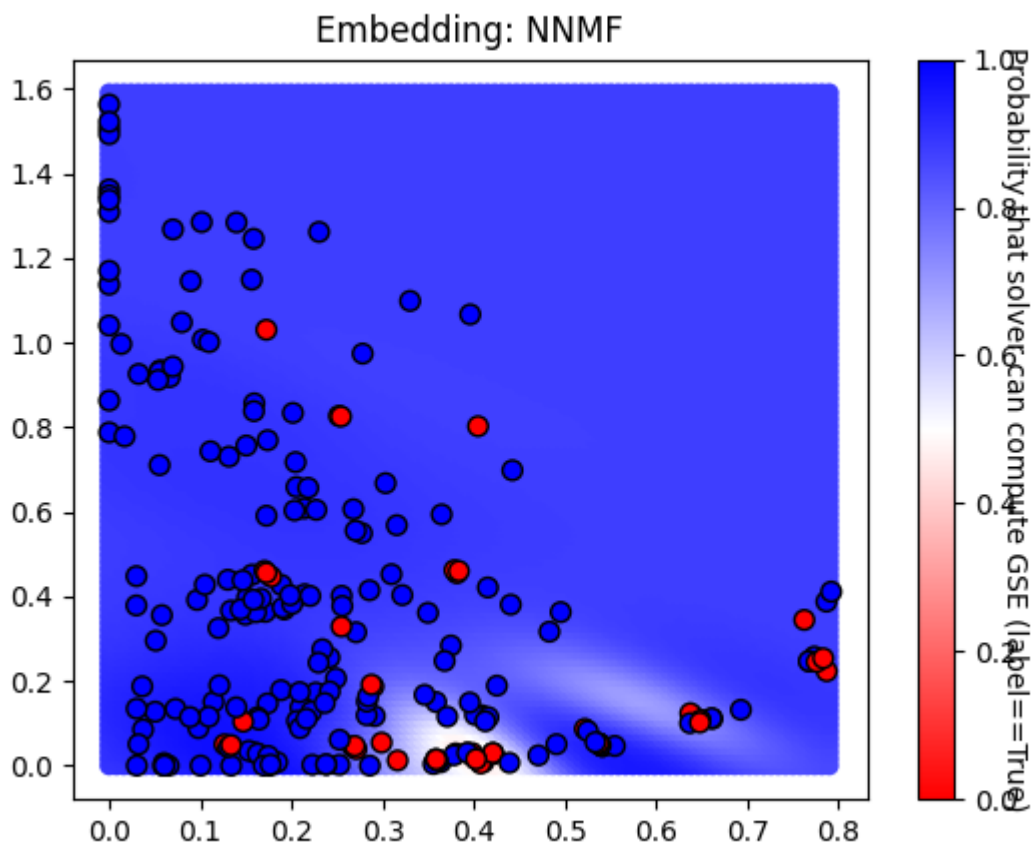


### Utility capture from CISD/418f...

(captured:  $\$8.2\text{e}+05/1.5\text{e}+07$ , approximately  $5.5\text{e}+00\%$ )







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: 54efd6d0-ed1b-4061-ac99-19c39a4ed4a0

creation\_timestamp: 2025-01-16T15:18:34.432203+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

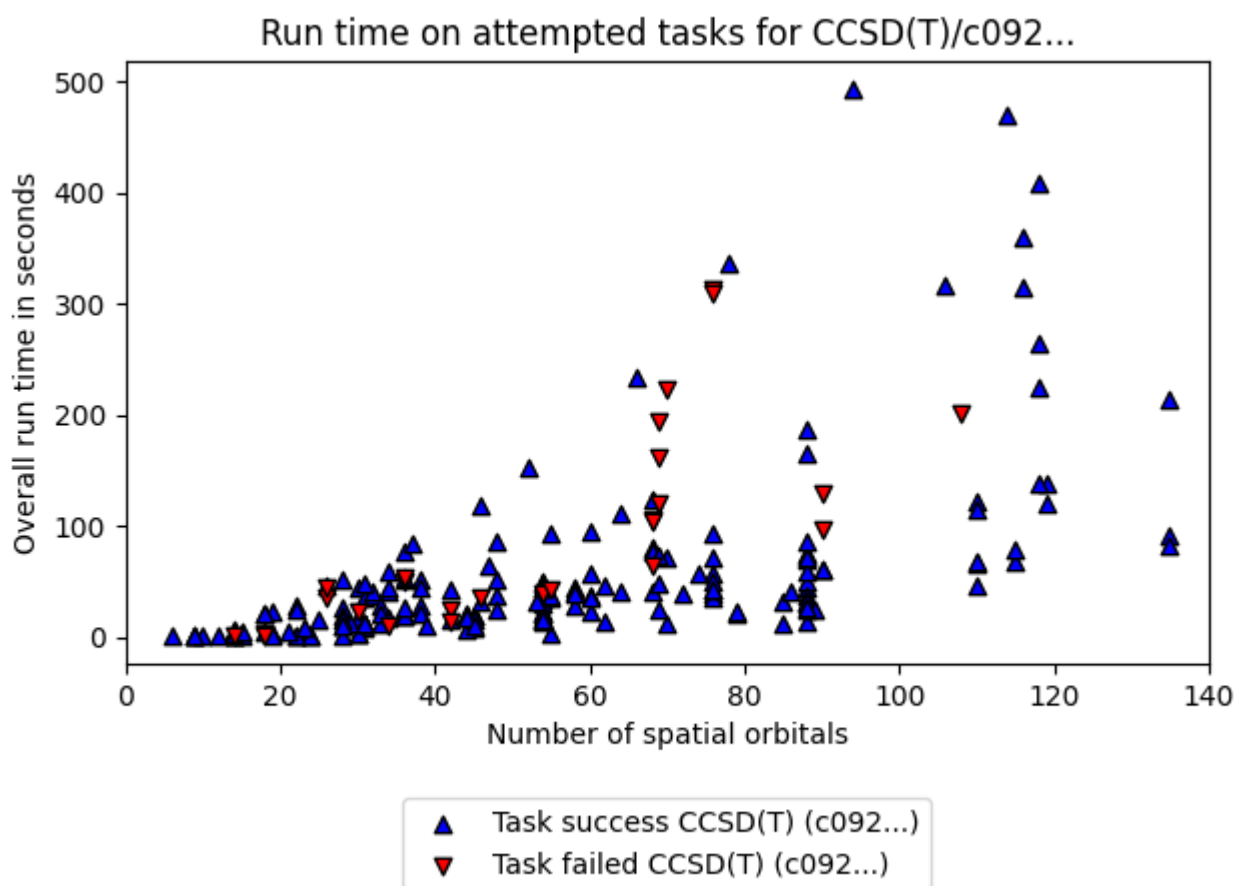
max\_run\_time\_of\_attempted\_tasks: 493.4080808162689

sum\_of\_run\_time\_of\_attempted\_tasks: 12968.4871737957

solvability\_ratio: 1.0

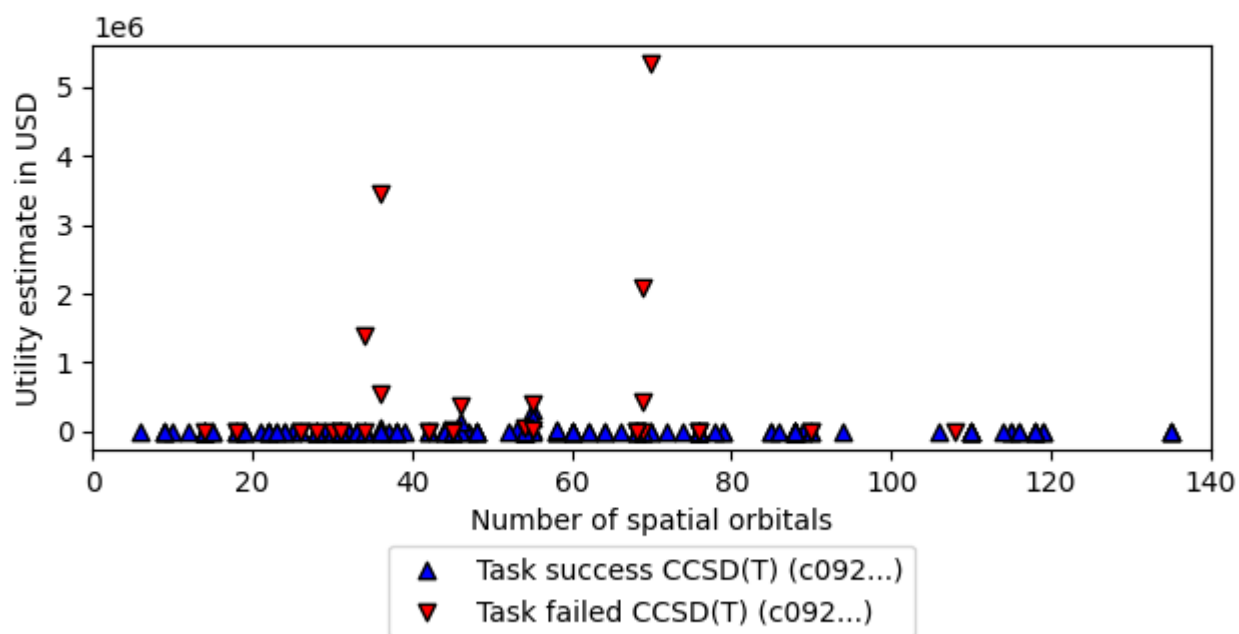
f1\_score: [0.0, 0.9176470588235294]

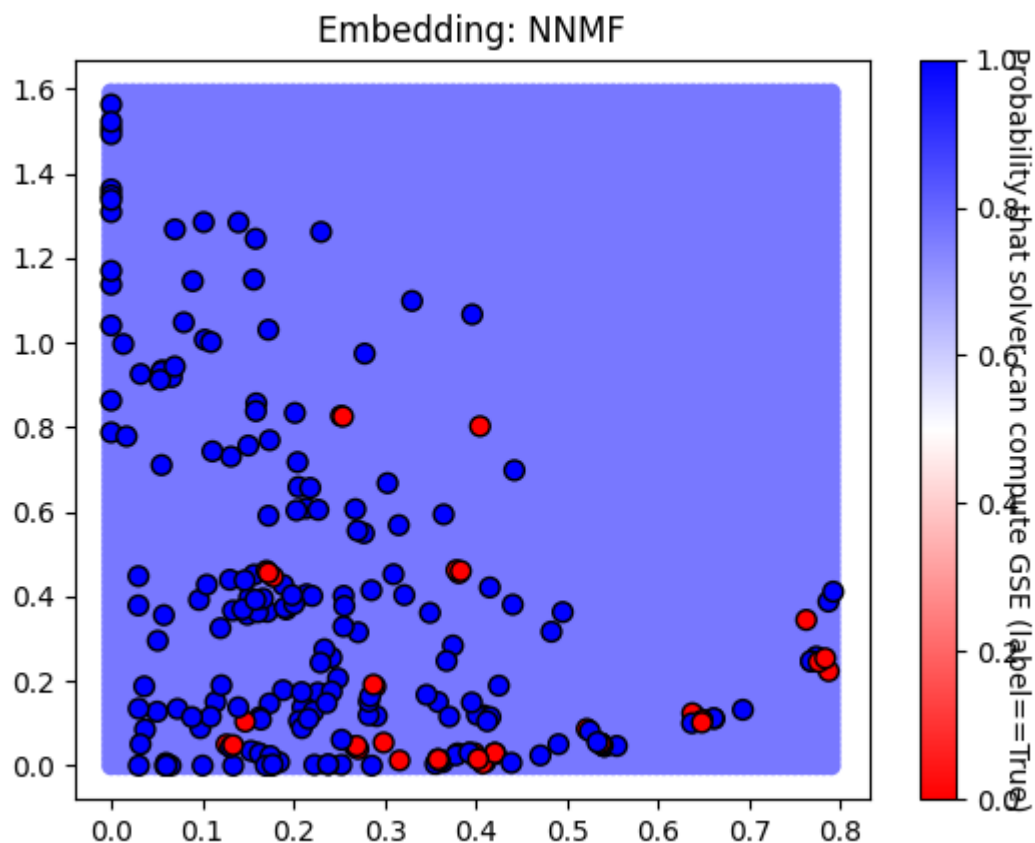
ml\_metrics\_calculator\_version: 1



### Utility capture from CCSD(T)/c092...

(captured:  $\$8.2\text{e}+05/1.5\text{e}+07$ , approximately  $5.5\text{e}+00\%$ )





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

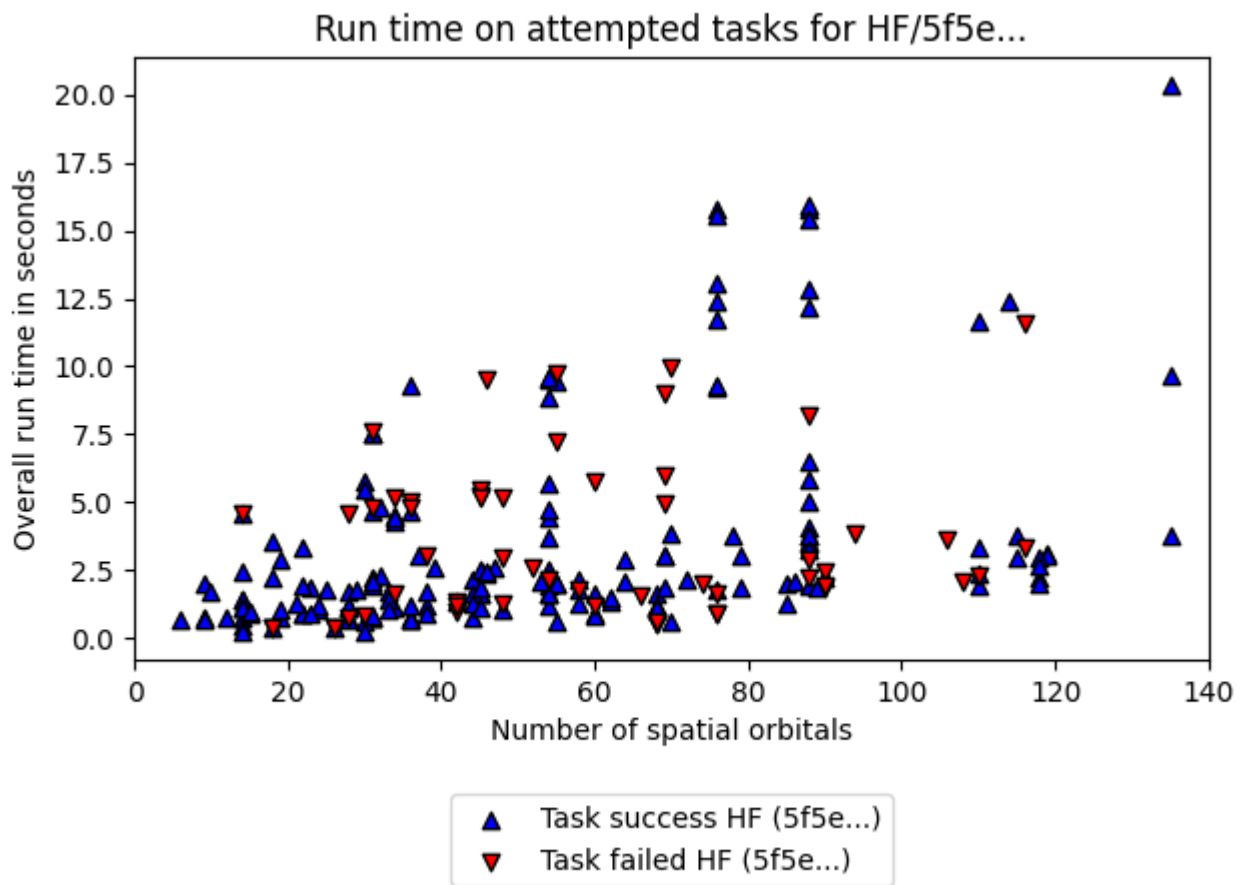
software\_details:pyscf (<https://github.com/pyscf/pyscf>).

performance\_metrics\_uuid: b667fdad-6c7a-4dd4-a68d-f034b11cce1f

creation\_timestamp: 2025-01-16T15:18:34.432203+00:00

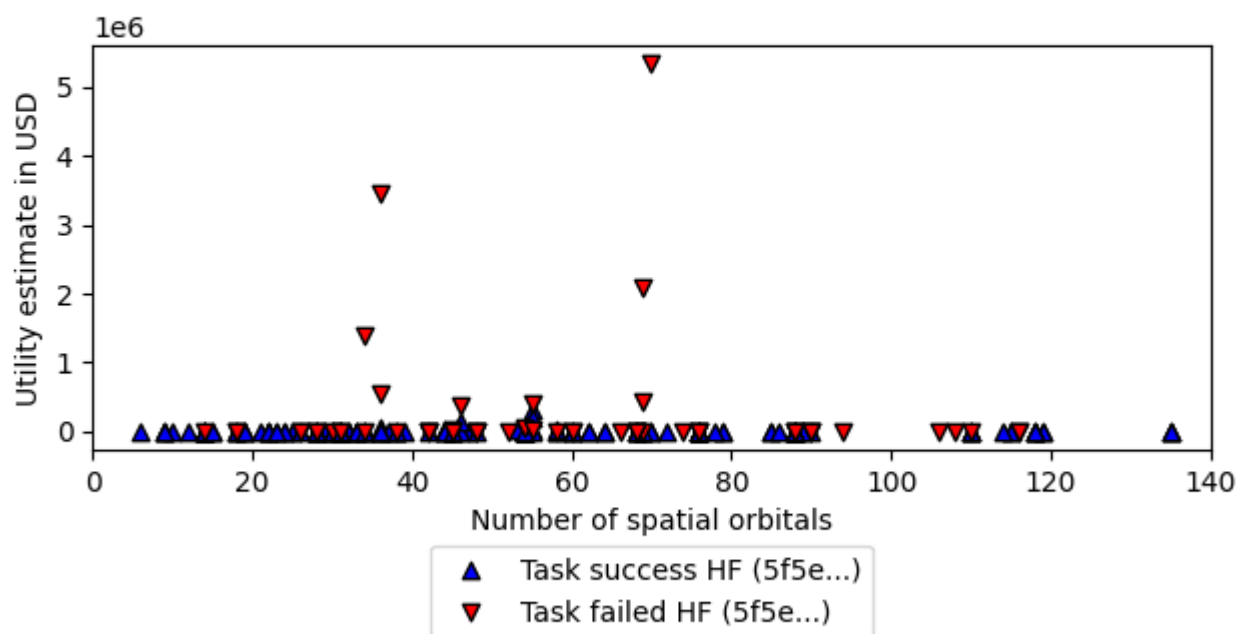
number\_of\_problem\_instances: 82

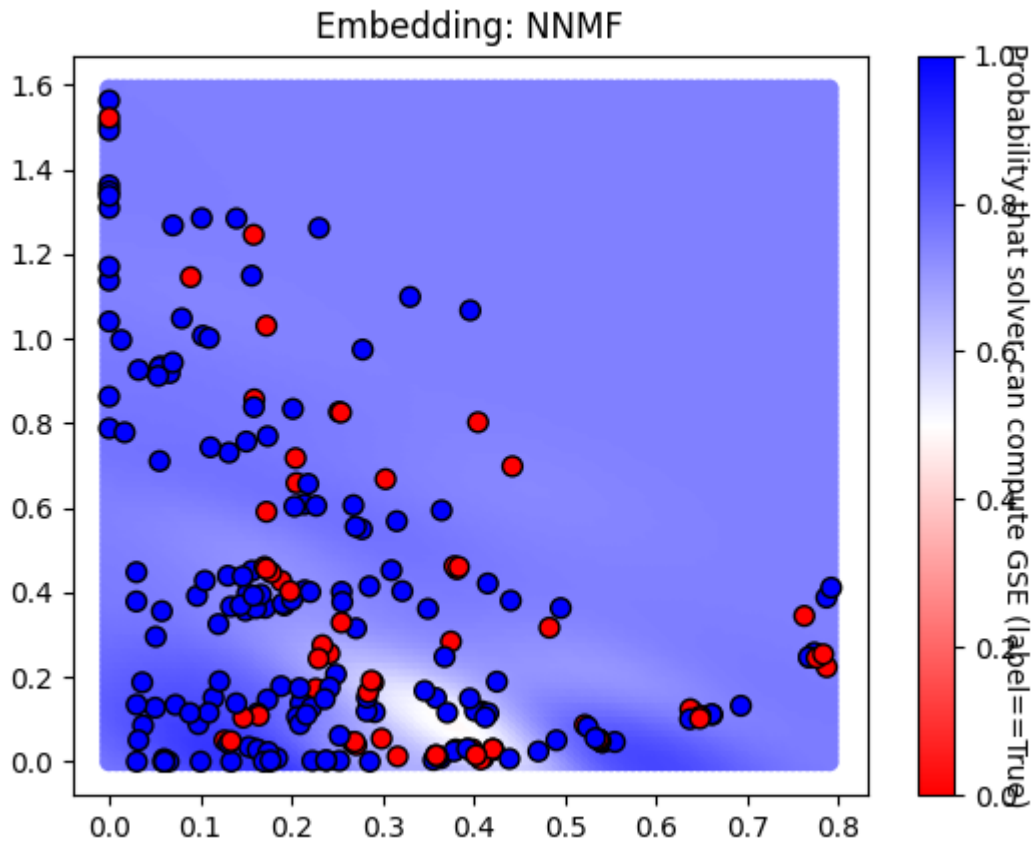
number\_of\_problem\_instances\_attempted: 82  
number\_of\_problem\_instances\_solved: 56  
number\_of\_tasks: 230  
number\_of\_tasks\_attempted: 230  
number\_of\_tasks\_solved: 174  
number\_of\_tasks\_solved\_within\_run\_time\_limit: 230  
number\_of\_tasks\_solved\_within\_accuracy\_threshold: 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:  $\$8.2\text{e}+05/1.5\text{e}+07$ , approximately  $5.5\text{e}+00\%$ )





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: 10960846-c7e8-4eb1-9656-574dc577aa2c

creation\_timestamp: 2025-01-16T15:18:34.432203+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

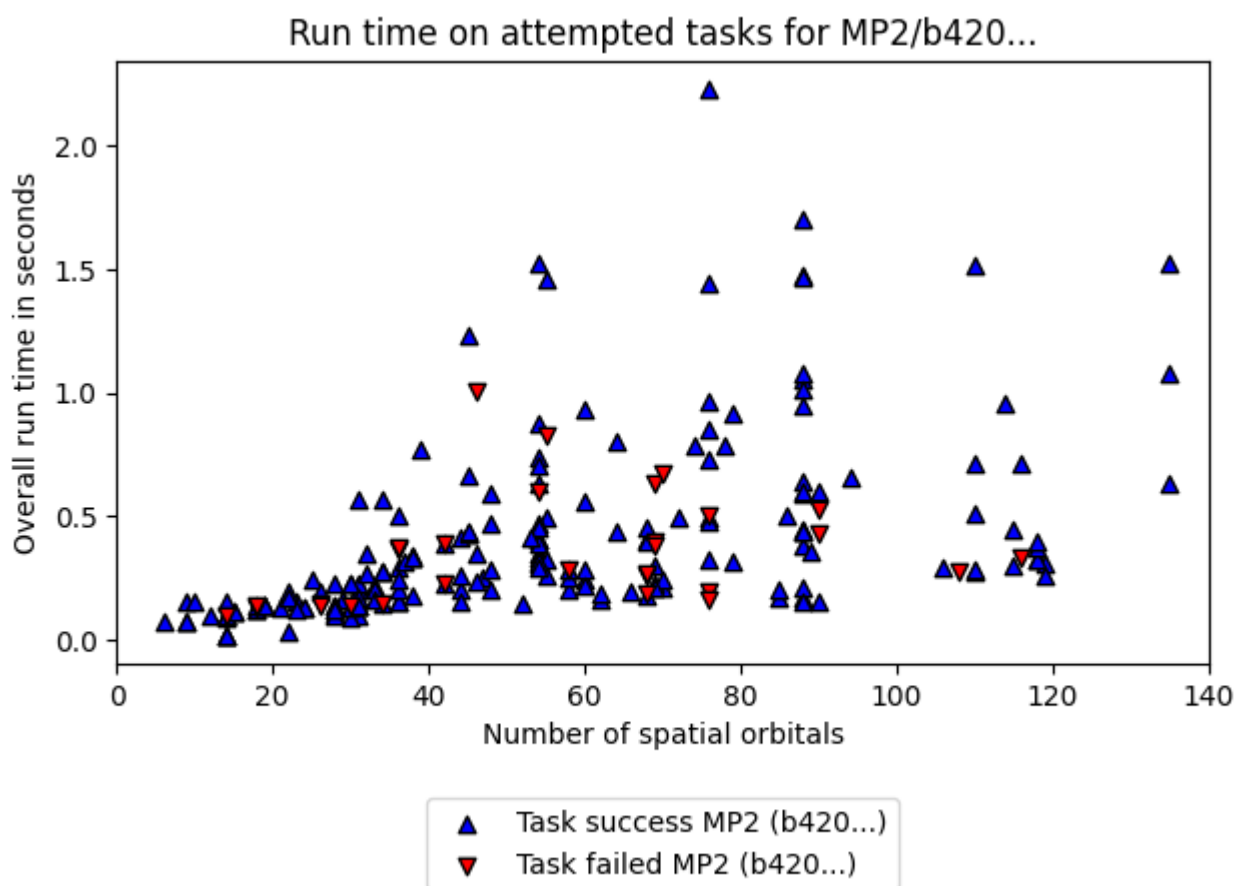
max\_run\_time\_of\_attempted\_tasks: 2.230440139770508

sum\_of\_run\_time\_of\_attempted\_tasks: 87.6544258594513

solvability\_ratio: 0.9958

f1\_score: [0.8131868131868132, 0.9539295392953929]

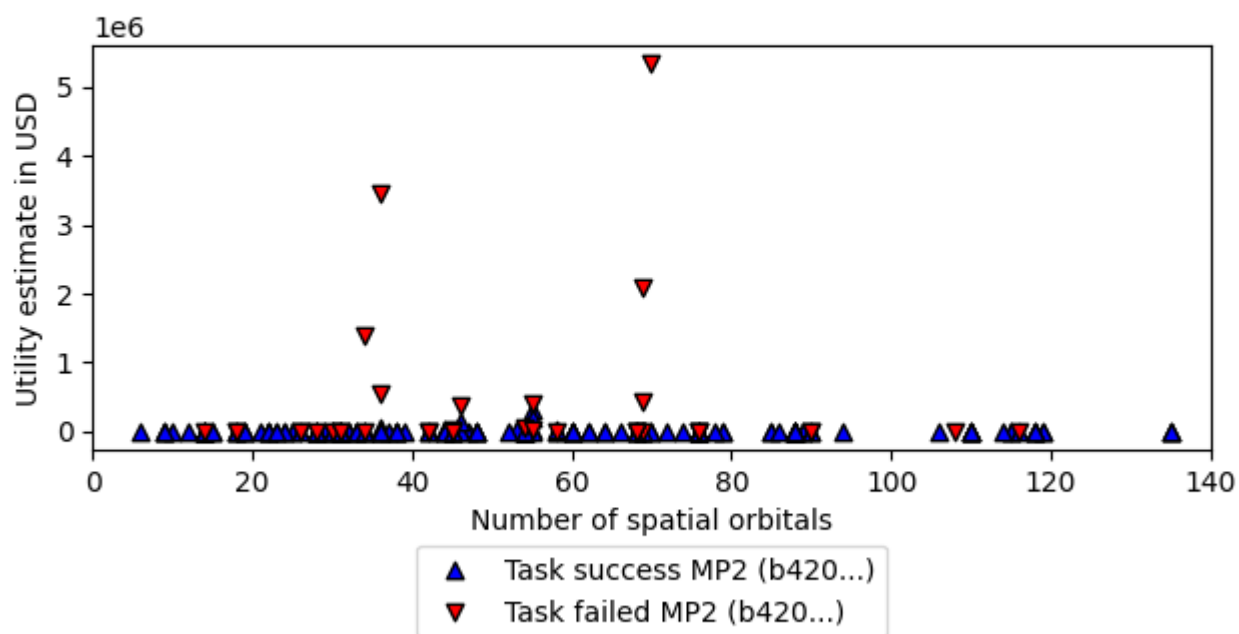
ml\_metrics\_calculator\_version: 1

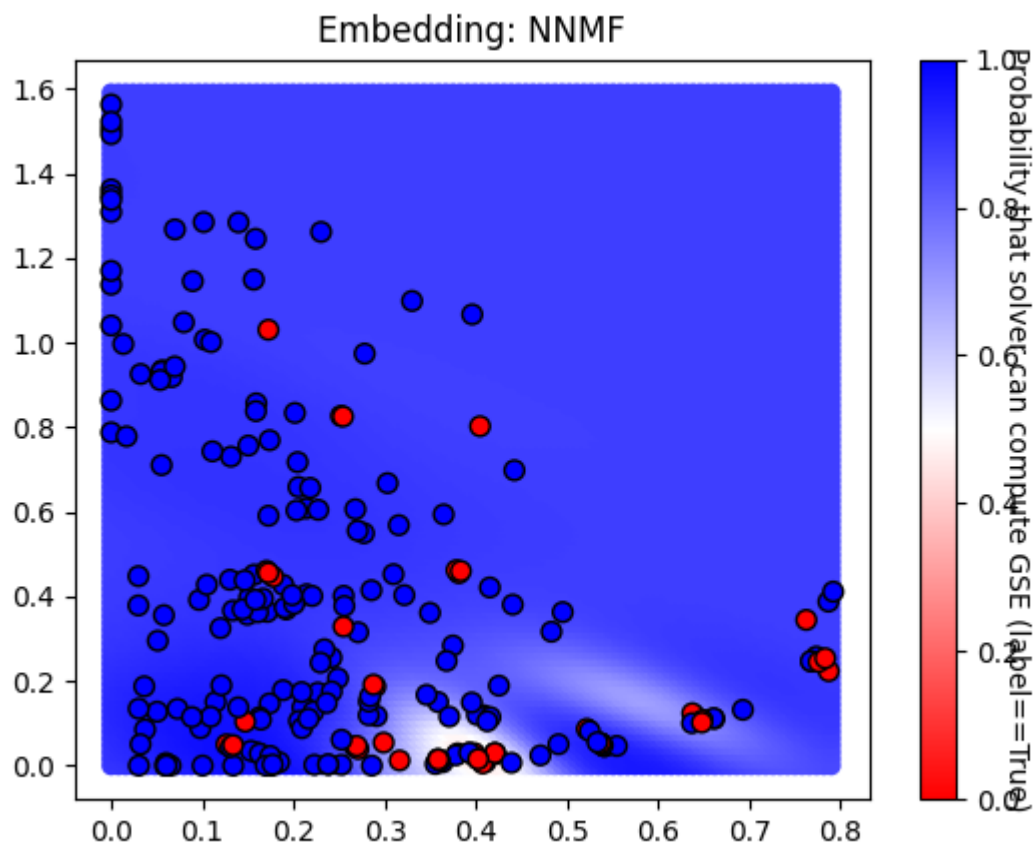




### Utility capture from MP2/b420...

(captured:  $\$8.2\text{e}+05/1.5\text{e}+07$ , approximately  $5.5\text{e}+00\%$ )





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: f6c3d5d5-2f7f-4521-bc89-ae3d3cd1283b

creation\_timestamp: 2025-01-16T15:18:34.432203+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

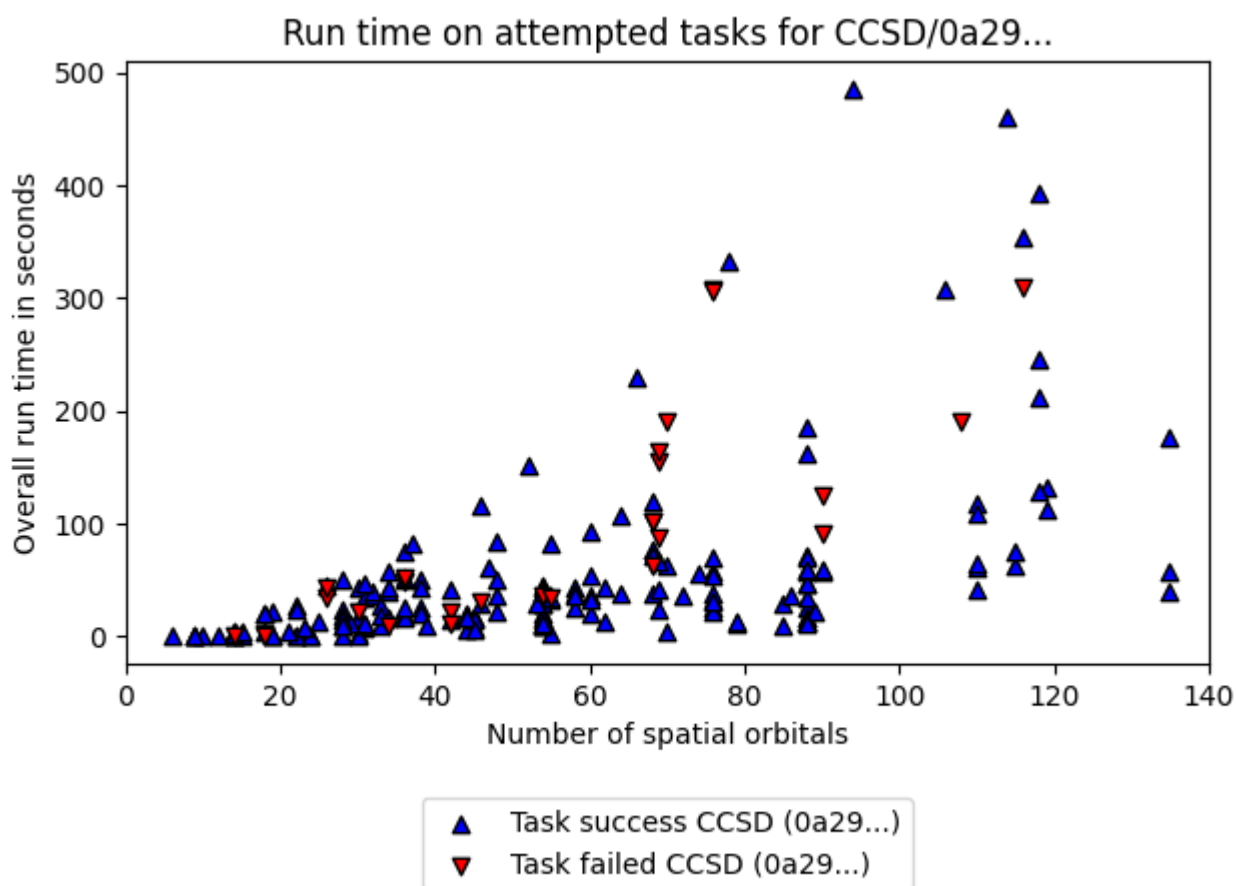
max\_run\_time\_of\_attempted\_tasks: 485.1982181072235

sum\_of\_run\_time\_of\_attempted\_tasks: 12029.76450586319

solvability\_ratio: 1.0

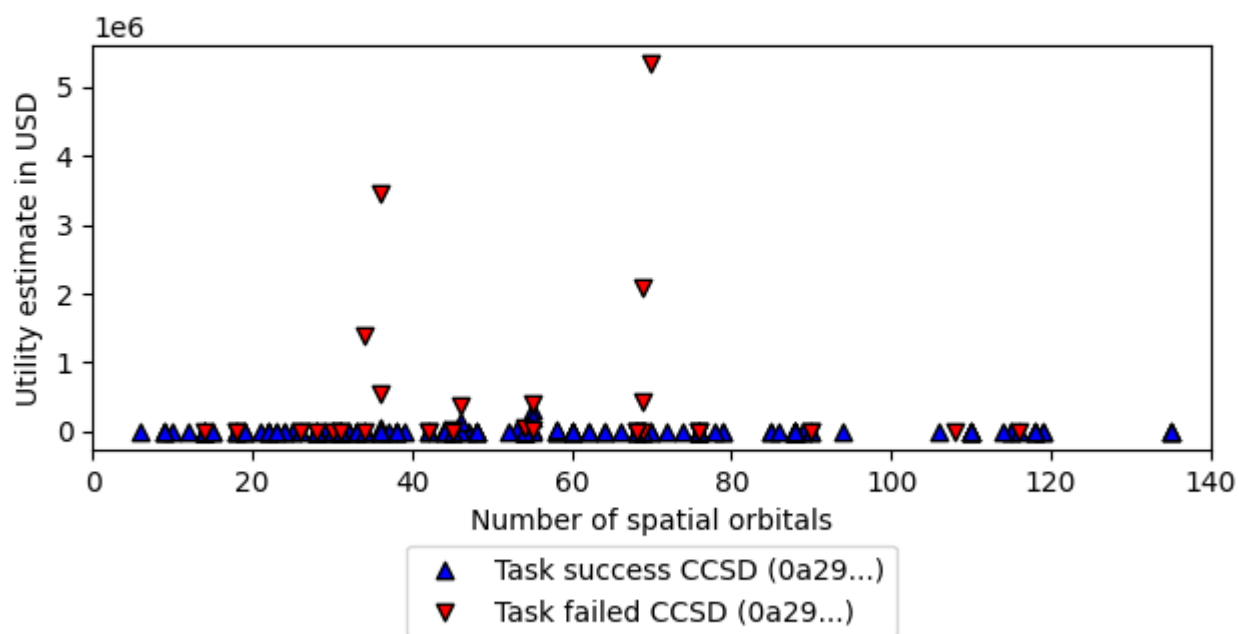
f1\_score: [0.2706766917293233, 0.0]

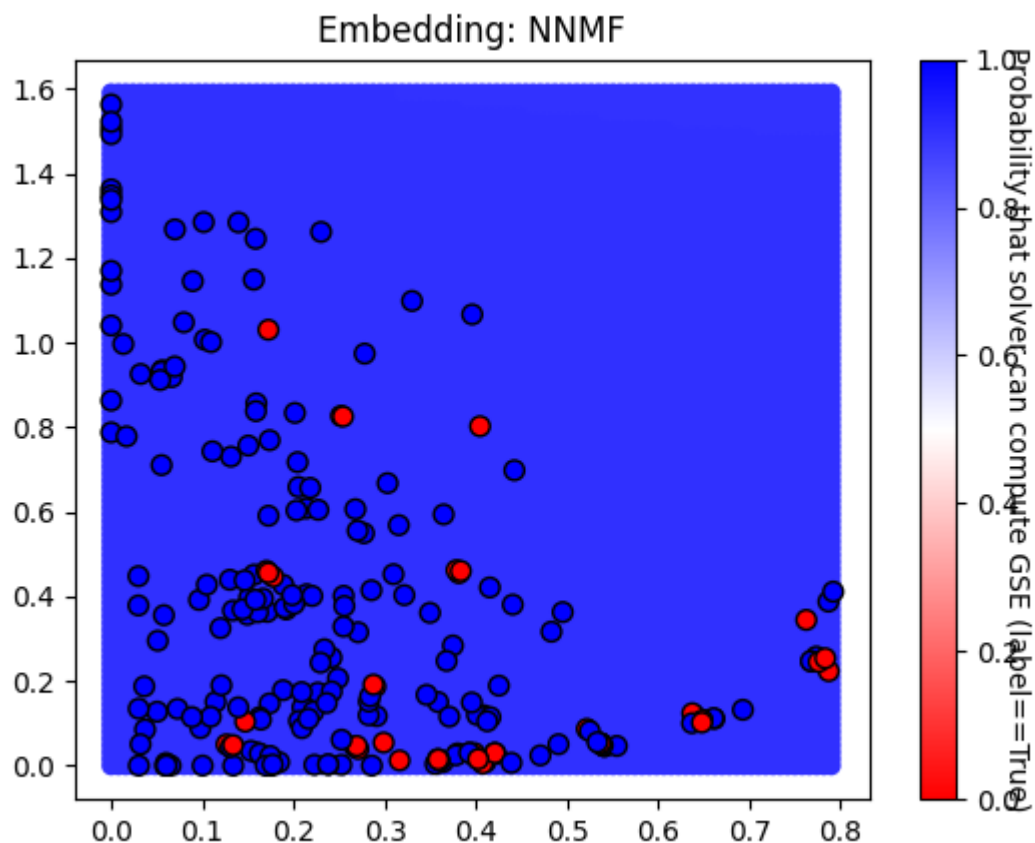
ml\_metrics\_calculator\_version: 1



### Utility capture from CCSD/0a29...

(captured:  $\$8.2\text{e}+05/1.5\text{e}+07$ , approximately  $5.5\text{e}+00\%$ )





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: 6519cb8c-a800-44a0-a218-018eec132eca

creation\_timestamp: 2025-01-16T15:18:34.432203+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

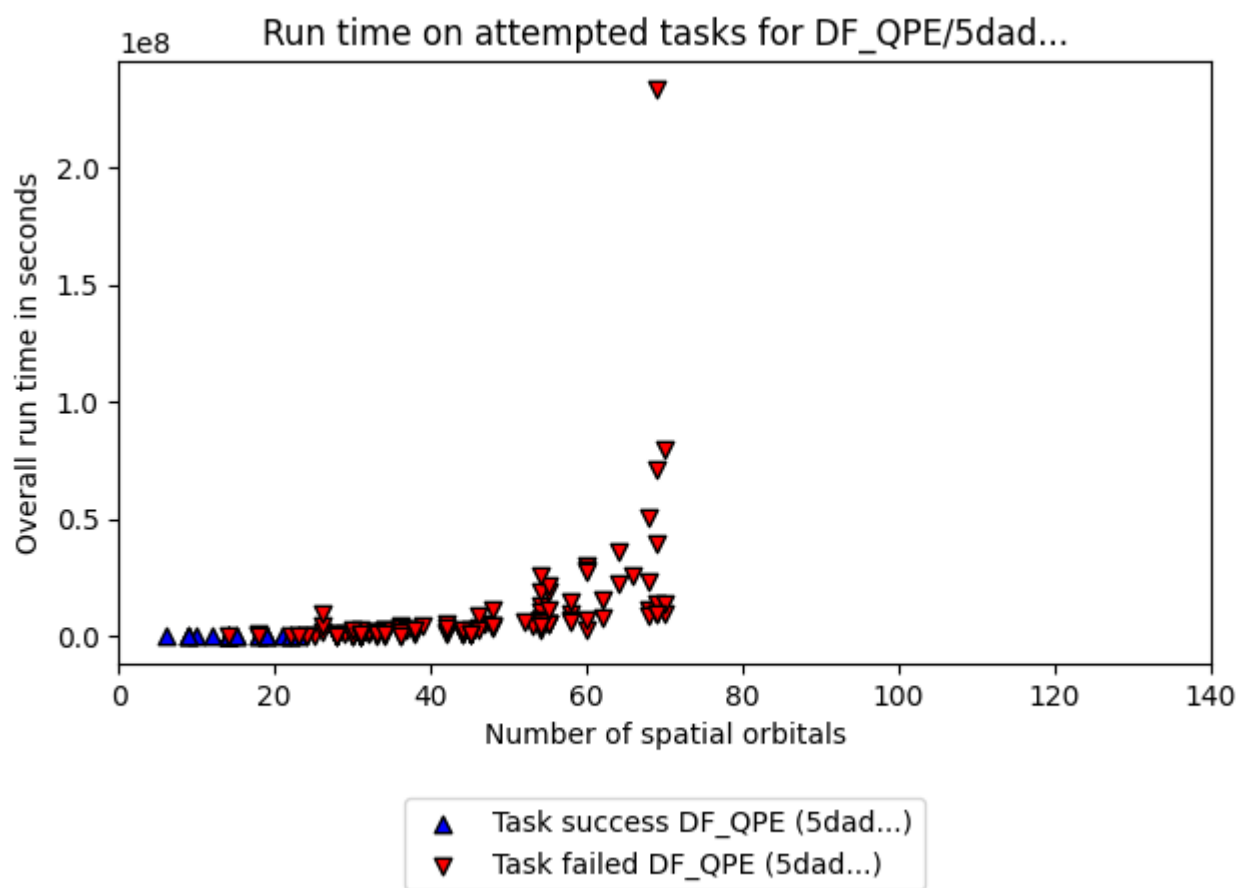
max\_run\_time\_of\_attempted\_tasks: 233737829.40462503

sum\_of\_run\_time\_of\_attempted\_tasks: 1180589418.3385448

solvability\_ratio: 0.0232

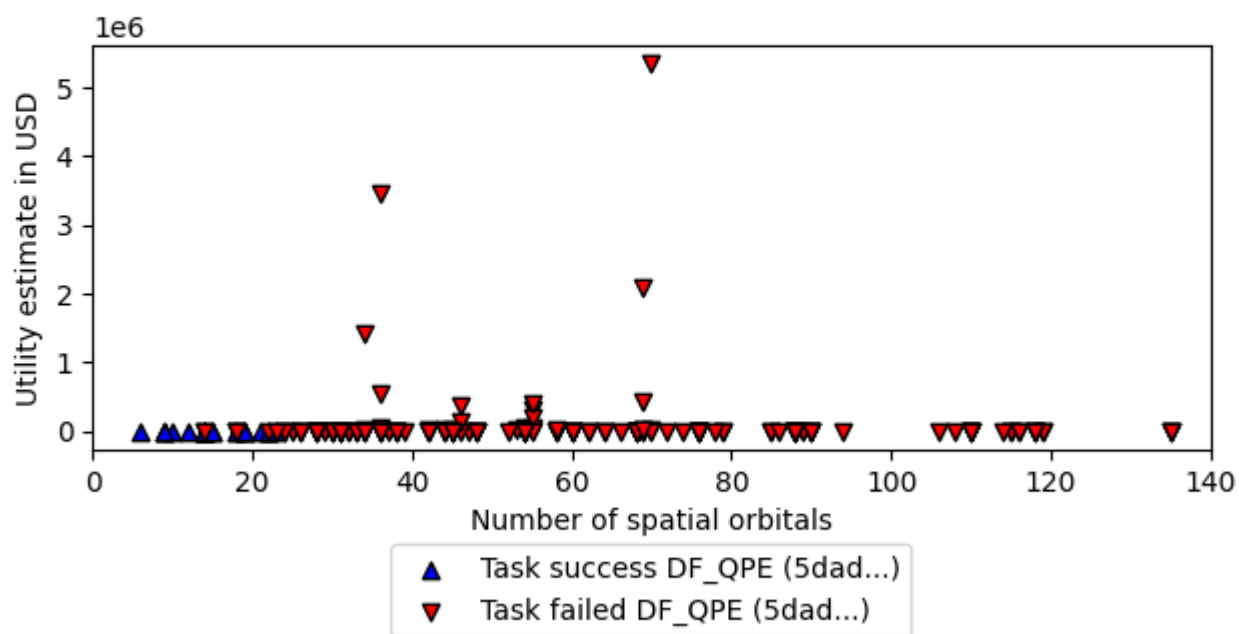
f1\_score: [0.9950738916256158, 0.9629629629629629]

ml\_metrics\_calculator\_version: 1

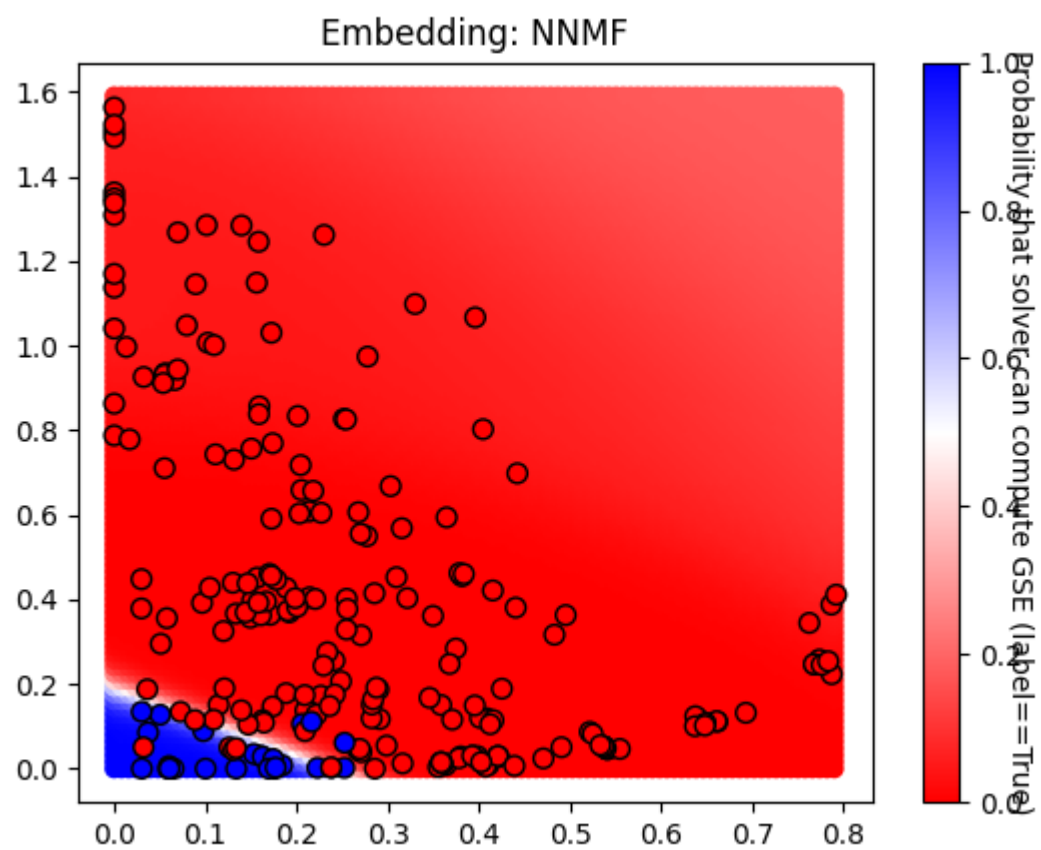


# Utility capture from DF\_QPE/5dad...

(captured:  $\$7.8\text{e-}01/1.5\text{e+}07$ , approximately  $5.2\text{e-}06\%$ )







SHAP summary plot