

Figure A.1: Relative differences in the algorithm training times between the standalone and integrated implementations of the SO-MCTS.

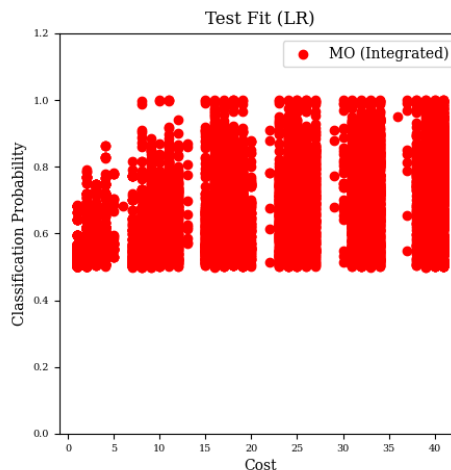


Figure A.2: Solutions for the MO-MCTS integrated implementation with the logistic regression classifier and fit strategy for the Heart Failure data set.

## A Experiments

### A.1 Experimental Results

#### Comparison of the Standalone and Integrated Implementations

The F1 AUCs of the SO-MCTS integrated implementation shows relative improvement of 4.6% and 1.8% for the logistic regression and neural network classifiers from the SO-MCTS standalone implementation. Solutions in the objective space do not show differences between the two implementations. In Figure A.1, we show the relative difference in the algorithm training times for the standalone implementation from the integrated implementation, where the standalone implementation has faster relative algorithm training times by 8.3% and 24.7% from the integrated implementation. When the algorithm training time is another constraint in the usage of the MCTS algorithm for feature acquisition, it is advantageous to use the standalone implementation with lower training times if there is an option of slightly higher AUC.

#### Comparison of the Classifier Strategies

For the Heart Failure, Coronary Heart Disease, and PhysioNet data sets, we use the fit strategy, where each subset of the feature set is used to train a single classifier. In comparison to the fit strategy, the best performing strategies with the SO-MCTS integrated implementation show relative performance improvements of 4.1% to 24.2%. For the MO-MCTS integrated implementation, the best performing strategies show relative improvements of 2.4% and 31.4%. We also plot the MO-MCTS solutions for the Heart Failure data set in the objective space in Figure A.2 for the logistic regression classifier with the fit strategy. In comparing the MO-MCTS solutions with the pretrain strategy, we observe that the solutions for the fit strategy are concentrated in the lower classification probability regions for all costs in Figure A.2. Thus, in the case when we use the MO-MCTS implementation for tight budget situations, it is also advantageous to use the fit strategy, as

solutions can be obtained for lower costs with slight decreases in confidence thresholds.

#### Comparison of the Strategies for the Unacquired Continuous Feature Values

As described in a previous section, we also optimize a function strategy for unacquired continuous feature values in the classifiers. The optimized hyperparameters are provided in the Appendix B.2. For the logistic regression classifiers, the quadratic cost function strategy has the highest train F1 AUCs for the Heart Failure, Coronary Heart Disease and PhysioNet data sets. For the neural network classifiers, the quadratic cost function strategy has the highest train F1 AUCs for the Heart Failure data set and constant function of 0 for the Coronary Heart Disease and PhysioNet data sets. Thus, it is advantageous to use the quadratic cost function strategies to set the values of unacquired continuous features.

## B Experimental Setup

### B.1 Network Architectures

The same network architectures are used for the neural network and convolutional neural network classifiers and policy and value networks in the algorithms, Table B.1 and B.2.

### B.2 Algorithm Hyperparameters

The algorithm hyperparameters are presented in Tables B.3-B.6.

### B.3 Continuous Unacquired Feature Values

We fitted four functions with quadratic maximum at 0 cost, quadratic minimum at full cost, linear, and constant. The choices are shown in Tables B.7-B.9.

Hyperparameter	Heart Failure	Coronary Heart Disease	PhysioNet
Feedforward1 Units	32	512	256
Activation	ReLU	ReLU	ReLU
Feedforward2 Units	16	256	128
Activation	ReLU	ReLU	ReLU
Feedforward3 Units	8	128	64
Activation	ReLU	ReLU	ReLU

Table B.1: Neural network architectures for classification and policy and value networks in the algorithms.

Layer	Hyperparameter	Value
Conv1	Filters	64
	Kernel	3
	Dilation	2
Activation	–	ReLU
Max Pooling	Pool	2
	Filters	128
Conv2	Kernel	3
	Dilation	2
	Activation	–
Max Pooling	Pool	2
	Filters	256
Conv3	Kernel	3
	Dilation	2
	Activation	–
Max Pooling	Pool	2
	Units	512

Table B.2: MNIST convolutional neural network architecture for classification and feature acquisition policy.

Hyperparameter	Heart Failure	Coronary Heart Disease	PhysioNet	MNIST
Number of simulations	100	100	100	100
$c$	1.0	1.0	1.0	1.0
Update frequency	18	20	36	100
Optimizer	Adam	Adam	Adam	Adam
Learning rate	$10^{-5}$	$10^{-5}$	$10^{-5}$	$10^{-5}$
Retrain frequency	54	180	324	10000

Table B.3: SO-MCTS hyperparameters.

Hyperparameter	Heart Failure	Coronary Heart Disease	PhysioNet	MNIST
Number of simulations	100	100	100	100
$c$	2.0	1.0	1.0	1.0
Update frequency	18	20	36	100
Optimizer	Adam	Adam	Adam	Adam
Learning rate	$10^{-5}$	$10^{-5}$	$10^{-5}$	$10^{-5}$
Retrain frequency	18	20	36	100

Table B.4: MO-MCTS hyperparameters.

Hyperparameter	Heart Failure	Coronary Heart Disease	PhysioNet	MNIST
Episodes	100	100	100	100
Batch size	6	20	18	25
Update frequency	6	20	18	25
$\gamma$	0.5	0.99	0.999	0.99
$\epsilon$ -decay	0.99	0.99	0.99	0.5
Learning rate	$10^{-6}$	$10^{-6}$	$10^{-6}$	$10^{-7}$
Optimizer	Adam	Adam	Adam	Adam
Retrain frequency	108	360	684	12000

Table B.5: DQN hyperparameters.

Hyperparameter	Heart Failure	Coronary Heart Disease	PhysioNet	MNIST
Episodes	100	100	100	100
Clip parameter	0.2	0.2	0.2	0.2
GAE parameter	0.95	0.95	0.95	0.95
Entropy coefficient	0.01	0.01	0.02	0.02
Value function coefficient	1.0	1.0	1.0	1.0
Learning rate	$10^{-5}$	$10^{-5}$	$10^{-5}$	$10^{-5}$
Optimizer	Adam	Adam	Adam	Adam
Retrain frequency	120	400	360	10000

Table B.6: PPO hyperparameters.

Algorithms	Unacquired Features (LR)	Unacquired Features (NN)
MO-MCTS Integrated	Quad Min at 41 with $-70$	Quad Min at 41 with $-70$
SO-MCTS Integrated	Quad Min at 41 with $-70$	Quad Min at 41 with $-70$
SO-MCTS Integrated	Quad Max at 0 with $-50$	Quad Min at 41 with $-50$
DQN	Quad Min at 41 with $-50$	Quad Min at 41 with $-70$
PPO-PG	Quad Max at 0 with $-70$	Quad Min at 41 with $-70$
PPO-AC	Quad Max at 0 with $-90$	Quad Min at 41 with $-70$

Table B.7: Heart Failure data set.

Algorithms	Unacquired Features (LR)	Unacquired Features (NN)
MO-MCTS Integrated	Quad Max at 0 with $-50$	0
SO-MCTS Integrated	Quad Min at 51 with $-70$	0
SO-MCTS Integrated	Quad Min at 51 with $-70$	0
DQN	Quad Max at 0 with $-10$	0
PPO-PG	Quad Min at 51 with $-20$	0
PPO-AC	Quad Max at 0 with $-90$	0

Table B.8: Coronary Heart Disease data set.

Algorithms	Unacquired Features (LR)	Unacquired Features (NN)
MO-MCTS Integrated	Quad Max at 0 with $-50$	0
SO-MCTS Integrated	Quad Min at 229 with $-70$	0
SO-MCTS Integrated	Quad Min at 229 with $-70$	0
DQN	Quad Min at 229 with $-60$	0
PPO-PG	Quad Min at 229 with $-60$	0
PPO-AC	Quad Min at 229 with $-60$	0

Table B.9: PhysioNet data set.

**Algorithm 1:** Single-objective Monte Carlo Tree Search Functions

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1 function MCTS( $v, I$ )
2   for iteration = 1, 2, ...,  $I$  do
3     train( $v$ )
4   end for

5 function train( $v$ )
6    $v_l = \text{select}(v)$ 
7   expand( $v_l$ )
8   reward = simulate( $v_l$ )
9   backprop( $v_l, \text{reward}$ )

10 function makeChild( $v, a$ )
11   Obtain the feature by  $a$  in  $s$  of  $v$  to set  $s'$ 
12   Create node  $v'$  with  $s'$  where  $a(v') = a$ 
13   return  $v'$ 

14 function select( $v$ )
15   while True do
16     if  $v$  unexplored or terminal do
17       return  $v$ 
18     end if
19      $v \leftarrow \arg \max_{v' \in C(v)} \frac{Q(v')}{N(v')} + c \sqrt{\frac{\ln N(v)}{N(v' )}}$ 
20   end while

21 function expand( $v$ )
22   for all unacquired actions  $a \in A(v)$  do
23      $v' \leftarrow \text{makeChild}(v, a)$ 
24     Add  $v'$  to  $C(v)$ 
25     Set  $a(v') = a$ 
26   end for

27 function simulate( $v$ )
28   reward = 0
29   while  $v$  not terminal do
30     Choose  $a \in A(v)$  uniformly at random
31      $v \leftarrow \text{make child}(v, a)$ 
32     reward +=  $Q(v)$ 
33   end while
34   return reward

35 function backprop( $v, \text{reward}$ )
36   while  $v$  not null do
37      $N(v) += 1$ 
38      $Q(v) += \text{reward}$ 
39      $v \leftarrow \text{parent of } v$ 
40   end while

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**Algorithm 2:** Multi-objective Monte Carlo Tree Search (Integrated)

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**Input :** Iteration number  $I$ , initial policy network weights  $\theta$ , policy network update frequency  $f$

- 1 Initialize policy network  $\phi$  with  $\theta$
- 2 Initialize list  $L$  of visited nodes and their  $R$  and visit counts  $N$
- 3 Initialize list  $M$  of global Pareto Front approximations  $P$
- 4  $i \leftarrow 0$

5 **function** **preprocess**( $L, M$ )

- 6 Make each node  $v$  in  $L$  to be distinct with non-dominated union for  $R(v)$  and  $N(v)$  for duplicates
- 7  $A = \vec{0}$
- 8  $S = v$  in  $L$
- 9 **for**  $v$  in  $L$  **do**
- 10     **for** action in  $A$  **do**
- 11         Find child nodes of  $v$  in  $L$
- 12         **for** node in child nodes **do**
- 13              $R(\text{node}) = [R(\text{node}), M]$
- 14              $A(\text{action}) \leftarrow A(\text{action}) + \mathbf{HV}(R(\text{node}))$
- 15         **end for**
- 16     **end for**
- 17 Normalize  $A$  with division by  $\max(A)$
- 18 **return**  $S, A$

19 **for** sample = 1, 2, ...,  $m$  **do**

- 20      $i \leftarrow i + 1$
- 21 Initialize state  $s_0$
- 22 Initialize global Pareto Front approximation  $P$
- 23 Create root node  $v_0$  with  $s_0$
- 24      $R(v_0)$ : local Pareto Front approximation
- 25      $N(v_0)$ : visit count of  $v_0$
- 26      $C(v_0)$ : children of  $v_0$
- 27      $a(v_0)$ : action of  $v_0$
- 28     **while**  $v_0$  not terminal **do**
- 29         **MO-MCTS**( $v_0, I$ )
- 30          $a \leftarrow \phi_\theta(s_0)$
- 31          $v_0 \leftarrow \mathbf{makeChild}(v_0, a)$
- 32     **end while**
- 33 Append  $R(v)$  and  $N(v)$  to  $L$
- 34  $M \leftarrow \mathbf{findGlobalP}(M, P)$
- 35 **if**  $f \% i == 0$  **do**
- 36      $S, A \leftarrow \mathbf{preprocess}(L, M)$
- 37     Train  $\phi_\theta$  on  $S$  and  $A$
- 38     **end if**
- 39 **end for**

40 **function** **MO-MCTS**( $v, I$ )

- 41     **for** iteration = 1, 2, ...,  $I$  **do**
- 42         **train**( $v$ )
- 43     **end for**

44 **function** **train**( $v$ )

- 45      $v_l = \mathbf{select}(v)$
- 46     **expand**( $v_l$ )
- 47     reward = **simulate**( $v_l$ )
- 48     **backprop**( $v_l, \text{reward}$ )

49 **function** **makeChild**( $v, a$ )

- 50     Obtain the feature by  $a$  in  $s$  of  $v$  to set  $s'$
- 51     Create node  $v'$  with  $s'$  where  $a(v') = a$
- 52     **return**  $v'$

53 **function** **HV**( $R(v)$ )

- 54     Set reference point at  $[-1.0, 0.0]$
- 55      $hv = 0$
- 56     **for** front in  $R(v)$  **do**
- 57          $h = \text{front}[i][0] - \text{reference}[0]$
- 58          $hv \leftarrow hv + (\text{front}[i][1] - \text{front}[i-1][1])h$
- 59     **return**  $hv$

60 **function** **select**( $v$ )

- 61     **while** True **do**
- 62         **if**  $v$  unexplored or terminal **do**
- 63             **return**  $v$
- 64         **end if**
- 65         **for**  $v' \in C(v)$  **do**
- 66              $R(v') \leftarrow \frac{R(v')}{N(v')} + c\sqrt{\frac{2\ln N(v)}{N(v')}}$
- 67              $v \leftarrow \arg \max_{v' \in C(v)} \mathbf{HV}(R(v'))$
- 68         **end while**

69 **function** **backprop**( $v, \text{reward}$ )

- 70     **while**  $v$  not null **do**
- 71          $N(v) \leftarrow N(v) + 1$
- 72          $R(v)[0] \leftarrow R(v)[0] + \text{reward}[0]$
- 73          $R(v)[1] \leftarrow R(v)[1] + \text{reward}[1]$
- 74          $P \leftarrow \mathbf{findGlobalP}(P, R(v'))$
- 75          $v \leftarrow \text{parent of } v$
- 76     **end while**

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