A Fast Branch-and-Bound Algorithm for U-Curve Feature Selection

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Abstract

We introduce a fast branch-and-bound algorithm for optimal feature selection based on a U-curve assumption for the cost function. The U-curve assumption, which is based on the peaking phenomenon of classification error, postulates that the cost over the chains of the Boolean lattice that represents the search space describe a U-shaped curve. The proposed algorithm is an improvement over the original algorithm for U-curve feature selection introduced recently. Extensive simulation experiments are carried out to assess the performance of the proposed algorithm (IUBB), and compare it to exhaustive search and the original algorithm (UBB). The results show that IUBB makes fewer evaluations and achieves better solutions under a fixed budget. We also show that IUBB is also quite robust with respect to a violation of the U-curve assumption. We propose and investigate the application of the IUBB algorithm in the design of imaging W-operators and in classification feature selection, using the average mean conditional entropy (MCE) as the cost function for the search.

Keywords: Branch-and-Bound Algorithm; Feature Selection; U-Curve Assumption; W-Operator Design.

1. Introduction

Feature selection is the problem of finding an optimal subset of a finite set of features that minimizes a cost function that is correlated to the classification error (e.g., the estimated classification error) [1]. Determining the optimal set of features can be a complicated task, since for a problem with n features, an exhaustive search requires considering all 2^n possible feature sets. The Cover-Campenhout theorem [2] stipulates that, to be guaranteed to find the optimal feature set, no algorithm can avoid the exponential complexity of exhaustive search, in a worst-case sense, unless there is extra information about the problem.

Algorithms have been proposed that use heuristics to attempt to find the optimal feature set in fewer evaluations than exhaustive search; among them are feature selection algorithms based on the well-known Branch-and-Bound (BB) paradigm for discrete and combinatorial optimization [3, 4]. A BB algorithm uses some property of the cost function, such as monotonicity, to accomplish a systematic enumeration of the features sets in the form of a *tree*. At each step of the algorithm, the tree is traversed (*Branch*) and the cost of the best feature set found until that step is recorded (*Bound*). If the cost of a node is smaller than the bound, its successor nodes are explored further and the bound is updated. Otherwise, the successors of that node can be safely discarded or *pruned*, by exploring the monotonicity of the cost. If the tree is organized in such a way that large sections

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of it can be pruned en masse, then the BB algorithm is successful. Different improvements have been proposed to enhance the performance of the basic BB algorithm [5]. Yu and Yuan [6] suggest avoiding the evaluation of intermediate single-branching nodes by obtaining a "minimum search tree." Also ordering the nodes in the tree based on the significance of the features is used in some of the variants of the BB algorithm [5]. In addition, to minimize the number of cost evaluations, some algorithms use analytical properties of the search space [7].

It is well-known that the optimal classification error is monotonically nonincreasing with an increasing the number of features [8], making it a perfect candidate for a cost function for a BB algorithm. However, the optimal classifier and optimal classification error are rarely known in practice, and the criterion used is typically the classification error for a classifier designed using sample data, which does not generally decrease monotonically. Rather, increasing the number of features used to design the classifier, with a fixed sample size, generally makes the expected error of the designed classifier decrease and then increase. This is known as the *peaking phenomenon*, which was first studied in [9].

Figures 1(a) and (b) show the peaking phenomenon for the Linear Discriminant Analysis (LDA) classification rule. In Figure 1(a) the features are slightly correlated. In this case, peaking occurs earlier (i.e., for a smaller number of features) or later depending on the sample size. For example, for sample size 30, peaking occurs with about 6 features, but when samples size increases to 100, peaking occurs at a larger feature size. In Figure 1(b) the features are highly correlated. As we see in this case, even for a large sample size, peaking occurs early.

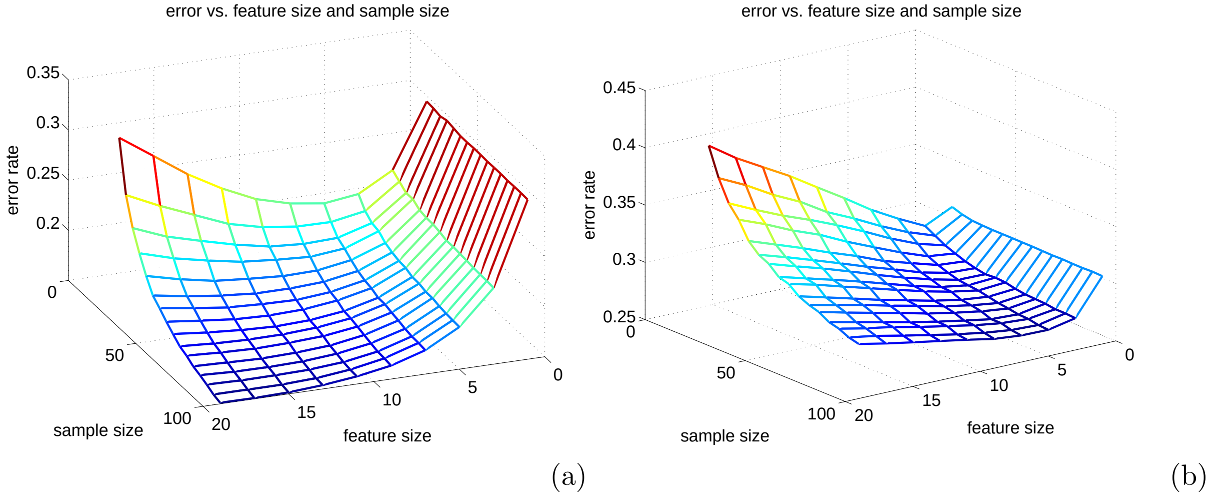


Figure 1: Peaking phenomenon. (a) Slightly correlated features. $\rho = 0.125$. (b) Highly correlated features. $\rho = 0.5$. Reproduced from [10].

Due to the peaking phenomenon, the error of the designed classifier (as opposed to the optimal classification error) is likely to display a U-shaped behavior along a chain of increasing nested feature sets. Thus, it is reasonable to make the assumption that all the chains of the Boolean lattice that represents the search space have a U-shaped behavior (U-curve assumption). The U-curve assumption was used by Ris and colleagues to formulate the *U-curve* optimization problem, which in turn can be employed to model the feature selection step of classifier design [11]. To solve this problem, the original BB algorithm, or its variants mentioned previously, are not suitable, as all of these algorithms assume that the cost function is monotone. Hence, the solution found by these algorithms will not necessarily be the globally best possible feature set. A feature selection algorithm based on a U-shaped cost function was proposed in [11]. They also presented some principles for a branch-and-bound procedure to tackle the U-curve problem, which were developed by Reis into the U-curve Branch-and-Bound (UBB) algorithm [12].

The purpose of this paper is to propose and evaluate a branch-and-bound algorithm for the U-curve optimization problem, which outperforms the original UBB algorithm, and propose its application in the design of imaging W-operators, as well as feature selection for classifier design. Section 2 presents a formal description of the U-curve optimization problem and also reviews the UBB algorithm. In Section 3, we introduce the Improved UBB (IUBB) algorithm, a fast method to solve the U-curve optimization problem that has two main innovations in relation to the original UBB algorithm: an iterative updating of optimal chains and the usage of bisection to find chain minima. In Section 4, we introduce a model for the U-curve feature selection problem and employ it as a synthetic benchmark to assess the performance of the IUBB algorithm, as well as compare it to the origina UBB algorithm; the case where the U-curve assumption is also investigated. Section 5 considers the application of the IUBB algorithm in the design of imaging W-operators using the average mean conditional entropy (MCE) as the cost function for the search. Section 6 assesses the performance of the IUBB algorithm in an actual classification problem using synthetic data. In all our experiments, we have observed that IUBB displays a qualitative superior performance to the original UBB algorithm. This and other conclusions and directions for future research are discussed in Section 7.

2. U-curve Branch and Bound Algorithm

In this section, we introduce the U-curve optimization problem formally, and review the UBB algorithm. Let S be a set of features, and let $\mathcal{P}(S)$ denote the set of all possible feature sets.

Definition 2.0.1 (Chain). *A chain is a collection of feature sets $\mathcal{F} = \{F_1, F_2, ..., F_k\} \subseteq \mathcal{P}(S)$, such that $F_1 \subseteq F_2 \subseteq ... \subseteq F_k$.*

Definition 2.0.2 (U-shaped curve). *Let $\mathcal{F} \subseteq \mathcal{P}(S)$ be a chain. A function $f : \mathcal{F} \to \mathbb{R}$ describes a U-shaped curve if $F_1 \subseteq F_2 \subseteq F_3$ implies that $f(F_2) \leq \max\{f(F_1), f(F_3)\}$, for $F_1, F_2, F_3 \in \mathcal{F}$.*

Definition 2.0.3 (Decomposability in U-shaped curves). *A cost function $c : \mathcal{P}(S) \to \mathbb{R}$ is decomposable in U-shaped curves if, for each chain $\mathcal{F} \subseteq \mathcal{P}(S)$, the restriction of c to $\mathcal{F}$ describes a U-shaped curve.*

Definition 2.0.4 (Minimum cost). *Let $F^* \in \mathcal{F} \subseteq \mathcal{P}(S)$ and let c be a cost function defined on $\mathcal{P}(S)$. If there does not exist another feature set $F \in \mathcal{F}$ such that $c(F) < c(F^*)$, then F^* is of minimum cost in $\mathcal{F}$. If $\mathcal{F} = \mathcal{P}(S)$, then we say that F^* is of minimum cost.*

Definition 2.0.5 (U-curve problem). *Given a cost function $c : \mathcal{P}(S) \to \mathbb{R}$ that is decomposable in U-shaped curves, find a feature set $F^* \in \mathcal{P}(S)$ of minimum cost.*

The previous definitions are illustrated in Figure 2. Part (a) displays a Boolean lattice corresponding to $\mathcal{P}(S)$, where S is a set of 5 features. Each node in the lattice denotes a distinct feature set $F \in \mathcal{P}(S)$, where "0" and "1" indicate whether the corresponding feature is absent or present, respectively. Four different chains are shown in red. The cost $c(F)$ of each feature set $F \in \mathcal{P}(S)$ is indicated next to the corresponding node. Noteice that c is decomposable in U-curves. The feature set F^* of minimum cost in this example has cost zero and is highlighted in yellow. Parts (b) and (c) display 2D and 3D representations of the lattice in part (a), respectively.

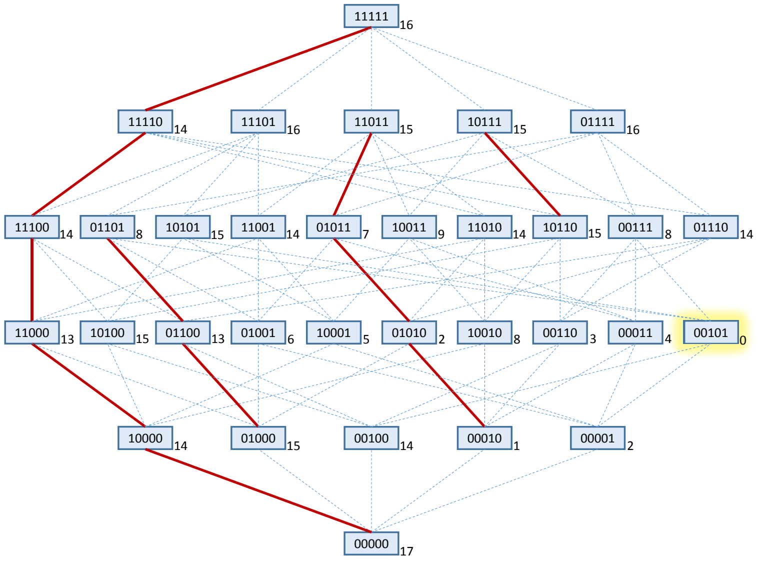


Figure 2: Lattice for 5 features, with 4 chains highlighted in red. The cost function for this example is decomposable in U-curves.

2.1. U-curve Branch and Bound (UBB) Algorithm

The UBB algorithm, proposed in [12], uses the U-assumption to find the feature set of minimum cost in $\mathcal{P}(S)$ without evaluating all the elements in $\mathcal{P}(S)$. Through a recursive enumeration scheme, it first constructs a tree and then uses it as the search space. The fact that c is decomposable in U-shaped curves is used to prune the tree during the search: the tree is pruned when the cost of an element in the search chain starts increasing. Although in the early iterations of the UBB algorithm, finding a minimum element in a chain leads to removal of many elements in the tree, in later iterations the search chains are not the best possible chains in the search space and the pruning becomes very slow. UBB iterates over the pruned tree until the search space is exhausted. Figure 3 illustrates the UBB algorithm, using the lattice in Figure 2. More details about the UBB algorithm, including pseudocode, can be found in [12].

3. Improved U-Curve Branch and Bound Algorithm

The results in [12] show that the UBB algorithm requires fewer function calls compared to Exhaustive Search (ES) in finding the global best solution of the U-curve problem. However, the number of function calls in UBB is still high: in the numerical experiments of [12], UBB required about half of the function calls of ES. To tackle the high number of function calls of UBB, an improved algorithm is proposed here. The Improved UBB (IUBB) algorithm is based on two main innovations:

1) **Iterative updating of optimal chains.**

To improve the pruning process, instead of limiting the search to the tree structure constructed through the enumeration process of UBB, at each step of IUBB, we determine a chain in the search space that leads to pruning the maximum number of elements; such chain is called optimal. In order to update the search after each pruning, at the beginning of each iteration, we need to update a data structure that manages the current state of the search space. This is done as follows. For a feature selection problem with n features, the search space can be represented by a Boolean lattice

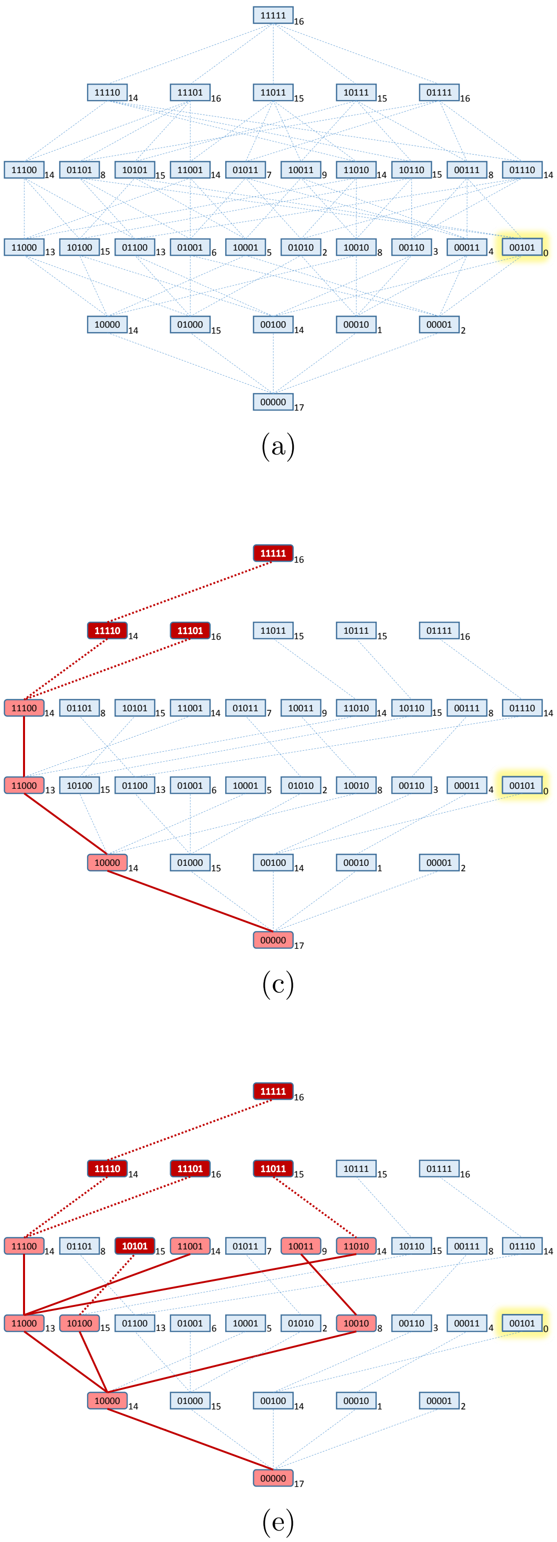


Figure 3: The UBB algorithm. (a) Search space. (b) The tree produced by enumeration scheme. (c-f) Four iterations of the algorithm. Visited nodes are colored pink, while pruned nodes are colored red.

$\mathcal{L}$ of degree n. Let $\mathcal{L}$ be organized in layers, as represented in Figures 2 and 3, where L_l denotes the l-th layer, for $l = 0, 1, \ldots, n$, that is, let L_l contain all possible feature sets of size l. The data structure contains vectors that store the pruning gain of each element in the current search space. Those vectors are computed recursively with the assistance of adjacency matrices. For $l = 0, 1, \ldots, n-1$, let $\mathbf{R}_l = [r_{ij}]$ be a matrix of size $\binom{n}{l} \times \binom{n}{l+1}$, with (i, j)-element given by

$$r_{ij} = \begin{cases} 1, & \text{if the Hamming distance between } F_j^l \text{ and } F_i^{l+1} \text{ is equal to 1,} \\ 0, & \text{otherwise,} \end{cases} \tag{1}$$

where F_i^l and F_j^{l+1} are elements of L_l and L_{l+1}, respectively. Thus, if $r_{ij} = 1$, then the two feature sets F_i^l and F_j^{l+1} are on the same chain. For each $l = 0, 1, \ldots, n$ let $\mathbf{V}_l = [v_{li}]$ be an auxiliary vector such that

$$v_{li} = \sum_{j=1}^{|L_{l+1}|} r_{ij}, \quad i = 1, \ldots, |L_l| \,. \tag{2}$$

Finally, let the main vectors to control the current search space be constructed recursively as

$$\begin{aligned} \mathbf{T}_n &= 0 \,, \\ \mathbf{T}_l &= \mathbf{V}_l + \mathbf{R}_l \times \mathbf{T}_{l+1} \,, \quad l = n-1, n-2, \ldots, 0 \,. \end{aligned} \tag{3}$$

The ith element of $\mathbf{T}_l$ indicates the pruning gain of its corresponding element in the search space. We use $\mathbf{T}_l$ to find chains for which finding the minimum element results in maximum pruning of the search space. At each step of the algorithm, an optimal chain $\mathcal{F}^*$ is found, and after determining the minimum element of the chain, all the states connected to the optimal element are removed from the search space. Then the matrices $\mathbf{R}_l$, $\mathbf{C}_l$ and $\mathbf{T}_l$ are updated, and the algorithm proceeds until there are no remaining elements in the search space.

2) **Use of bisection to find chain minimum.**

A drawback of UBB is that in finding the minimum element of a chain, it searches all the nodes in a chain before reaching a feature set that shows an increase in cost value. That is, for a chain $\mathcal{F} = \{F_1, F_2, \ldots, F_k\}$, if the U-curve cost function has a minimum $F^* = F_{i^*}$, the algorithm evaluates the cost function $(i^* + 1)$ times to find F^*. When dealing with a large number of features, the algorithm will tend to need a large number of unnecessary function calls to find F^*. To use the U-curve assumption efficiently, a faster method based on bisection is proposed to find the minimum element of the chain. Bisection changes the complexity of finding the minimum of the chain $\mathcal{F}$ from $O(|\mathcal{F}|)$ to $O(\log(|\mathcal{F}|))$.

Figure 4 diplays the number of the function calls required to find the minimum-cost feature set F^* in the chain when i^* is uniformly distributed in the set $2, \ldots, |\mathcal{F}| - 1$ and the cost function is $c(F_i) = (i - i^*)^2$. As we see, at $|\mathcal{F}| = 500$, bisection requires on average 17 function evaluations, while $|\mathcal{F}|/2 = 250$ function evaluations are needed on average by the method in UBB to find the minimum-cost feature set F_i^*.

With the aforementioned modifications to increase efficiency, the IUBB pseudocode is displayed below as Algorithm 1.

Compared to the original UBB algorithm, the proposed IUBB algorithm uses the U-assumption efficiently by first using a different search structure which focuses on an optimal chain $\mathcal{F}^*$ in the search space at each step of the algorithm. Then using the U-assumption for not only pruning the search space, but also for finding the minimum element F^* of each chain (`Bisection` module). This improved and efficient use of U-curve assumption enables the proposed algorithm to outperform

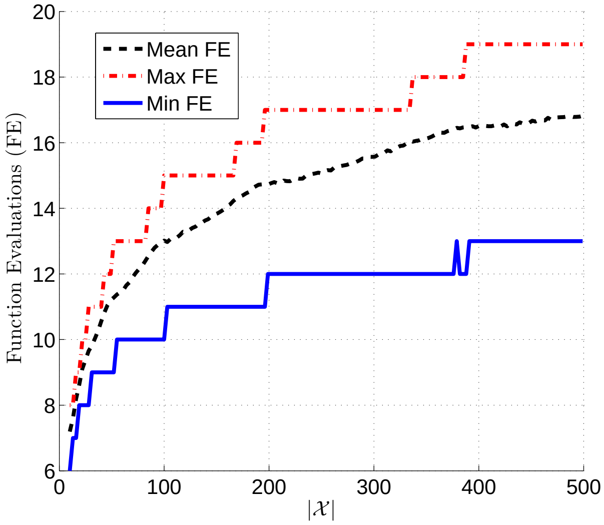


Figure 4: Number of function evaluations required by bisection to find the minimum-cost feature set F_{i^*} of the chain $\mathcal{F}$ vs. $|\mathcal{F}|$, when i^* is uniformly distributed in the set $2, \ldots, |\mathcal{F}| - 1$ and the cost function is $c(F_i) = (i - i^*)^2$.

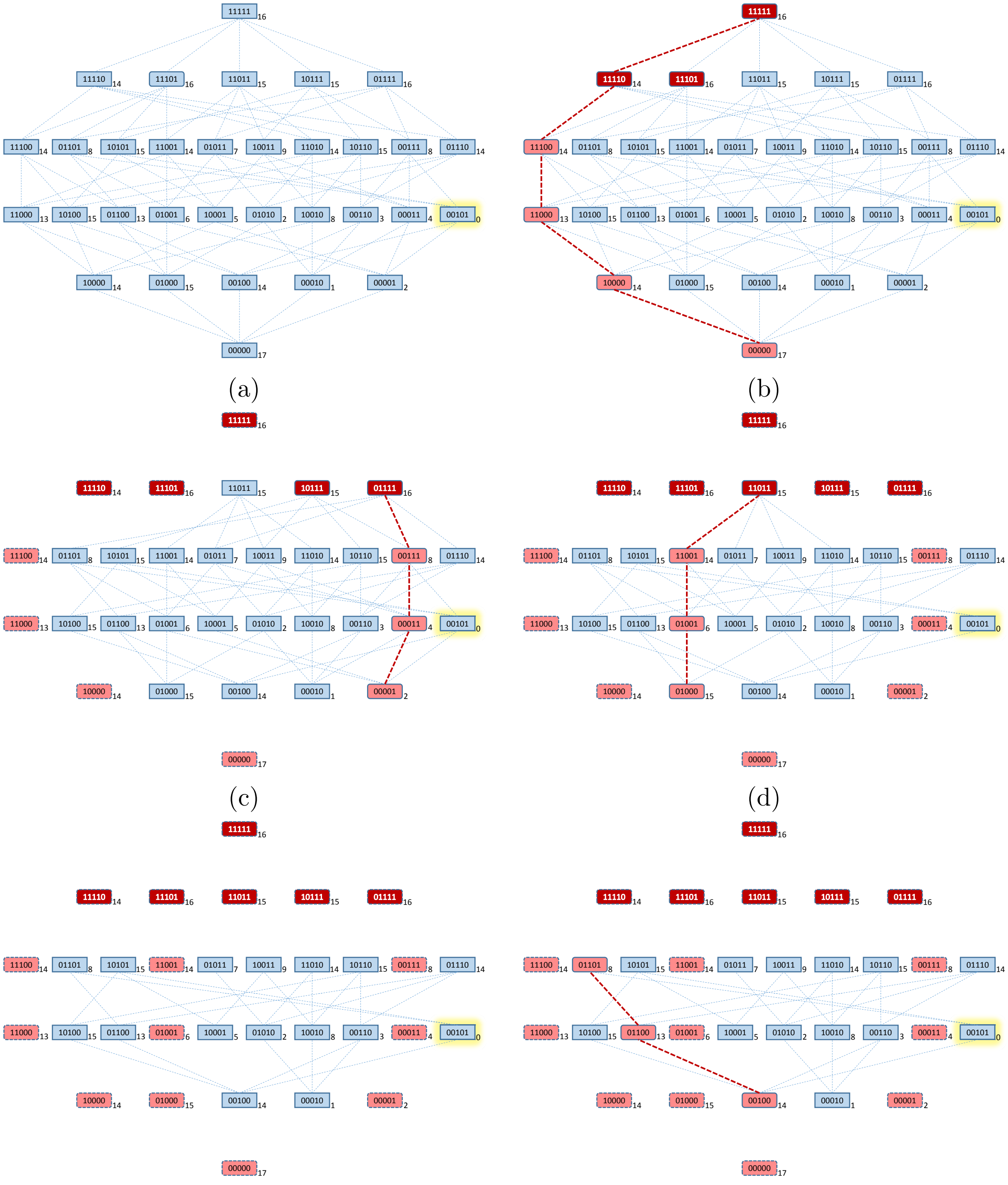
Algorithm 1 IUBB Algorithm

```
Initialize Boolean lattice $\mathcal{L}$ of degree $n$.
$N_r \Leftarrow$ Number of elements is the search space that are not visited.
$c^{opt} \Leftarrow \infty$
while $N_r \geq 0$ do
  Find the optimal chain $\mathcal{F}^*$
  Bisection($\mathcal{F}^*$) $\Rightarrow F^*$
  if $c(F^*) < c^{opt}$ then
    $c^{opt} \Leftarrow c(F^*)$
    $F^{opt} \Leftarrow F^*$
  end if
  Prune($\mathcal{L}, \mathcal{F}^*, F^*$) $\Rightarrow (\mathcal{L}, N_r)$
end while
return $F^{opt}$ and $c^{opt}$
```

UBB in most problems. Figure 5 illustrates the UBB algorithm, using the lattice in Figure 2. In the next section, feature selection experiments are conducted to assess the performance of both algorithms.

4. Feature Selection Experiments

In this section the performances of the proposed IUBB algorithm and the original UBB algorithm are compared in various feature selection experiments. The analysis is broken into two different parts. First, the algorithms are compared in a set of synthetic benchmark U-curve problems. The parameters in the synthetic problems allow us to study the effects the U-shape assumption can have on the underlying cost function and their impact on the behavior of the algorithms. Next, the robustness of the algorithms are studied under violation of the U-curve assumption, which would typically happen in wrapper feature selection [13] when the estimated classification error is used



(a) (b)

(c) (d)

(e) (f)

Figure 5: The IUBB algorithm. (a) The original search space. (b-f) Five iterations of the algorithm. Visited nodes are colored pink, while pruned nodes are colored red. The selected optimal chain in each iteration is shown by a red dashed line in all the diagrams.

as the cost.

4.1. Synthetic Benchmark

In this section, we perform numerical experiments to compare the performances of the UBB and IUBB algorithms.

4.1.1. Cost Function

The model for the cost function is given by:

$$c(F \mid F_0, \mathbf{W}, c_{\max}) \;=\; c_{\max}\left[1 - \exp\left(-\frac{1}{2}(F - F_0)^T \mathbf{W}(F - F_0)\right)\right] \tag{4}$$

where

$$\begin{array}{l} F \in \{0,1\}^n : \text{Feature set (binary string representation)} \\ F_0 \in \{0,1\}^n : \text{Global minimum of the cost function} \\ \mathbf{W} \in \mathbb{R}^{(n\times n)} : \text{Positive-definite weighting matrix (shaping matrix)} \\ c_{\max} : \text{Cost scale, or ideal maximum value of cost} \end{array} \tag{5}$$

The density of 1's in the global minimum,

$$\alpha \;=\; \frac{1}{n}\sum_{i=1}^{n} F_0(i)\,, \tag{6}$$

with $0 \le \alpha \le 1$, indicates how late peaking occurs. Note that $n\alpha$ is the number of features in the optimal feature set.

4.1.2. Performance Metrics

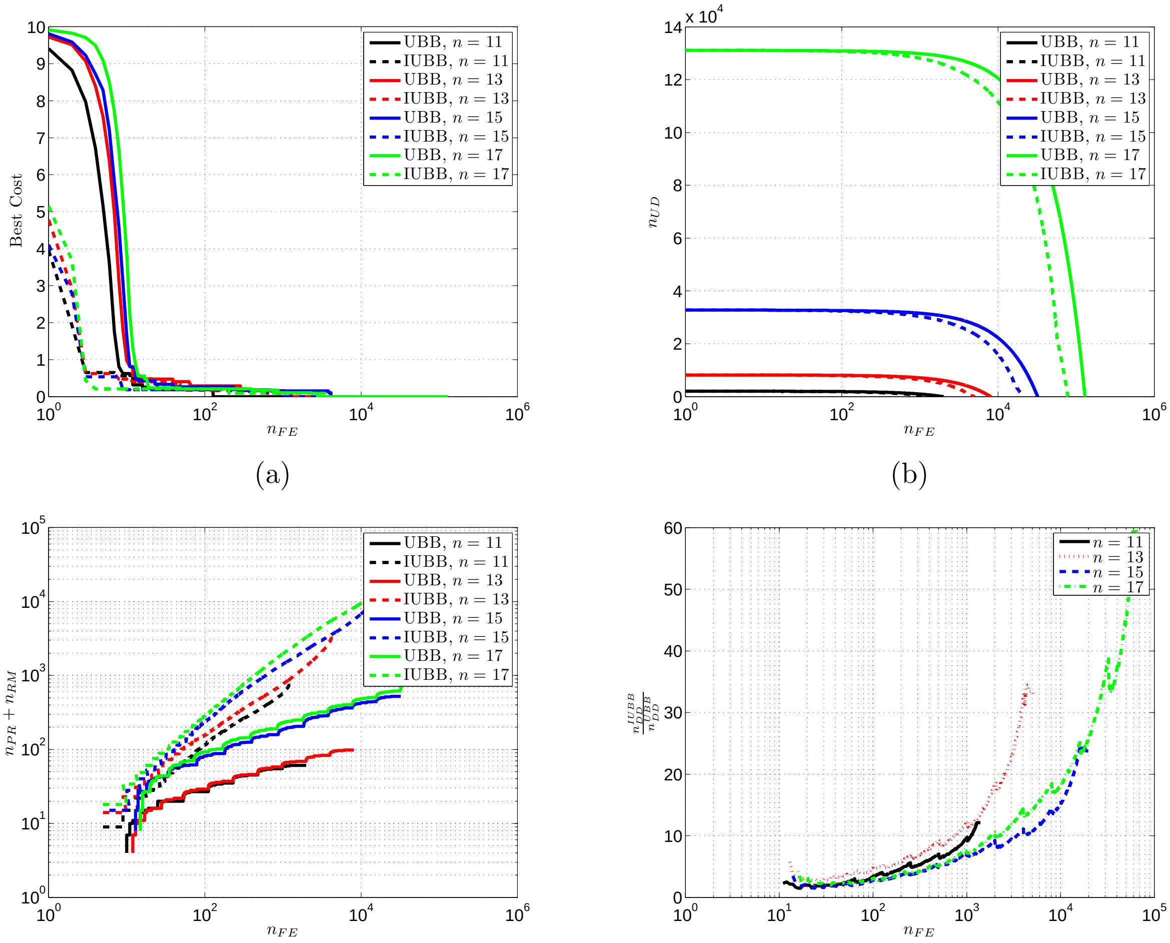
Let n_{FE} be the number of function evaluations, i.e., the number of feature sets visited and evaluated by the algorithm, let n_{PR} be the number of feature sets pruned by applying the U-curve assumption on the search, and let n_{RM} be the number of feature sets removed from the search for reasons other than pruning; for example, removal of feature sets from a chain using bisection to find the minimum element.

The algorithms will be compared using the following metrics

- The cost of best feature set found by the algorithm.
- Number of feature sets pruned or removed: $n_{DD} = n_{PR} + n_{RM}$.
- Number of feature sets not visited, pruned or removed: $n_{UD} = 2^n - n_{FE} - n_{PR} - n_{RM}$.
- The number of function evaluations required to find the optimal feature set.
- Search Efficiency (SE):

  $$SE = \frac{n_{FE} + n_{DD}}{n_{FE}}\,. \tag{7}$$

  The SE measures how efficiencient the algorithm is in using the U-curve assumption to discard undesired solutions from the search space. The minimum value $SE = 1$ is achieved by an exhaustive search, when $n_{DD} = 0$. A small value of SE will show that the algorithm uses the assumption inefficiently.



(a)

(b)

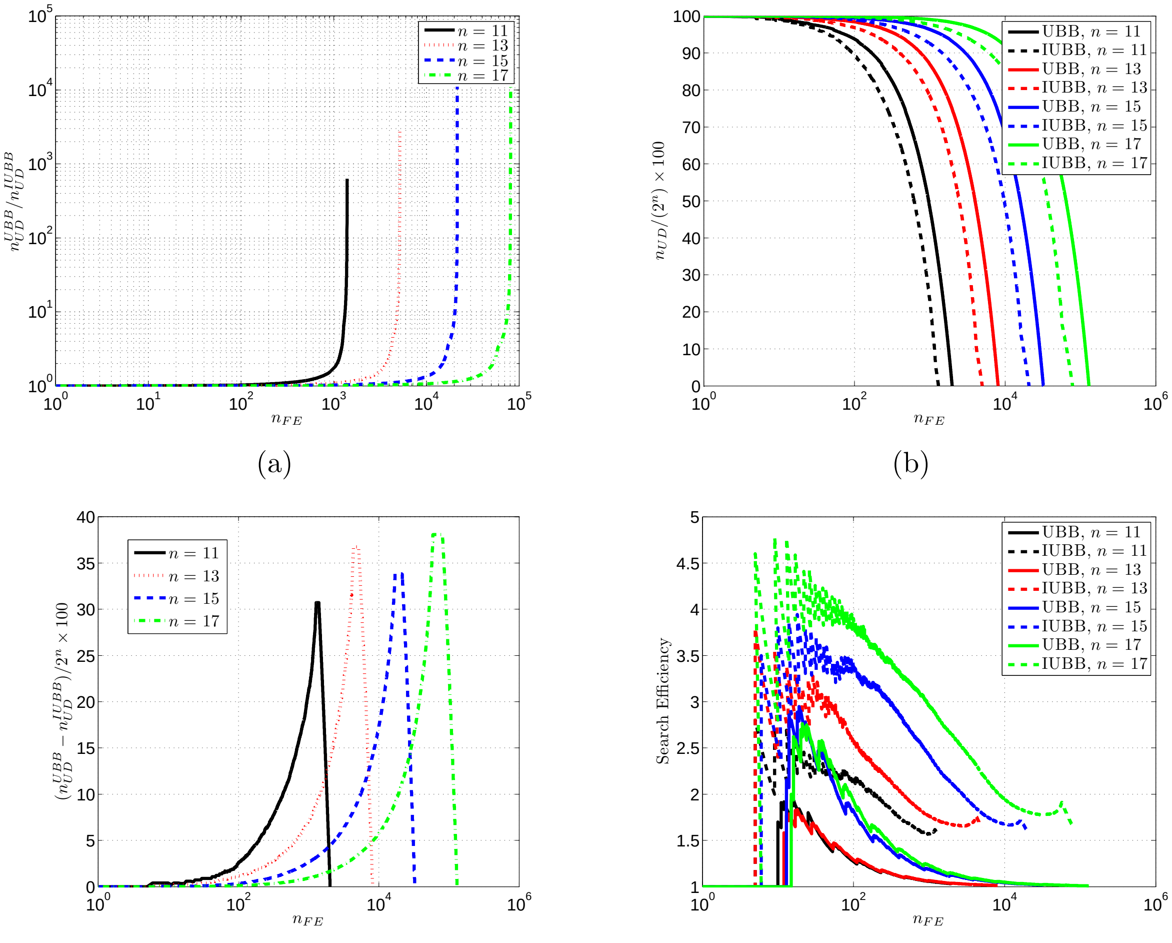
(c)

(d)

Figure 6: Performance of the IUBB and UBB algorithms for $\alpha = 0.75$ and different values of n. All quantities are plotted against the number of feature sets visited n_{FE}. (a) Best cost found by each algorithm. (b) Number of feature sets not visited, pruned or removed n_{UD}. (c) Number of feature sets pruned or removed n_{DD}. (d) Ratio of n_{DD} for IUBB over n_{DD} for UBB.

4.1.3. Results

Figures 6 and 7 display plots of several of the metrics discussed in the previous section vs. the number of feature sets visited, for $\alpha = 0.75$ and varying n. One can observe that IUBB presents a high search gain for small n_{FE}, which is important as this represents the case of limited computational resources.



(a)

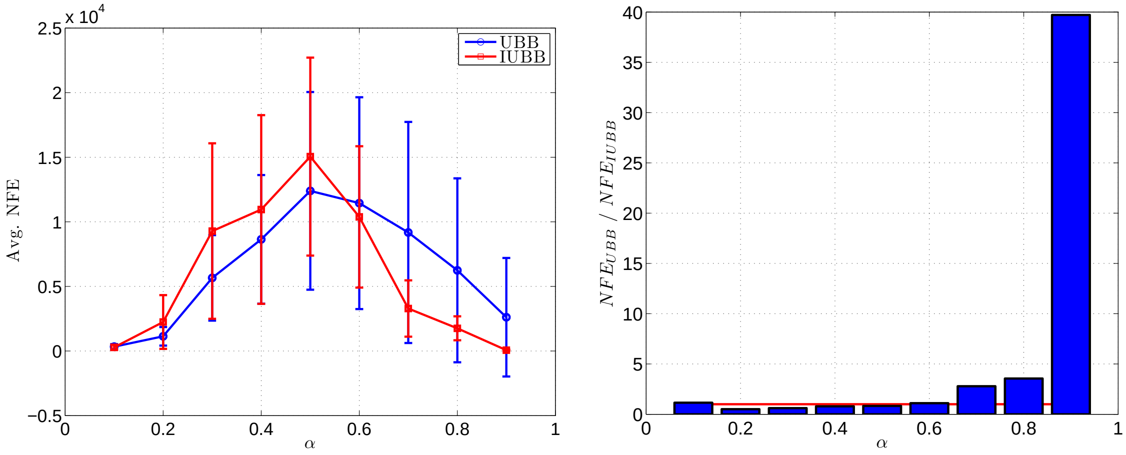
(b)

(c)

(d)

Figure 7: Performance of the IUBB and UBB algorithms for $\alpha = 0.75$ and different values of n. All quantities are plotted against the number of feature sets visited n_{FE}. (a) Ratio of n_{UD} for IUBB over n_{UD} for UBB. (b) Number of feature sets not visited, pruned or removed n_{UD} as a percentage of the entire search space. (c) Difference between n_{UD} for UBB and n_{UD} for IUBB as a percentage of the entire search space. (d) Search efficiency.

Figure 8 displays the average number of function evaluations needed to find the best feature set, as a function of α, for $n = 15$. Varying *alpha* allows us to observe the relative performance of the algorithms with respect to early and late peaking. We can see in Figure 8(a) that the increase of α from 0 to 0.5 increases the number of feature set evaluations required by each algorithm. This behavior is expected, as the increase of α delays success in finding the best feature sets. Both algorithms have the worst performance when α is about 0.5. However, increasing α in the interval $[0.5, 1]$ improves the performance of the two algorithms. When α is close to 1, the optimal solution is in the first selected chains and both algorithms perform well, but with a noticeable superiority of IUBB. Figure 8 (b) shows that UBB might require about 40 times more feature set evaluations for a problem with late peaking.



(a) (b)

Figure 8: (a) Plot of the average feature set evaluations required by each algorithm to find the optimal feature set, for $n = 15$. (b) Barplot of the average gain in efficiency displayed by IUBB over UBB in terms of feature set evaluations required to find the global best feature set.

Figure 9 compares the two algorithms using the minimum cost found, search efficiency SE, and SE ratio plots as a function of α, for $n_{FE} = 5\%$ and $n_{FE} = 10\%$ of the search space, and $n = 15$. Limiting the total number of functions evaluations models the realistic scenario of limited computational resources. We can see that IUBB has a better performance in terms of minimum cost found and search efficiency, over the entire range of α. We also see that the two algorithms display high search efficiency for low values of α and, as α increases, the search efficiency decreases very fast for both algorithms.

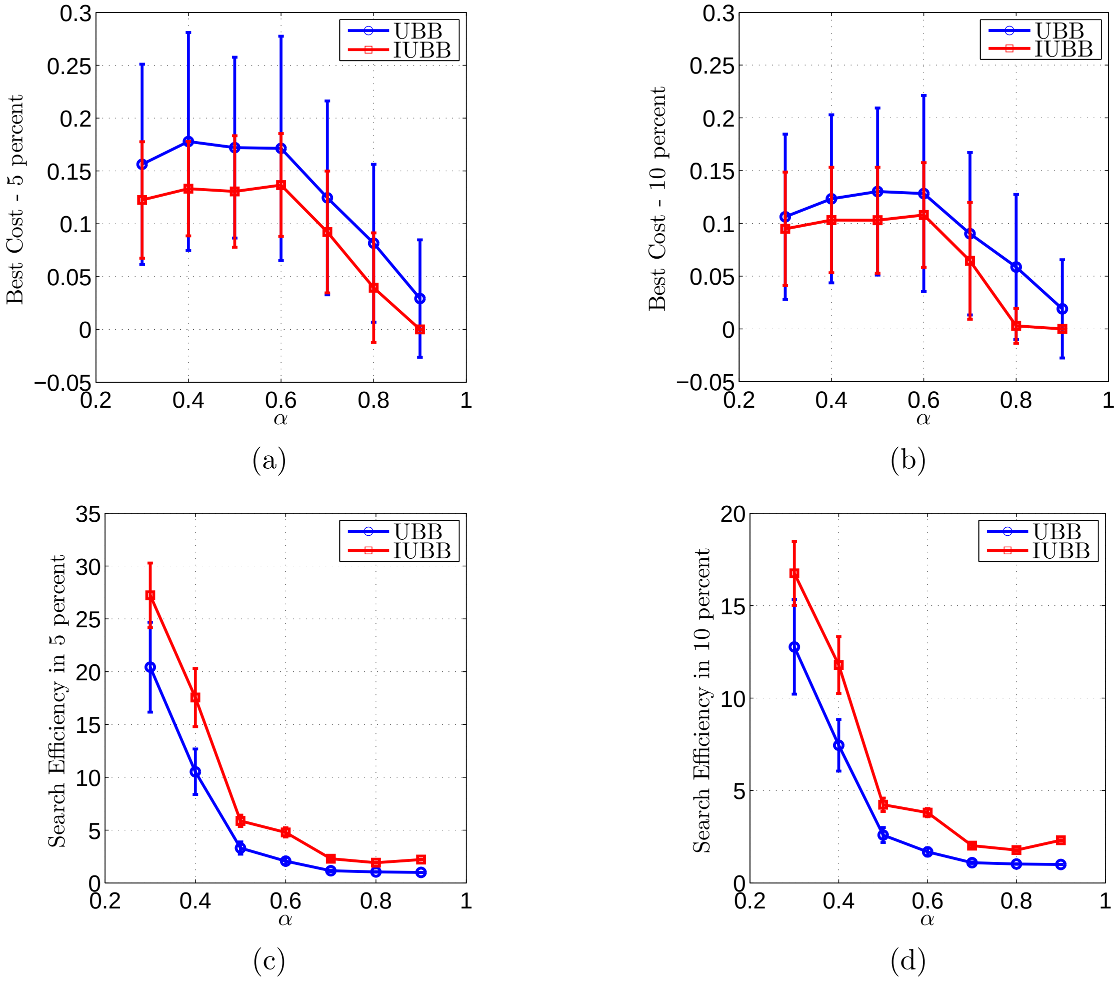
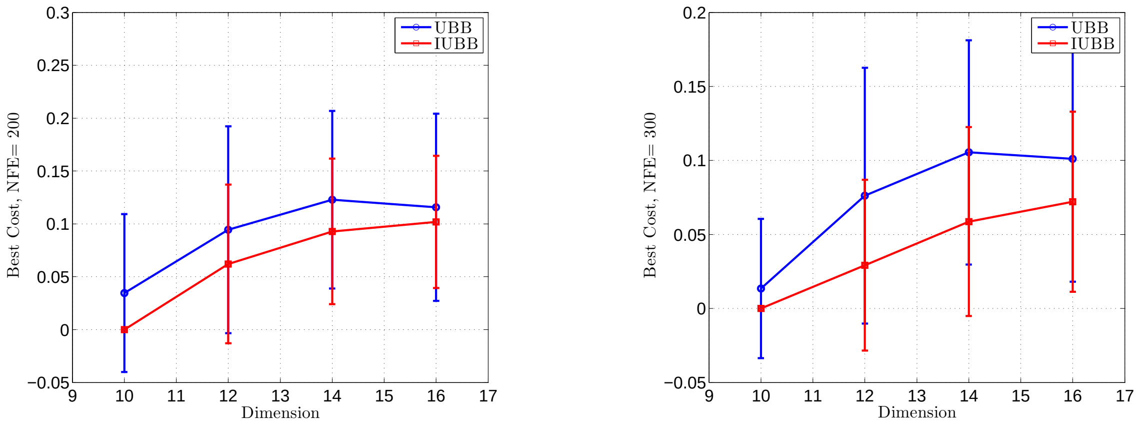


Figure 9: Performance for fixed number of visited feature sets, $n_{FE} = 5\%$ and $n_{FE} = 10\%$ of the search space, and $n = 15$. All quantities are plotted against α. (a,b) Average minimum cost found. (c,d) Search efficiency.

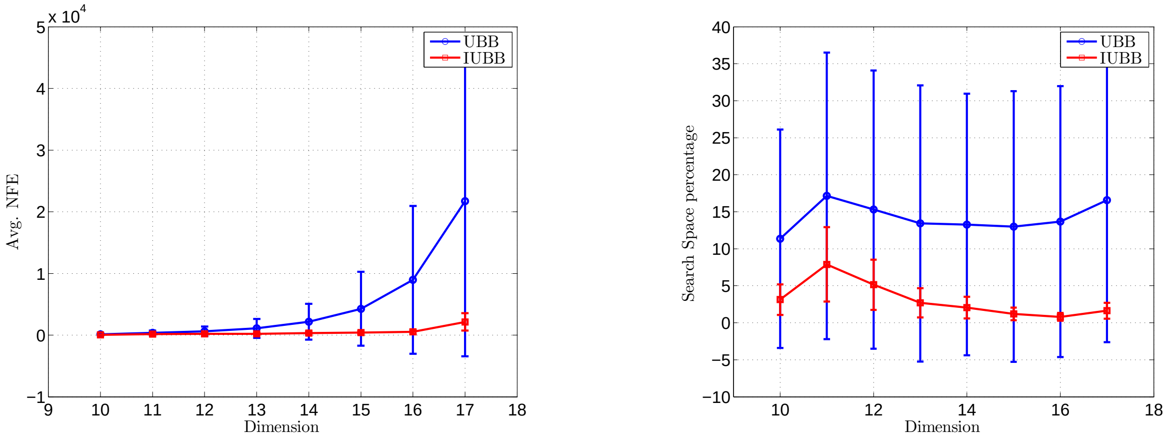
Figure 10 allows us to examine the loss of performance typically presented by branch-and-bound algorithms to increasing dimensionality, by plotting the average minimum cost found (with error bars) as a function of the number of features, with $\alpha = 0.85$. We can see that IUBB outperforms UBB, but that the performance of both algorithms degrade as dimensionality increases.



(a) (b)

Figure 10: Average minimum cost vs. dimension for fixed number of function evaluations, (a) $n_{FE} = 200$ and (b) $n_{FE} = 300$

Figure 11 displays the number of function calls and the percentage of the search space evaluated by each algorithm in order to find the best feature set, as a function of the dimensionality, for $\alpha = 0.85$. One can observe that, on average, IUBB makes a smaller number of function evaluations and explores a smaller percentage of the search space than UBB in finding the optimal feature set. The difference tends to increase with larger dimensionality. The smaller error bars displayed by IUBB indicating good stability with respect to random changes in the structure of the problem.



(a) (b)

Figure 11: Number of function calls and the percentage of the search space evaluated by each algorithm in order to find the best feature set, as a function of the dimensionality, for $\alpha = 0.85$. (a) Number of function evaluations used by each algorithm. (b) Percentage of the search space evaluated by each algorithm.

4.2. Violation of the U-Curve Assumption

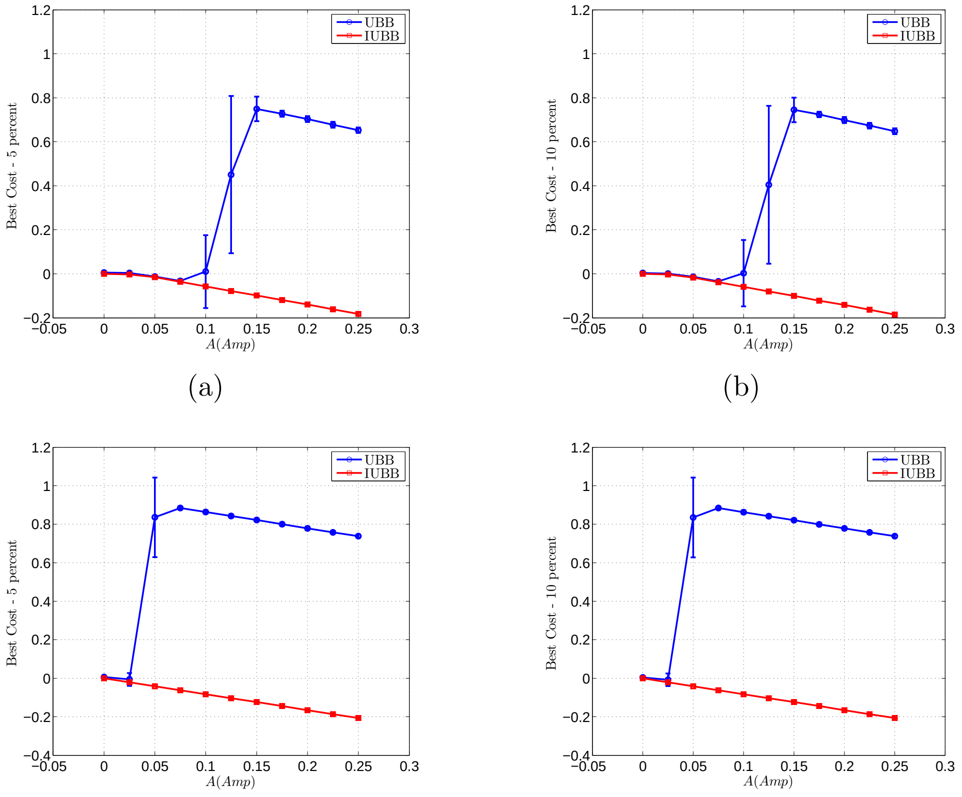
In order to study the robustness of the algorithms, in this section we allow violation of the U-curve assumption; for instance, this would be the case in wrapper feature selection when classifier error estimators are used to obtain the cost function. This is accomplished by adding a sinusoidal disturbance to the cost model to allow violation of the U-assumption assumption:

$$c(F \mid F_0, \mathbf{W}, c_{\max}) \;=\; c_{\max}\left[1 - \exp\left(-\frac{1}{2}(F-F_0)^T\mathbf{W}(F-F_0)\right) + A\cos(2\pi f\beta(F))\right] \tag{8}$$

where

$$\begin{aligned} &\beta(F) \;=\; \tfrac{1}{n}\textstyle\sum_{i=1}^{n} F(i) \\ &A : \text{Amplitude of the sinusoidal disturbance} \\ &f : \text{Frequency of the sinusoidal disturbance} \end{aligned} \tag{9}$$

and the other parameters are as before. The value of f controls the number (frequency) of local minima and A controls the depth of the local minima. If A is set to 0, then the U-curve assumption is not violated, whereas if $A > 0$, then the problem does not satisfy the U-curve assumption and each chain might have more than one local minimum. A robust branch-and-bound algorithm should be able to avoid most of these minima and display a small reduction in its ability of finding the global minimum of each chain and pruning the search space, provided that A and f are not too large. In Figure 12, we display the average cost of the best feature sets found as the value of A increases. As we see, for $A \leq 0.075$ and $f = 2$ the two algorithms are able to tolerate the violation of the U-curve assumption. However, as A becomes greater than 0.075, the performance of UBB degrades suddenly while IUBB is robust. With $f = 3$, even a small value of deviation from U-assumption is enough for UBB to get stock in local minimums of the function.



(a)

(b)

(c)

(d)

Figure 12: Average minimum cost for fixed number of function evaluations, $n_{FE} = 5\%$ and $n_{FE} = 10\%$ of the search space, and $n = 15$. All quantities are plotted against A. Top row: $\alpha = 0.75$, $f = 2$. Bottom row: $\alpha = 0.85$, $f = 3$.

5. Application to the Design of Imaging W-operators

In this section, we employ the IUBB algorithm to the design a W-operator, a type of morphological imaging operator that is locally defined inside a window and also is translation invariant [14]. The design of a W-operator involves a feature selection procedure, which requires the choice of a suitable cost function. Previous results have shown that an effective cost function for W-operator window design is the minimization of mean conditional entropy [15].

The cost function to be employed is the (estimated) *mean conditional entropy* [16]. The conditional entropy of a discrete random variable Y taking values in $\mathcal{Y}$ given a realization of another discrete random variable $\mathbf{X}$ taking values in $\mathcal{X}$ is defined by

$$H(Y|\mathbf{X} = \mathbf{x}) = -\sum_{y\in\mathcal{Y}} P(Y = y|\mathbf{X} = \mathbf{x}) \log P(Y = y|\mathbf{X} = \mathbf{x})\,, \quad \text{for } \mathbf{x} \in \mathcal{X}, \tag{10}$$

so that the mean conditional entropy (MCE) of Y given $\mathbf{X}$ is expressed by

$$\begin{aligned} E[H(Y|\mathbf{X})] &= \sum_{\mathbf{x}\in\mathcal{X}} H(Y|\mathbf{X} = \mathbf{x}) P(\mathbf{X} = \mathbf{x}) && (11) \\ &= -\sum_{\mathbf{x}\in\mathcal{X}} P(\mathbf{X} = \mathbf{x}) \sum_{y\in\mathcal{Y}} P(Y = y|\mathbf{X} = \mathbf{x}) \log P(Y = y|\mathbf{X} = \mathbf{x}) && (12) \\ &= -\sum_{\mathbf{x}\in\mathcal{X}} \sum_{y\in\mathcal{Y}} P(Y = y, \mathbf{X} = \mathbf{x}) \log \frac{P(Y = y, \mathbf{X} = \mathbf{x})}{P(\mathbf{X} = \mathbf{x})}\,, && (13) \end{aligned}$$

where $0 \log c/0$, for $c \geq 0$, is to be interpreted as zero. Since $P(Y = y, \mathbf{X} = \mathbf{x}) \leq P(\mathbf{X} = \mathbf{x})$, one has $E[H(Y|\mathbf{X})] \geq 0$. It can be shown that the minimum value of zero is obtained if and only if Y is completely determined by $\mathbf{X}$.

Given t i.i.d. pairs $(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_t, Y_t)$ distributed as $(\mathbf{X}, Y)$, plugging in the standard sample-based estimators for the probabilities in (13) leads to an estimator $\hat{E}[H(Y|\mathbf{X})]$ for the MCE of Y given $\mathbf{X}$. However, since t is usually small, the estimation error is typically high. To minimize this, we penalize pairs that are observed only once by considering such occurrences as following a uniform distribution, which leads to maximum entropy. Given that the probability of a pair $(\mathbf{X}_i, Y_i)$ occurring only once is $1/t$ and the fact that the number of such pairs is m, the total penalty contribution to the MCE estimator is m/t. Therefore, the final MCE estimator is given by

$$\hat{E}[H(Y|\mathbf{X})] = \frac{m}{t} - \sum_{\mathbf{x}\in\mathcal{X}} \sum_{y\in\mathcal{Y}} \hat{P}(Y = y, \mathbf{X} = \mathbf{x}) \log \frac{\hat{P}(Y = y, \mathbf{X} = \mathbf{x})}{\hat{P}(\mathbf{X} = \mathbf{x})} I_{\hat{P}(Y=y,\mathbf{X}=\mathbf{x}) \geq \frac{2}{t}}\,. \tag{14}$$

Now, consider an ideal binary image I and a corresponding noisy binary image I_N. Let W be a window centered on a pixel $x \in I$, and let $\mathbf{X}$ be a set of pixels in W. A W-operator $\psi : \mathbf{X} \mapsto \{0, 1\}$ tries to predict the value $Y = I(x) \in \{0, 1\}$ using the values taken by I_N on $\mathbf{X}$. The W-operator is assumed to be translation-invariant, that is, the same set of pixels $\mathbf{X}$ (relative to the translated window) is used for all $x \in I$. The design of a W-operator, for a given window W, involves determining the appropriate subset of pixels $\mathbf{X}$ and the mapping ψ. Now assume that a sample realization of an image pair (I, I_N) is available. By assuming stationarity, one can slide the window W across the images and obtain t approximately i.i.d. realizations of the pair $(\mathbf{X}, Y)$, for a given subset of pixels $\mathbf{X}$, where t is the number of pixels in the image I (ignoring border effects), which allows one to compute the MCE estimator $\hat{E}[H(Y|\mathbf{X})]$ in (14), for the given $\mathbf{X}$. We propose to apply the IUBB algorithm to select the best $\mathbf{X}$ using the MCE estimator as the cost function — once the best $\mathbf{X}$ is selected, the value of $\psi(\mathbf{X})$ is determined by majority voting over the t realizations of $(\mathbf{X}, Y)$.

We conducted an experiment where the noisy image I_N was created by adding 30% salt-and-pepper noise to the original ideal image I — an example is shown in Figure 13. Such pairs of images were screened considering windows of size ranging from 8 to 16 pixels, some of which are displayed in Figure 14.

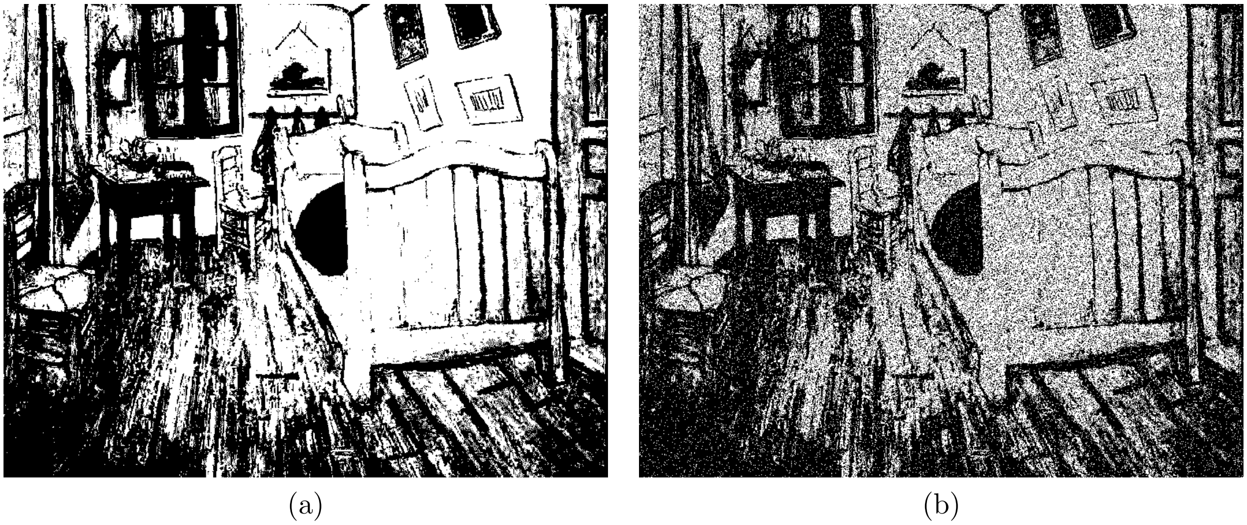

(a) (b)

Figure 13: An example of a pair of images that was used in the design of imaging W-operators. (a) Ideal image I. (b) Noisy image I_N.

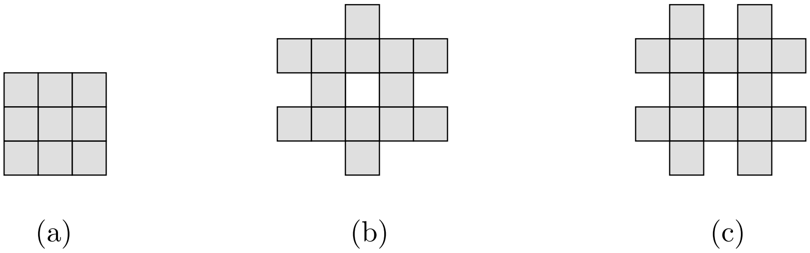
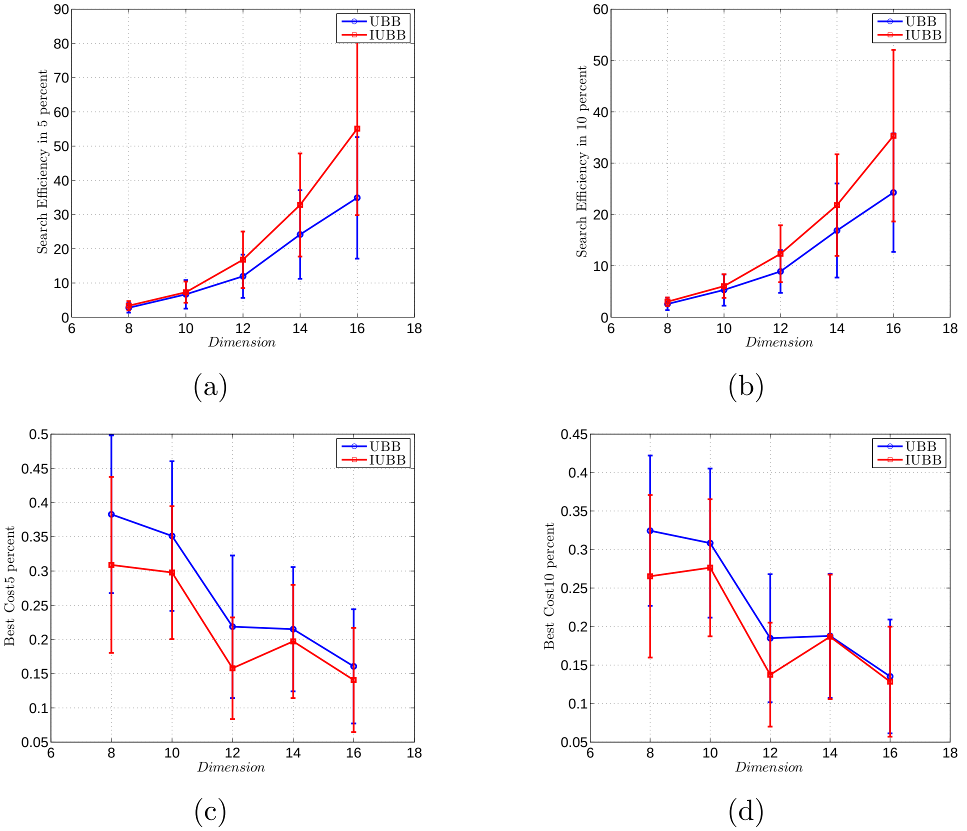

(a) (b) (c)

Figure 14: A few of the W-operator windows used in the experiment. (a) 9-pixel window. (b) 14-pixel window. (c) 16-pixel window.

Performance was evaluated by means of the search efficiency and best cost criteria defined previously, averaged over a set of fifty pairs of ideal/noisy images. We also computed the results obtained by the original UBB algorithm, for comparison. Figure 15 displays the values of the performance metrics as a function of the window size, which plays the role of dimensionality in this case. The left and right columns depict results for 5% and 10% of the search space explored, respectively. We can see that both the average search efficiency and the average minimum value of MCE found improve with an increasing window size — there will usually be a point at which increasing window size further will not improve performance and may indeed degrade it, for a fixed image size, but the window sizes employed in the experiment were small enough, compared to the image size, to avoid this peaking phenomenon. We can also see that IUBB outperforms UBB in each case.



(a) (b) (c) (d)

Figure 15: Performance of W-operator design. All quantities plotted as a function of the window size.

6. Application to Classification Feature Selection

In this section, we show the results of a feature selection experiment in the classification of synthetic data generated from a Gaussian model, using the Mean Conditional Entropy (MCE) criterion, introduced in the previous section, as the cost function.

We generate synthetic data according to the model proposed in [17]. The individual features are divided into two different groups, *markers* and *non-markers* (i.e. "noise"). A Gaussian block model is used for the abundance of markers and non-markers, with the latter group being divided into two groups, high-variance and low-variance. There are altogether D_{gm} global markers. The class-conditional distributions for the markers are D_{gm}-dimension Gaussian: $N(\mu_0^{gm}, \Sigma_0^{gm})$ for class 0 and $N(\mu_1^{gm}, \Sigma_1^{gm})$ for class 1, where μ_0^{gm} and μ_1^{gm} are the mean vectors of class 0 and 1, respectively, and Σ_0^{gm} and Σ_1^{gm} are the covariance matrices. The means are set to $\mu_0^{gm} = (0, 0, ..., 0)$ and $\mu_1^{gm} = (1, 1, ..., 1)$, while a block-based structure is used to define the covariance matrices, whereby markers are divided into groups of D_m markers each. Markers from different groups are uncorrelated and markers of the same group possess the same correlation ρ between each other. More specifically, we define Σ_0^{gm} and Σ_1^{gm} as $\Sigma_0^{gm} = \sigma_0^2 \times \Sigma$ and $\Sigma_1^{gm} = \sigma_1^2 \times \Sigma$, with

$$\Sigma = \begin{bmatrix} R_\rho & 0 & \cdots & 0 \\ 0 & R_\rho & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_\rho \end{bmatrix}, \tag{15}$$

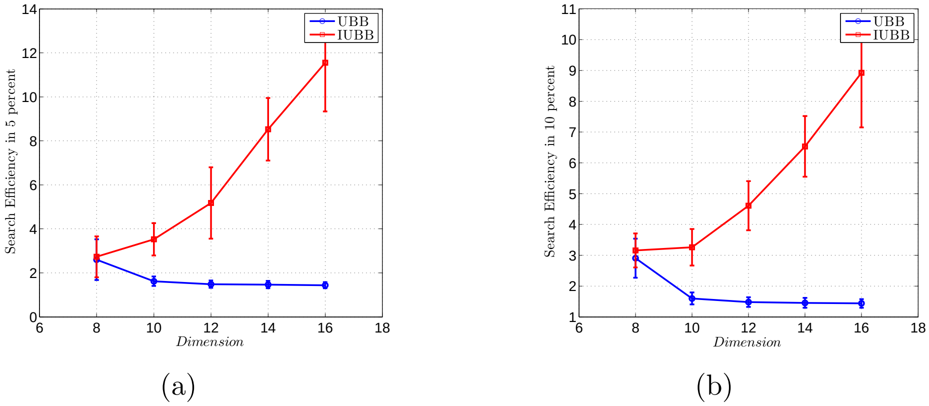
where R_ρ is a $D_m \times D_m$ matrix with 1's on the diagonal and ρ's elsewhere. On the other hand, the non-markers are features that provide no discriminating power between two classes. The high-variance non-markers are uncorrelated. For any feature, the distribution will be a mixture of Gaussians, $N(0, \sigma_0^2)$ and $N(1, \sigma_1^2)$, where σ_0^2 and σ_1^2 are the same values used for the markers. The number of high-variance non-markers is denoted by D_{hv}. The low-variance non-markers are also uncorrelated. For any feature, the distribution is $N(0, \sigma_0^2)$. The number of low-variance non-markers is $D_{lv} = D - D_{gm} - D_{hv}$.

Using this data model and the estimated MCE as the cost function, the IUBB algorithm was used to find the best feauture set. Results are also computed for the original UBB algorithm for comparison. The specific parameter values used in the simulation are displayed in Table 6.

Table 1: Summary of parameters

Parameter		**Value**
No. of sample size	nTr	100
Block Size	D_m	2
Correlation	ρ	0.5
Variances	$\sigma_0^2 = \sigma_1^2$	0.3^2

Figures 16 displays the results of the experiment. As we can see, increasing the dimension decreases the search efficiency of UBB while IUBB has an efficient use of the problem assumptions and prunes the search space very fast.



(a)

(b)

Figure 16: Search Efficiency vs. Dimension, (a) $NFE = 5\%$ of search space, and (b) $NFE = 10\%$ of search space.

7. Conclusion

In this paper, we proposed a new and improved branch and bound algorithm for the U-curve optimization problem, assessed its performance by means of simulated optimization problems, and demonstrated its aplication to the design of imaging W-operators and in feature selection for classification. The proposed algorithm (IUBB) improves on a previous algorithm (UBB), which requires fewer number of function calls compared to exhaustive search. However, the experiments in the present paper show that the UBB algorithm does not use the U-curve assumptions efficiently. The IUBB algorithm uses the U-assumption efficiently by reorganizing the tree structure in optimal fashion and using bisection to find the minimum along the chains. Different indices were used to evaluate the performance of the proposed algorithm. The number of function calls needed to find the best feature set, the minimum cost vs. number of function calls, and the search efficiency were three major indices used to asses performance. The results showed that the proposed IUBB algorithm requires a qualitatively smaller number of function evaluations to find the optimal solution than UBB. In addition, for a fixed budget, i.e., with the same number of function evaluations, IUBB generally reaches a feature set with lower cost value compared to UBB.

References

[1] A. Jain and D. Zongker, "Feature selection: Evaluation, application, and small sample performance," *IEEE Trans. on Pattern Analysis and Machine Intelligence*, vol. 19, no. 2, pp. 153–158, 1997.

[2] T. Cover and J. van Campenhout, "On the possible orderings in the measurement selection problem," *IEEE Trans. on Systems, Man, and Cybernetics*, vol. 7, pp. 657–661, 1977.

[3] P. M. Narendra and K. Fukunaga, "A branch and bound algorithm for feature subset selection," *Computers, IEEE Transactions on*, vol. 100, no. 9, pp. 917–922, 1977.

[4] A. Frank, D. Geiger, and Z. Yakhini, "A distance-based branch and bound feature selection algorithm," in *Proceedings of the Nineteenth conference on Uncertainty in Artificial Intelligence.* Morgan Kaufmann Publishers Inc., 2002, pp. 241–248.

[5] S. Nakariyakul and D. P. Casasent, "Adaptive branch and bound algorithm for selecting optimal features," *Pattern Recognition Letters*, vol. 28, no. 12, pp. 1415–1427, 2007.

[6] B. Yu and B. Yuan, "A more efficient branch and bound algorithm for feature selection," *Pattern Recognition*, vol. 26, no. 6, pp. 883–889, 1993.

[7] P. Somol, P. Pudil, and J. Kittler, "Fast branch & bound algorithms for optimal feature selection," *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, vol. 26, no. 7, pp. 900–912, 2004.

[8] L. Devroye, L. Gyorfi, and G. Lugosi, *A Probabilistic Theory of Pattern Recognition.* New York: Springer, 1996.

[9] G. Hughes, "On the mean accuracy of statistical pattern recognizers," *Information Theory, IEEE Transactions on*, vol. 14, no. 1, pp. 55–63, 1968.

[10] C. Sima and E. R. Dougherty, "The peaking phenomenon in the presence of feature-selection," *Pattern Recognition Letters*, vol. 29, no. 11, pp. 1667–1674, 2008.

[11] M. Ris, J. Barrera, and D. C. Martins Jr, "U-curve: A branch-and-bound optimization algorithm for U-shaped cost functions on Boolean lattices applied to the feature selection problem," *Pattern Recognition*, vol. 43, no. 3, pp. 557–568, 2010.

[12] M. S. Reis, "Minimization of decomposable in U-shaped curves functions defined on poset chains – algorithms and applications," Ph.D. dissertation, Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, Brazil, 2012, (in Portuguese).

[13] R. Kohavi and G. John, "Wrappers for feature subset selection," *Artificial Intelligence*, vol. 97, no. 1–2, pp. 273–324, 1997.

[14] J. Barrera, R. Terada, R. Hirata-Jr., and N. Hirata, "Automatic programming of morphological machines by PAC learning," *Fund. Inform.*, pp. 229–258, 2000.

[15] D. Martins-Jr, R. Cesar-Jr, and J. Barrera, "W-operator window design by minimization of mean conditional entropy," *Pattern Anal. Appl.*, vol. 9, no. 2, pp. 139–153, 2006.

[16] T. Cover, *Elements of Information Theory*, 2nd ed. New York, NY: Wiley, 2006.

[17] J. Hua, W. D. Tembe, and E. R. Dougherty, "Performance of feature-selection methods in the classification of high-dimension data," *Pattern Recognition*, vol. 42, no. 3, pp. 409–424, 2009.