A Fast Algorithm for Unsupervised Feature Value Selection

Kilho Shin[1], Kenta Okumoto[2], David Lowrence Shepard[3], Tetsuji Kuboyama[1], Takako Hashimoto[4] and Hiroaki Ohshima[5]

[1]*Gakushuin University, Tokyo, Japan*

[2]*Japan Post Bank, Tokyo, Japan*

[3]*UCLA, Scholary Innovation Lab., CA, U.S.A.*

[4]*Chiba University of Commerce, Chiba, Japan*

[5]*University of Hyogo, Kobe, Japan*

Keywords: Unsupervised Learning, Feature Selection.

Abstract: The difficulty of unsupervised feature selection results from the fact that many local solutions can exist simultaneously in the same dataset. No objective measure exists for judging the appropriateness of a particular local solution, because every local solution may reflect some meaningful but different interpretation of the dataset. On the other hand, known accurate feature selection algorithms perform slowly, which limits the number of local solutions that can be obtained using these algorithms. They have a small chance of producing a feature set that can explain the phenomenon being studied. This paper presents a new method for searching many local solutions using a significantly fast and accurate algorithm. In fact, our feature value selection algorithm (UFVS) requires only a few tens of milliseconds for datasets with thousands of features and instances, and includes a parameter that can change the local solutions to select. It changes the scale of the problem, allowing a user to try many different solutions and pick the best one. In experiments with labeled datasets, UFVS found feature value sets that explain the labels, and also, with different parameter values, it detected relationships between feature value sets that did not line up with the given labels.

1 INTRODUCTION

Feature selection has been an area of considerable research in machine learning. In the era of big data, feature selection algorithms must be both highly efficient with large, complex datasets and independent of class labels.

In addition, data found in the cloud often includes more categorical values and numerical values than traditional statistical data. Categorical data can easily be converted into numeric data and vice-versa: one-hot encoding is a common algorithm for converting categorical values into vectors of numerical values. Many discretization algorithms are known for the conversion of numerical values into categorical (discrete) values. In this paper, we focus on feature selection for categorical data and assume that numerical values in datasets have been appropriately discretized beforehand. Hence, we assume that all features in each dataset take only a finite number of categorical values. Feature selection on categorical data in supervised learning has been studied intensively. In supervised learning, feature selection is a process for finding a subset of the features of a dataset that maximizes the relevance, or correlation, of the subset to class labels. In fact, Almualllim et al. (Almuallim and Dietterich, 1994) propose an algorithm that performs a breadth first search of the Hasse diagram of an entire feature set. Almuallim's algorithm starts from the empty set node and stops when it reaches a feature set whose Bayesian risk vanishes. Bayesian risk is used as a measure of correlation of feature set to class labels: the smaller the Bayesian risk of a feature set is, the more relevant the set is to class labels. However, this algorithm is inefficient with a large number of features because the size of a Hasse diagram increases exponentially with the number of features.

On the other hand, Hall (Hall, 2000) and Peng et al. (Peng et al., 2005) propose a view of feature selection as a process for building a set of relevant features without redundancy. A relevant feature is a feature highly correlated to class labels, while

Shin, K., Okumoto, K., Shepard, D., Kuboyama, T., Hashimoto, T. and Ohshima, H.
A Fast Algorithm for Unsupervised Feature Value Selection.
DOI: 10.5220/0008981702030213
In *Proceedings of the 12th International Conference on Agents and Artificial Intelligence (ICAART 2020) - Volume 2*, pages 203-213
ISBN: 978-989-758-395-7; ISSN: 2184-433X

a redundant feature in a feature set has strong correlation with other features in the same set. According to Battiti's recommendation (Battiti, 1994), the correlation is measured using mutual information. In fact, Maximum-Relevance-Minimum-Redundancy (mRMR) (Peng et al., 2005) is a forward-selection algorithm and iterates selection of a feature that shows the best balance between mutual information to class labels (relevance) and a sum of mutual information to the features selected so far (redundancy). This greedy algorithm has improved the efficiency of the feature selection algorithms known so far, partly because it avoids evaluation of correlation for feature sets: the number of pairs of distinct features is $n(n-1)/2$, while the number of feature subsets is determined by 2^n.

One problem with this approach is that it does not incorporate interaction among features into the determination of relevance. Two or more features are said to mutually interact when each individual feature has no strong correlation to class labels but all the features together strongly correlate to class label. Zhao et al. (Zhao and Liu, 2007a) propose a practically fast algorithm that incorporates such interaction into the results of selection, while Shin et al. (Shin et al., 2017) further improved the efficiency and propose significantly fast algorithms that can scale to real big data.

Study of unsupervised feature selection is, on the other hand, more challenging, because class labels cannot be used to guide selection. As a substitute for class labels, pseudo-labels generated by clustering can be used to convert unsupervised problems into supervised problems (Qian and Zhai, 2013; LI et al., 2014; Liu et al., 2016). Also, some studies use preservation of manifold structures (He et al., 2005; Cai et al., 2010; Zhao and Liu, 2007b) and data-specific structures (Wei et al., 2016; Wei et al., 2017) as criteria of selection. In many cases, however, computationally-intensive procedures such as matrix decomposition are used to solve optimization problems. More importantly, the proposed algorithms aim to find a single answer which is merely a local solution. Since pseudo-labels and structures are derived from the entire feature set, which can include data that should be understood as noise or outliers for the purpose of selection, the solution can be inappropriate.

In contrast, this paper aims to develop a significantly fast algorithm for unsupervised feature selection that is equipped with an adjustable parameter to change local solutions that the algorithm selects. By leveraging these attributes of the algorithm, we can test a number of different parameter values. As a result, we can choose better solutions from the pool of solutions that the algorithm finds.

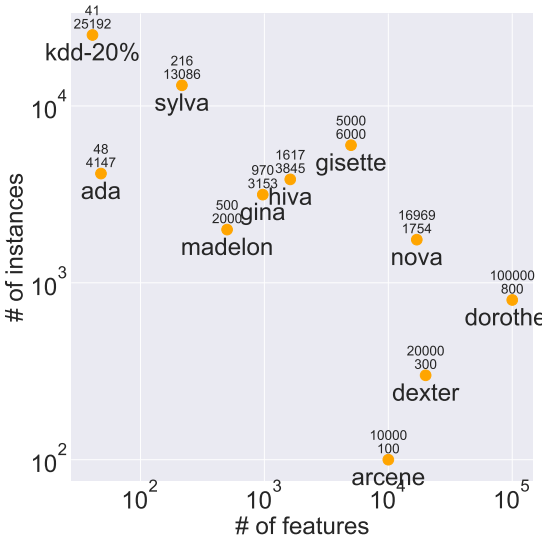


Figure 1: Eleven datasets used in our experiment.

2 PRELIMINARY ASSUMPTIONS AND NOTATIONS

In this paper, we assume that all continuous values specified in a dataset are discretized beforehand, and a feature always takes a finite number of categorical values.

For the purpose of analysis, we use 11 relatively large datasets of various types taken from the literature (Fig. 1): five from NIPS 2003 Feature Selection Challenge, five from WCCI 2006 Performance Prediction Challenge, and one from KDD-Cup. For continuous features included in the datasets, we categorize the values of such features into five equally long intervals before using them. The instances of all of the datasets are annotated with binary labels.

In this paper, a dataset D is a set of instances and $\mathcal{F}$ denotes the entire set of the features that describe D. A feature $f \in \mathcal{F}$ is a function $f : D \to R(f)$, where $R(f)$ denotes the range of f, which is a finite set of values. Also, we often treat f as a random variable with the empirical probability distribution derived from the dataset. That is, when $N(f = v)$ denotes the number of instances in a dataset D that have the value v at the feature f, $\Pr(f = v) = N(f = v)/|D|$ determines the empirical probability.

A feature set $S \subseteq \mathcal{F}$ can be viewed as a random variable associated with the joint probability for the features that belong to S: for a value vector $\boldsymbol{v} = (v_1, \ldots, v_n) \in R(f_1) \times \cdots \times R(f_n)$, $\Pr(S = \boldsymbol{v}) = N(f_1 = v_1, \ldots, f_n = v_n)/|D|$ determines the joint probability for $S = \{f_1, \ldots, f_n\}$. Furthermore, we introduce a random variable C to represent class labels of instances,

when the dataset is labeled.

Our method uses several measures from information theory defined for the random variables X and Y. The entropy of X is determined and denoted by

$$H(X) = -\sum_x \Pr(X=x)\log_2 \Pr(X=x), \quad (1)$$

and mutual information (MI) between X and Y is given by

$$I(X;Y) = \sum_x \sum_y \left[\Pr(X=x, Y=y) \cdot \log_2 \frac{\Pr(X=x, Y=y)}{\Pr(X=x)\Pr(Y=y)} \right]. \quad (2)$$

$I(X;Y)$ quantifies the portion of the information of X that also describes Y, and therefore, evaluates the relevance of X to Y.

To evaluate the extent to which X and Y are identical (isomorphic), we evaluate not only $I(X;Y)$ but also $H(X)$ and $H(Y)$. In fact, the normalized mutual information of X and Y is the harmonic mean of $I(X;Y)/H(X)$ and $I(X;Y)/H(Y)$, and is therefore defined as

$$\mathrm{NMI}(X;Y) = \frac{2 \cdot I(X;Y)}{H(X)+H(Y)}. \quad (3)$$

We have $\mathrm{NMI}(X;Y) \in [0,1]$, and $\mathrm{NMI}(X;Y) = 1$ holds, if, and only if, X and Y are isomorphic as random variables.

To measure the relevance of X to Y, we can also use the complement of Bayesian risk, defined as

$$\overline{\mathrm{Br}}(X;Y) = 1 - \mathrm{Br}(X;Y) = \sum_x \max_y \Pr(X=x, Y=y). \quad (4)$$

The following inequality describes the relationship between $I(X;Y)$ and $\overline{\mathrm{Br}}(X;Y)$ (Shin and Xu, 2009):

$$-\log_2 \overline{\mathrm{Br}}(X;Y) \le H(Y) - I(X;Y) \le -\overline{\mathrm{Br}}(X;Y)\log_2 \overline{\mathrm{Br}}(X;Y) + \mathrm{Br}(X;Y)\log_2 \frac{\mathrm{Br}(X;Y)}{|R(Y)|-1}. \quad (5)$$

In particular, $\overline{\mathrm{Br}}(X;Y) = 1$ and $I(X;Y) = H(Y)$ are mutually equivalent.

3 FEATURE VALUE SELECTION IN UNSUPERVISED LEARNING

To investigate the problem of unsupervised feature selection, we introduce two new principles: feature value selection instead of feature selection, and control of the support of feature value subsets to replace measures of relevance of feature subsets to class labels (class relevance).

D

f_0	f_1	C
0	2	1
0	1	1
0	0	0
1	0	2
2	0	2

D^b

$0_{@f_0}$	$1_{@f_0}$	$2_{@f_0}$	$0_{@f_1}$	$1_{@f_1}$	$2_{@f_1}$	C
1	0	0	0	0	1	1
1	0	0	0	1	0	1
1	0	0	1	0	0	0
0	1	0	1	0	0	2
0	0	1	1	0	0	2

Figure 2: An example dataset.

3.1 Feature Value Selection

Feature value selection selects feature *values* instead of features. Formally defined, given a dataset D, feature value selection is the introduction of new binary features to describe D using one-hot encoding. Note that we assume that D includes only categorical features, and hence, the range $R(f)$ of any feature f is a finite set.

Definition 1. *For a value $v \in R(f)$, $v_{@f}$ denotes a binary feature such that for an instance $x \in D$, $v_{@f}(x) = 1$ if $f(x) = v$; otherwise, $v_{@f}(x) = 0$.*

Thus, we can convert a dataset D into a new dataset D^b, which consists of the same instances but is described by $\mathcal{F}^b = \{v_{@f} \mid f \in \mathcal{F}, v \in R(f)\}$. Thus, we can equate feature value selection on a dataset D to feature selection on D^b.

Feature value selection has particular advantages in supervised learning, although it can be applied to other areas of machine learning. For an illustration, we will use the dataset shown in Fig. 2: two features f_0 and f_1 whose range is $\{0,1,2\}$ describe the dataset D, and five instances are annotated by the labels of 0, 1 and 2.

3.1.1 Clearer Model Interpretation

Feature value selection explains how features contribute to the determination of class labels more clearly. Even if a feature f is selected through feature selection, not all of the possible values of f necessarily contribute to the determination equally. In particular, only a small portion of values may be useful for explaining class labels.

In Fig. 2, neither f_0 nor f_1 alone determines class labels; hence, feature selection cannot help in selecting the entire features $\{f_0, f_1\}$. On the

other hand, among the six feature values, the feature values $\{0_{@f_0}, 0_{@f_1}\}$ fully determine class labels by $class\_label\_of(x) = 0_{@f_0}(x) + 2 \cdot 0_{@f_1}(x) \bmod 3$. This implies that in f_0 and f_1, the value 0 has more significance in explaining the class labels than the other values of 1 and 2.

3.1.2 Further Reduction of Entropy

The purpose of feature selection can be described simply as finding $S \subseteq \mathcal{F}$, where S has high relevance to class labels and low entropy $H(S)$. Feature value selection can select sets with less entropy than feature selection. To illustrate, we assume that feature value selection selects S' and let S be the minimum $S \subseteq \mathcal{F}$ with $S' \subseteq S^b = \{v_{@f} \mid f \in S, v \in R(f)\}$. Then, we have

Theorem 1. $H(S) = H(S^b)$.

Proof. The assertion follows from $\Pr(v_{1@f_1} = 1, \ldots, v_{n@f_n} = 1) = \Pr(f_1 = v_1, \ldots, f_n = v_n)$ and $\Pr(v_{@f} = 1, w_{@f} = 1) = 0$ for $v \neq w$. □

Hence, $H(S') \leq H(S^b) = H(S)$ holds by monotonicity of entropy.

For the example dataset, feature selection will select $\{f_0, f_1\}$, while feature value selection will select $\{0_{@f_0}, 0_{@f_1}\}$. Both consist of two elements, but the entropy scores are different. In fact, we have $H(\{f_0, f_1\}) = 2.32$ and $H(\{0_{@f_0}, 0_{@f_1}\}) = 1.52$. As a result, $\mathrm{NMI}(\{f_0, f_1\}; C) = 0.79$ and $\mathrm{NMI}(\{0_{@f_0}, 0_{@f_1}\}; C) = 1$ follows from $H(C) = I(\{0_{@f_0}, 0_{@f_1}\}; C) = 1.52$, and in particular, $\{0_{@f_0}, 0_{@f_1}\}$ turns out to be isomorphic to C as random variables.

3.2 Constraint by Support of Feature Subsets

In supervised learning, feature selection can leverage class relevance of feature sets As we saw in Section 2, we can use $\overline{\mathrm{Br}}(S;C)$ as a measure to evaluate the class relevance of S. To illustrate, we simply formalize supervised feature selection as the optimization problem of finding a feature subset S that minimizes $H(S)$ subject to $\overline{\mathrm{Br}}(S;C) = \overline{\mathrm{Br}}(\mathcal{F};C)$.

Because $S \subseteq S'$ implies $\overline{\mathrm{Br}}(S;C) \leq \overline{\mathrm{Br}}(S';C)$, $\overline{\mathrm{Br}}(\mathcal{F};C)$ is the upper bound of $\overline{\mathrm{Br}}(S;C)$. Therefore, solving the optimization problem means finding a feature subset S with minimum entropy that does not reduce class relevance. Although CWC and Lcc (Shin et al., 2011; Shin et al., 2015) implement this formalization, use of $\mathrm{Br}(S;C)$ was first introduced in INTERACT (Zhao and Liu, 2007a). MRMR (Peng et al., 2005) and CFS (Hall, 2000) use $I(S;C)$ instead of $\overline{\mathrm{Br}}(S;C)$.

We can restate the meaning of the constraint $\overline{\mathrm{Br}}(S;C) = \overline{\mathrm{Br}}(\mathcal{F};C)$: $\overline{\mathrm{Br}}(S;C)$ is calculated from a subset of instances such that the value vectors of S can uniquely determine their class labels in the subset. In other words, S can explain their class labels. In fact, $\overline{\mathrm{Br}}(S;C)$ is defined as the maximum ratio of the size of such subsets to $|D|$. Thus, we see that the constraint requires that the elimination of features from $\mathcal{F}$ to obtain S does not reduce the maximum number of instances explainable by S.

We intend to formalize unsupervised feature value selection based on the same idea, but we cannot leverage class relevance of feature sets as a guide. Hence, we need a substitute for $\overline{\mathrm{Br}}(S;C)$ that yields a constraint when minimizing $H(S)$. In fact, minimizing $H(S)$ with no constraint leads us to the trivial answer $S = \emptyset$.

For this purpose, we introduce the support of feature value subsets S:

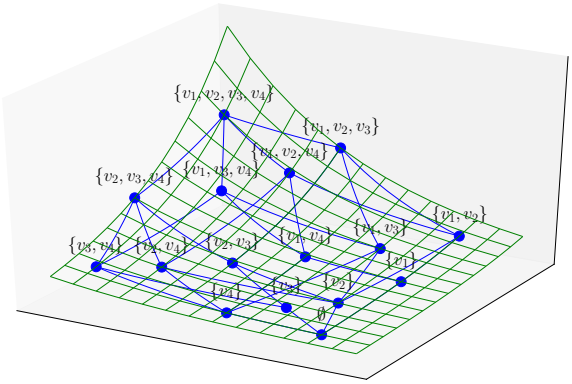
Definition 2. *For $S \subseteq \mathcal{F}^b$, the support of S is determined by* $\mathrm{supp}_D(S) = \{x \in D \mid \exists (v_{@f} \in S)[f(x) = v]\}$.

The support $\mathrm{supp}_D(S)$ consists of the instances that possess at least one feature value included in S, or, in other words, are explained by the feature values in S. Thus, we can determine a constraint for unsupervised feature value selection by the condition that the elimination of feature values from $\mathcal{F}^b$ to obtain S does not reduce the number of instances explainable by S. Specifically, because $\mathrm{supp}_D(\mathcal{F}^b) = D$ holds, we have the following formalization:

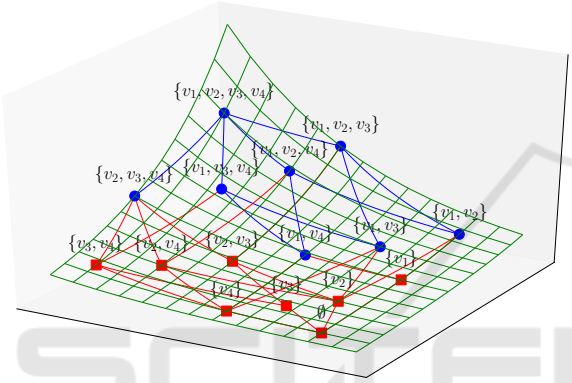
Unsupervised Feature Value Selection

Given an unlabeled dataset D described by a feature set $\mathcal{F}$, find $S \subseteq \mathcal{F}^b$ that minimizes $H(S)$ subject to $\mathrm{supp}_D(S) = D$.

The constraint actually restricts the search space of unsupervised feature value selection. As a result, it leads us to one or more non-trivial local solutions, as Fig. 3 illustrates. In the example, we assume $\mathcal{F}^b = \{v_1, v_2, v_3, v_4\}$ and consider the Hasse diagram of $\mathcal{F}^b$. The Hasse diagram of $\mathcal{F}^b$ is a directed graph (V_H, E_H) such that V_H is the power set of $\mathcal{F}^b$, and $(S,T) \in V_H \times V_H$ is in E_H, if, and only if, $S \supset T$ and $|S| - |T| = 1$ hold. Fig. 3 (a) depicts the Hasse diagram, and the height of a plot of $S \subseteq \mathcal{F}^b$ represents the magnitude of $H(S)$. On the other hand in Fig. 3 (b), the sets $S \subseteq \mathcal{F}$ with $\mathrm{supp}_D(S) \neq D$ are displayed in red, and we see that there are more than one minimal selections S in the sense that $\mathrm{supp}_D(S) = D$ holds but $\mathrm{supp}_D(T) \subsetneqq D$ holds for arbitrary $T \subsetneqq S$. One of these minimal S is the answer to the UFVS problem. Finding exact solutions to a UFVS problem, however, requires too much time both in theory and in practice. We need an approximation algorithm that works in practice.



(a) The Hasse diagram of $\{v_1, v_2, v_3, v_4\}$



(b) Restriction by complete coverage

Figure 3: Search space of UFVS.

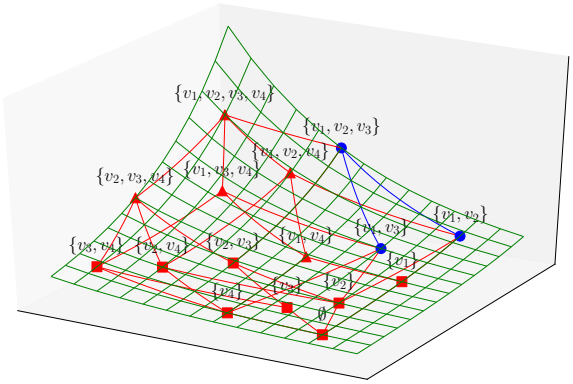


Figure 4: Restriction by a threshold.

4 A NEW FAST ALGORITHM FOR UNSUPERVISED FEATURE VALUE SELECTION

The approximation algorithm that we propose here is based on a gradient descent search. The following two points are the key components of our algorithm.

1. The approximation $\widetilde{H}(S) = \sum_{v \in S} H(v)$ substitutes for $H(s)$;
2. A threshold parameter t is used to cut off feature values with $H(v) \leq t$ before search.

The first component improves time efficiency so that our algorithm only has to evaluate $H(v)$ $v \in S$ to search the steepest downward edge from a selection $S \subseteq \mathcal{F}^b$ to an update. For example, in Fig. 3 (b), our algorithm can determine whether to move from $\mathcal{F}$ to $\mathcal{F} \setminus \{v_1\}$ by verifying only $H(v_1) > H(v_2) > H(v_3) > H(v_4)$, where the scores of $H(v_i)$ are computed once at the beginning.

The introduction of the threshold t, on the other hand, prevents the search from being captured by the same local minimum. When we place subsets S of the same size in increasing order of $\widetilde{H}(S)$ from left to right in a Hasse diagram, gradient descent always leads us to the leftmost minimal selection. In fact, $S = \{v_2, v_3, v_4\}$ is the solution of UFVS in Fig. 3 (b). To make a move among local solutions, we introduce the threshold parameter t, and our algorithm cuts off the feature values v with $H(v) \leq t$ before starting the search. For example, in Fig. 4, with a threshold t such that $H(v_3) > t \geq H(v_4)$, additionally, the vertices displayed as red triangles are eliminated, and the solution will be changed to $\{v_1, v_3\}$.

We can also frame our algorithm in the following way. Since $H(v)$ is an increasing function of $\Pr(v=1)$ if $\Pr(v=1) < \frac{1}{2}$, feature values v with too small $H(v)$ describe only a tiny portion of instances and will not be useful to describe the dataset. For example, if v identifies a particular instance, $H(v)$ is the minimum. Such feature values are eliminated by the initial cut-off based on the threshold. On the other hand, feature values with too great $\Pr(v=1)$ are common among instances and may not be useful for discriminating between instances. The gradient descent method eliminates feature values in the search space in decreasing order of $H(v)$, and therefore, feature values with greater $H(v)$ are more likely to be eliminated.

Algorithm 1 describes our algorithm. Due to the monotonicity property of $\mathrm{supp}_D(S) \subseteq \mathrm{supp}_D(T)$ for $S \subset T$, we can take advantage of a binary search to find the next feature value to leave in S. As a result, the algorithm is significantly fast as shown in Section 5.1.

The time complexity of Algorithm 1 can be estimated as follows: the complexity of computing $H(v_i)$ and the coverage of $\mathcal{F}^b[i, |\mathcal{F}^b|]$ for all i is $O(|\mathcal{F}^b| \cdot |D|)$; By updating the coverage of $S \cap \mathcal{F}^b[1,l]$ whenever we update l, $\mathrm{supp}_D(S \setminus \mathcal{F}^b[l+1, j]) = D$ can be investigated in $O(|D|)$-time, and the average

complexity to execute the while loop is estimated by $O((\log_2 |\mathcal{F}^b|)^2 \cdot |D|)$.

Algorithm 1: Unsupervised Feature Value Selection (our algorithm).

Require: An unlabeled dataset D described by $\mathcal{F}$; a threshold parameter $t \geq 0$.
Ensure: A minimal feature value set $S \subseteq \mathcal{F}^b$.
1: Let $\overline{S} = \mathcal{F}^b \setminus \{v_{@f} \in \mathcal{F}^b \mid H(v_{@f}) \leq t\}$.
2: Number the feature values of $\overline{S}$ so that $\overline{S} = \{v_1, \ldots, v_{|\overline{S}|}\}$ and $H(v_i) \geq H(v_j)$ for $i < j$.
3: Let $l = 0$ and $S = \overline{S}$.
4: **while** $l < |\overline{S}|$ **do**
5: Let $k = \max\{j \mid \mathrm{supp}_D(S \setminus \overline{S}[l+1, j]) = D, j = l, \ldots, |\overline{S}|\}$ by binary search.
6: Let $S = S \setminus \overline{S}[l+1, k]$ and $l = k+1$.
7: **end while**
8: **return** S.

5 EVALUATION OF PERFORMANCE

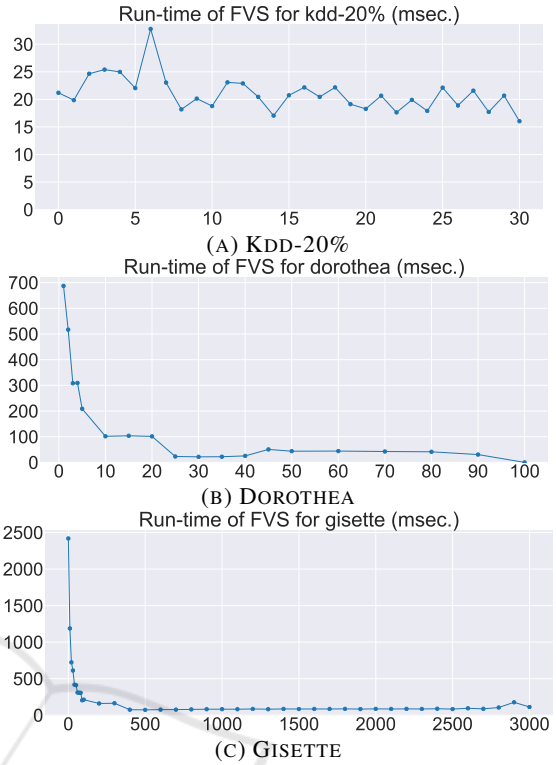
We ran experiments to evaluate the performance of our algorithm UFVS. In the experiments, we used the 11 datasets depicted in Fig. 1, selected from challenges of major conferences to make the evaluation fair. The evaluation is conducted from both efficiency and selection accuracy points of view.

5.1 Runtime Performance

Fig. 5 describes the runtime of Algorithm 1 in milliseconds for three typical datasets: KDD-20% with significantly many instances, DOROTHEA with significantly many features, and GISETTE with both many instances and many features (Fig. 1). The scores include only the time for search. For all 11 datasets we investigated, the runtime is no greater than 100 milliseconds, except for very small thresholds. We see that our algorithm is extremely fast. Although the x axis of Fig. 1 and the charts that follow it represents the threshold t, the displayed values are the number n with $t = -\frac{n}{|D|}\log_2\frac{n}{|D|} - \left(1-\frac{n}{|D|}\right)\log_2\left(1-\frac{n}{|D|}\right)$ and $n \leq |D|/2$; for a feature value v, $H(v) \leq t$, if, and only if, the number of the instances that have v is no greater than n.

5.2 Selection Performance

Several affinities appear in the results of nine of these eleven datasets (Fig. 6 to 10). We describe



(A) KDD-20%
(B) DOROTHEA
(C) GISETTE

Figure 5: Change in runtime measurements according to changes in threshold t.

the affinities taking GISETTE as an example (Fig. 6). For GISETTE, we changed the threshold t from 0 to 3,000 since GISETTE consists of 60,000 instances, the threshold of 3,000 is as small as 5%. Fig. 8 to 10 show the results for the other datasets.

1. The selection by our algorithm was performed without using the label information of the dataset at all. Even so, it found feature value sets that can explain the labels well. In fact, $I(S;C)$ remains close to $I(\mathcal{F};C)$, until t exceeds a certain limit (Fig 6 (b)). This property is significant evidence that our algorithm has an excellent ability to select *appropriate feature values*, because the label information initially given to the datasets is a *perfect summary* of the dataset.
2. Fig 6 (b) also shows that our algorithm can give different views of the dataset by changing t. In fact, when t exceeds the said limit, $I(S;C)$ rapidly decreases, and therefore, the feature values selected yield different clustering results than the initial clusters determined by the labels.
3. As t increases, $I(S;C)$ and $H(S)$ synchronously decrease (Fig. 6 (a) and (b)). This can be understood, if we assume that the dataset only includes feature values relevant to the labels, and

therefore, our algorithm starts to eliminate non-redundant and relevant feature values after it has eliminated all the redundant feature values.

4. $H(S)$ remains very close to its upper bound $H(\mathcal{F})$ (the orange line in Fig. 6 (a)), until t reaches the said limit. By contrast, the number of feature values selected decreases significantly rapidly as t increases (Fig. 6 (d)). Hence, an overwhelming majority of feature values v with small $H(v)$ are redundant, and eliminating them does not reduce the information that the dataset carries.
5. Fig. 6 (d) also shows that the feature values selected for $t \geq 1,000$ are fewer than the 35 features selected by CWC (Shin et al., 2011; Shin et al., 2015) (the green line) and significantly fewer than the 350 feature values of these features (the orange line).

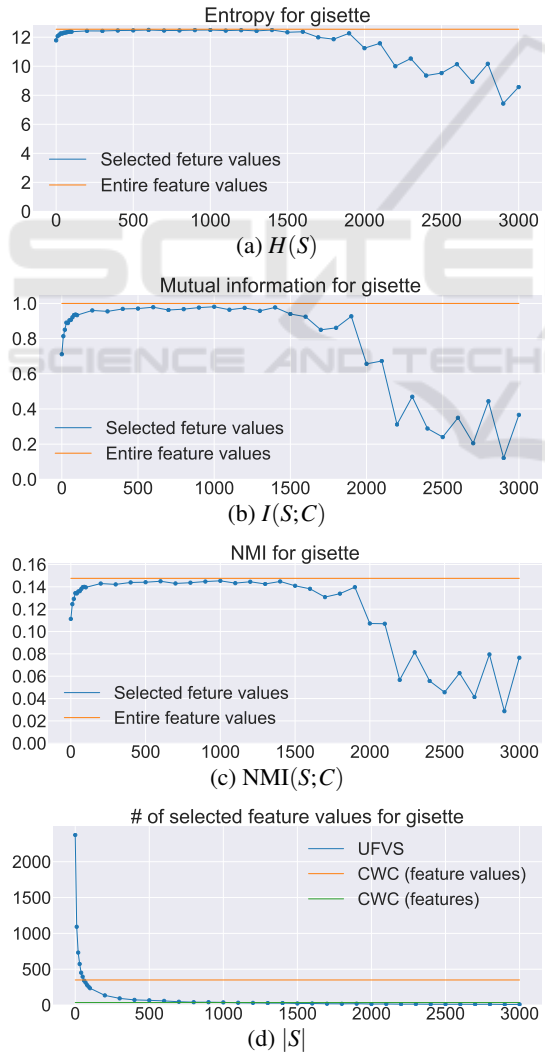


Figure 6: GISETTE.

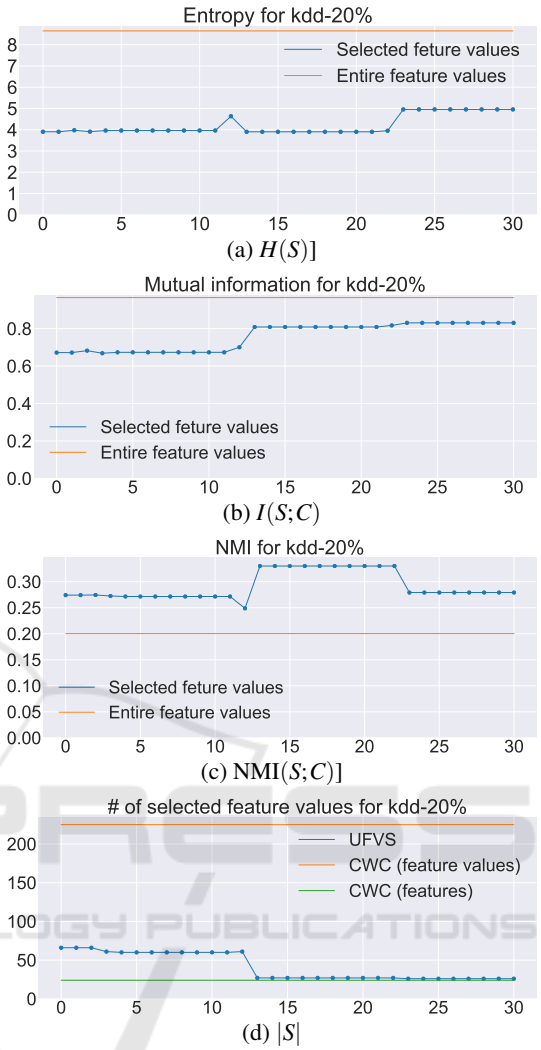


Figure 7: KDD-20%.

Also, the evaluation result of KDD-20% interests us. The dataset was created for study of intrusion detection. Hence, the features describe values specified in packet headers, and the instances (packets) are annotated relating to whether they are normal or anomalous. As opposed to the other datasets, the score of $H(S)$ moves around half of $H(\mathcal{F})$ (Fig. 7 (a)), while $I(S;C)$ remains close to $I(\mathcal{F};C)$ (Fig. 7 (b)). In fact, KDD-20% and ADA are the only datasets that could exhibit higher NMI$(S;C)$ than NMI$(\mathcal{F};C)$ (Fig. 7 (c)). With high $I(S;C)$ and low $H(S)$, the feature values selected could have good classification capability when used with a classifier. Also, it is surprising that the number of feature values selected is smaller than 30, when they show the highest score of NMI$(S;C)$. The figure is significantly lower than the 225 feature values that CWC selects for this dataset (Fig. 7 (d)), and hence, could provide a much more

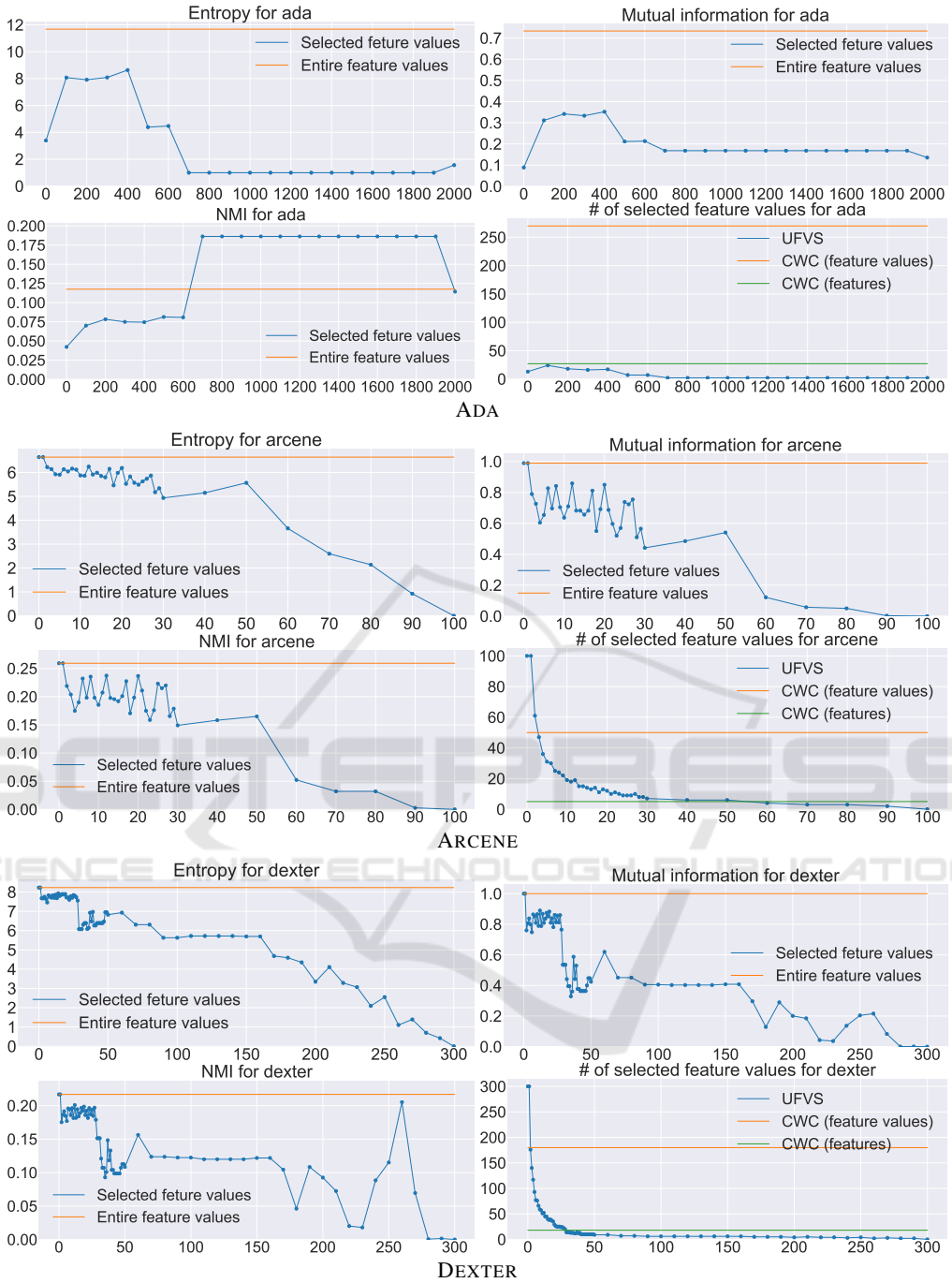


Figure 8: Experimental results for ADA, ARCENE and DEXTER.

interpretable model. Although it is out of the scope of this paper, applying our algorithm to intrusion detection will be an interesting direction for future research.

6 CONCLUSION

This paper introduced the principle of complete coverage and formally defined unsupervised feature value selection as an optimization problem: finding a minimal set of feature values that minimizes entropy un-

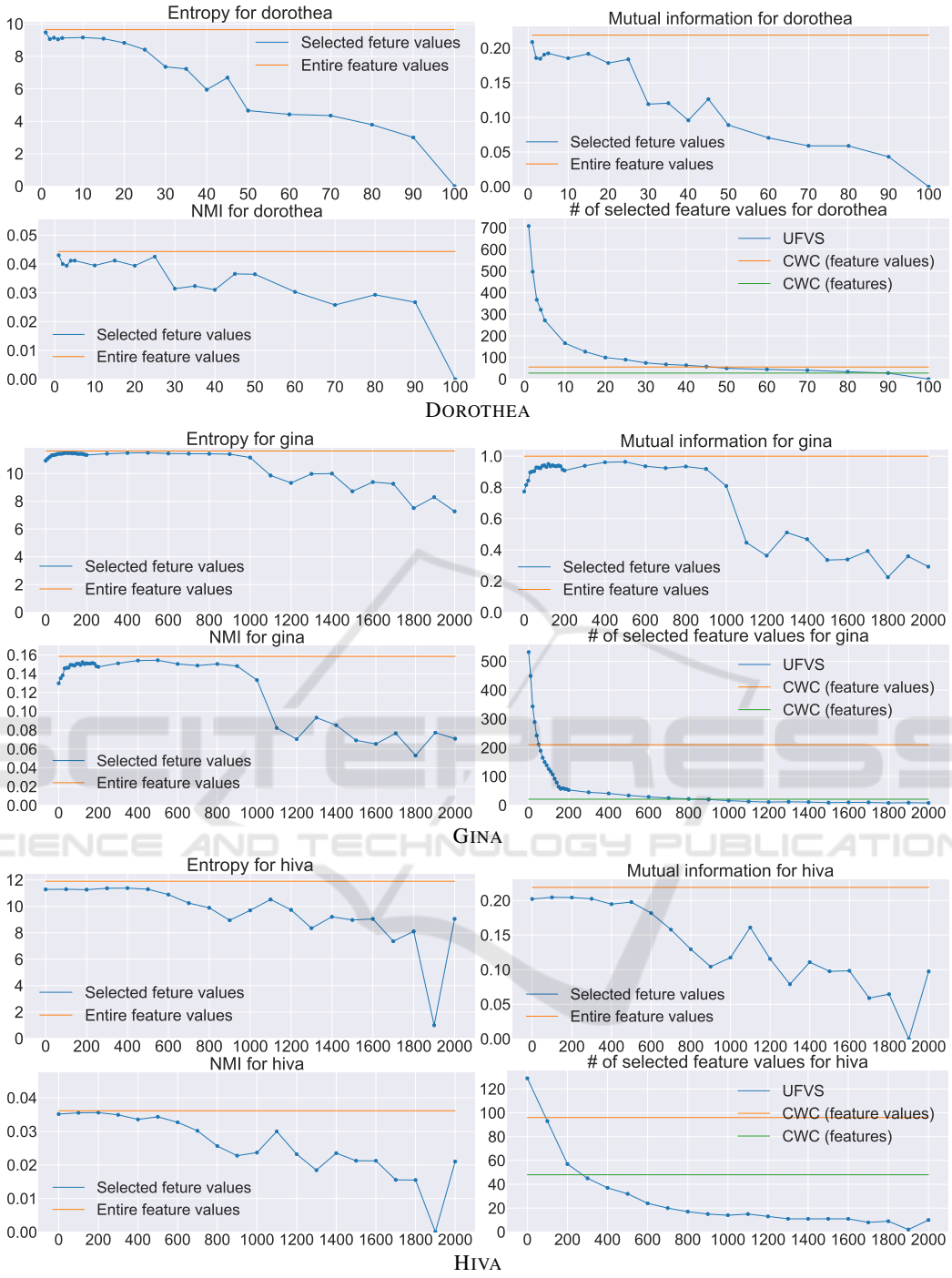


Figure 9: Experimental results for DOROTHEA, GINA and HIVA.

der the constraint. Without the constraint, the problem has a trivial meaningless solution, and hence, the constraint is essential to the definition of unsupervised feature value selection. Since the problem cannot be efficiently solved in theory and in practice, we have proposed a fast approximation algorithm, The algorithm's efficiency makes testing a number of different values for the threshold parameter practical, which avoids the need for a theoretically rigorous approach. Because no theoretically right solution for unsupervised feature value selection exists, the problem is intractable for unsupervised learning; by testing differ-

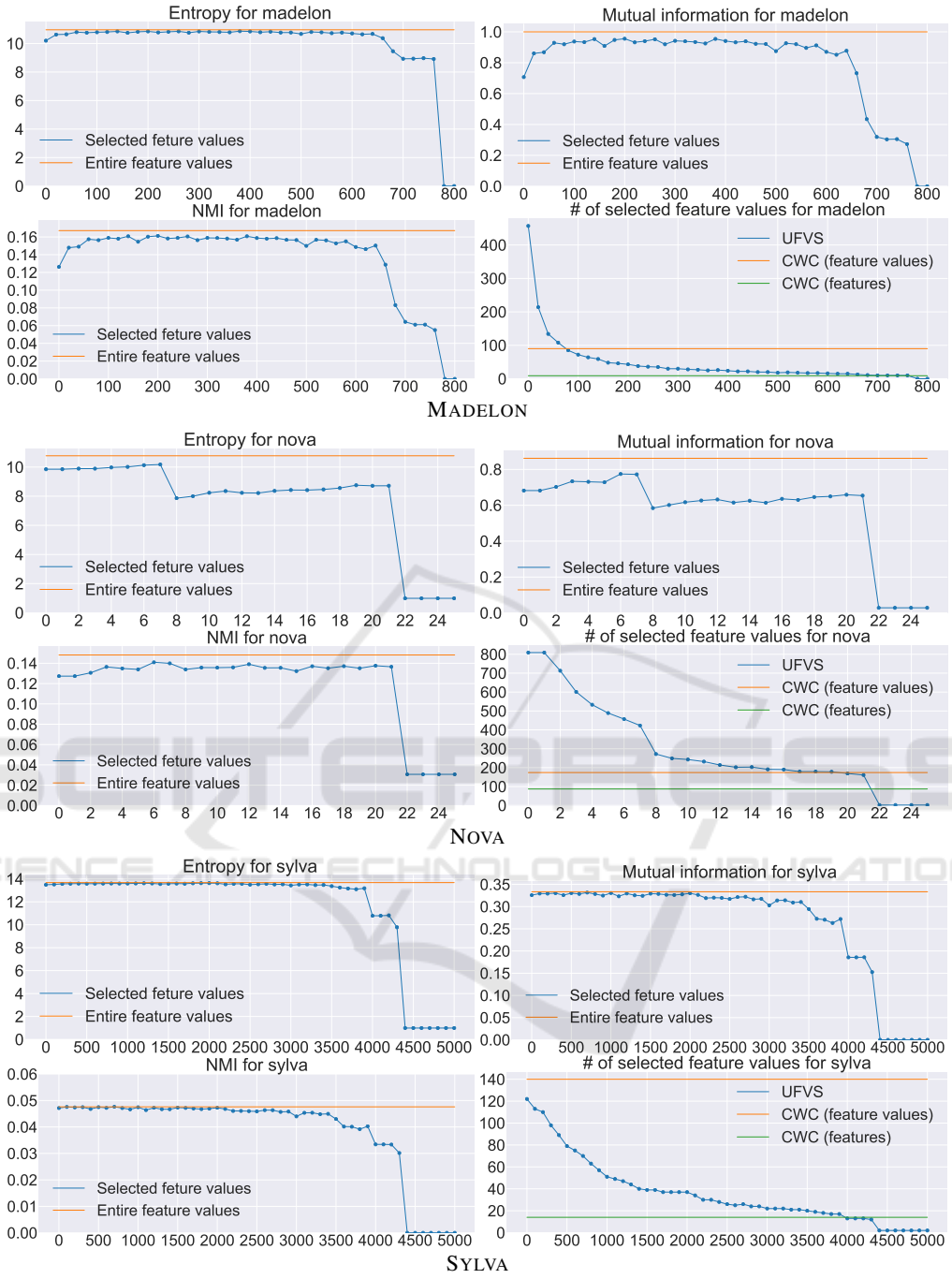


Figure 10: Experimental results for MADELON, NOVA and SYLVA.

ent threshold values, a human user is able to discover appropriate solutions by trying a varity of different values.

ACKNOWLEDGEMENTS

This work was partially supported by the Grant-in-Aid for Scientific Research (JSPS KAKENHI Grant Numbers 16K12491 and 17H00762) from the Japan Society for the Promotion of Science.

REFERENCES

Almuallim, H. and Dietterich, T. G. (1994). Learning boolean concepts in the presence of many irrelevant features. *Artificial Intelligence*, 69(1 - 2).

Battiti, R. (1994). Using mutual information for selecting features in supervised neural net learning. *IEEE Transactions on Neural Networks*, 5(4):537–550.

Cai, D., Zhang, C., and He, X. (2010). In *PIroceedings of the 16th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD 2010)*, pages 333–342.

Hall, M. A. (2000). Correlation-based feature selection for discrete and numeric class machine learning. In *ICML 2000*.

He, X., Cai, D., and Niyogi, P. (2005). Laplacian score for feature selection. In *Advances in Neural Information Processing Systems (NIPS 2005)*, pages 507–514.

LI, Z., Liu, J., Yang, Y., Zhou, X., and Liu, H. (2014). Clustering-guided sparse structural learning for unsupervised feature selection. *IEEE Transactions on Knowledge Data Engineering*, 26(9):2138–2150.

Liu, H., Shao, M., and Fu, Y. (2016). Consensus guided unsupervised feature selection. In *Proceedings of the 28th AAAI Conference on Artificial Intelligence (AAAI 2016)*, pages 1874–1880.

Peng, H., Long, F., and Ding, C. (2005). Feature selection based on mutual information: Criteria of max-dependency, max-relevance and min-redundancy. *IEEE Transaction on Pattern Analysis and Machine Intelligence*, 27(8).

Qian, M. and Zhai, C. (2013). Robust unsupervised feature selection. In *Proceedings of 23rd International Joint Conference on Artificial Intelligence (IJCAI 2013)*, pages 1621–1627.

Shin, K., Fernandes, D., and Miyazaki, S. (2011). Consistency measures for feature selection: A formal definition, relative sensitivity comparison, and a fast algorithm. In *22nd International Joint Conference on Artificial Intelligence*, pages 1491–1497.

Shin, K., Kuboyama, T., Hashimoto, T., and Shepard, D. (2015). Super-cwc and super-lcc: Super fast feature selection algorithms. In *Big Data 2015*, pages 61–67.

Shin, K., Kuboyama, T., Hashimoto, T., and Shepard, D. (2017). sCWC/sLCC: Highly scalable feature selection algorithms. *Information*, 8(4).

Shin, K. and Xu, X. (2009). Consistency-based feature selection. In *13th International Conferece on Knowledge-Based and Intelligent Information & Engineering System*.

Wei, X., Cao, B., and Yu, P. S. (2016). Unsupervised feature selection on networks: A generative view. In *Proceedings of the 28th AAAI Conference on Artificial Intelligence (AAAI 2016)*, pages 2215–2221.

Wei, X., Cao, B., and Yu, P. S. (2017). Multi-view unsupervised feature selection by cross-diffused matrix alignment. In *Proceedings of 2017 International Joint Conference on Neural Networks (IJCNN 2017)*, pages 494–501.

Zhao, Z. and Liu, H. (2007a). Searching for interacting features. In *Proceedings of International Joint Conference on Artificial Intelligence (IJCAI 2007)*, pages 1156 – 1161.

Zhao, Z. and Liu, H. (2007b). Spectral feature selection for supervised and unsupervised learning. In *Proceedings of the 24th International Conference on Machine Learning (ICML 2007)*, pages 1151–1157.