Information Sufficiency via Fourier Expansion

Mohsen Heidari
Purdue University
mheidari@purdue.edu

Jithin Sreedharan
Wadhwani AI
jithin@wadhwaniai.org

Gil Shamir
Google Inc.
gshamir@google.com

Wojciech Szpankowski
Purdue University
szpan@purdue.edu

***Abstract*—We take an information-theoretic approach to identify nonlinear feature redundancies in unsupervised learning. We define a subset of features as sufficiently-informative when the joint entropy of all the input features equals to that of the chosen subset. We argue that the rest of the features are redundant as all the accessible information about the data can be captured from sufficiently-informative features. Next, instead of directly estimating the entropy, we propose a Fourier-based characterization. For that, we develop a novel Fourier expansion on the Boolean cube incorporating correlated random variables. This generalization of the standard Fourier analysis is beyond product probability spaces. Based on our Fourier framework, we propose a measure of redundancy for features in the unsupervised settings. We then, consider a variant of this measure with a search algorithm to reduce its computational complexity as low as $O(nd)$ with n being the number of samples and d the number of features. Besides the theoretical justifications, we test our method on various real-world and synthetic datasets. Our numerical results demonstrate that the proposed method outperforms state-of-the-art feature selection techniques.**

I. Introduction

A central challenge in learning with feature selection is to jointly identify nonlinear *redundancies* within the features and the *dependencies* in the feature-label relation. Many well-known feature selection approaches (supervised or unsupervised) are based on measures that capture only linear relations or focus on the features individually [1]–[3]. Kernel-based methods are exception; however, are prohibitive in large datasets as the computational complexity of computing a kernel grows super linearly with the number of the samples [4]. Alternatively, information-theoretic metrics are powerful candidates in quantifying nonlinear dependencies among the random variables. However, typically estimating such quantities has high sample complexity.

In this work, we take an alternative approach and adapt a discrete Fourier analysis with information theoretic measures. Hence, capturing nonlinear relations with low sample complexity, while avoiding kernel computations. The discrete Fourier expansion (on the Boolean cube) provides an essential tool to characterize different levels of "nonlinearities" in a function. In this expansion, any real-valued function on the Boolean cube can be written as a linear combination of monomials (*parities*) [5], [6]. Highly nonlinear functions have Fourier expansion with large coefficients for high-degree parities. Thus, the Fourier expansion is potentially a powerful tool in learning problems. However, there are limitations making it impractical. First, it is developed for product probability spaces (mutually independent input variables). Secondly, this expansion is defined only for deterministic functions. These assumptions are too strong, as learning problems, often, involve correlated features with stochastic labeling.

In this work, we make a connection between the two approaches and aim to address these challenges. That said, the contributions of this paper are summarized below. A full version of the paper can be found in [7].

1) Fourier expansion for correlated random variables: The standard Fourier expansion on the Boolean cube has been central in a wide range of applications such as computational learning theory [8]–[12], noise sensitivity [5], [13], and other information-theoretic problems [14].

We develop a generalized Fourier expansion for functions of *correlated binary* random variables (Proposition 1). For this purpose, we adopt a Gram-Schmidt-type orthogonalization and construct a set of orthogonal basis functions. Further, we adapt our Fourier expansion to the more general space of stochastic mappings (e.g., mappings from one probability space to another). To the best of our knowledge, this is the first generalization of the Fourier expansion for correlated binary random variables. Although this Fourier expansion is defined on the Boolean cube, our algorithms are applicable to non-binary features too. We view the Binary Fourier as a framework that captures a special class of nonlinearities — those characterized via the *parities*. Alternatively, we could generalize our Fourier expansion to discrete features and, based on it, design feature selection algorithms. However, such a generalization requires character theory, which is beyond the scope of this paper. We note that there are other forms of orthogonal decomposition including the Hoeffding-Sobel decomposition [15]–[17]. However, such decompositions are basis-free. Our Fourier expansion is defined by constructing a set of *orthonormal* basis functions which makes it suitable for feature selection.

2) Sufficiently Informative: In the unsupervised setting, we take an information-theoretic perspective, and group the features into *redundant* and *sufficiently informative*. All the accessible *information* about the data can be captured from the later group. More precisely, we define a subset of features as sufficiently-informative when the joint entropy of all the input features equals to that of the chosen subset. The former group is statistically a function of the later, hence can be removed without affecting the learning's performance. This approach extends the notion of *Markov blanket* for "redundant" features to the unsupervised setting [18]–[20]. We then develop a characterization of sufficiently informative features based on

our Fourier expansion (Theorem 1). Built upon this, we design an Unsupervised Fourier Feature Selection (UFFS) algorithm, which captures the redundant features in our new formulation. Instead of ranking the features, the UFFS finds redundant features and declares the rest of the features as sufficiently informative. Through comprehensive numerical experiments in Section V, we show that the UFFS outperforms well-known methods for unsupervised feature selection.

A. Related Works

The literature in this area is extensive. Here we can only give pointers to some of the best known approaches. Some common approaches in unsupervised feature selection are pseudo-label based, "column subset selection", and spectral/manifold based. Methods in the first approach such as [21], [22] attempt to generate pseudo-labels via certain clustering methods. However, such methods focus on linear transformations between features and the pseudo labels and ignore the nonlinear relations.

The second approach, "column subset selection", assumes only linear dependencies among the features and solves an optimization problem that is similar to principal component analysis (PCA) [23], [24]. Although methods in the third approach, such as [25], [26], capture nonlinear relations, they ignore the interaction between the features.

We emphasize here that although dimension reduction methods such as Kernel PCA captures non-linear redundancies, they are not feature selection as the output is a mixture of the features.

In the supervised settings, several measures and approaches has been introduced. Among them are similarity-based measures (e.g., Pearson correlation, Fisher Score), information-theoretic measures [18], [27]–[30], and Kernel-based measures [31]–[33]. A nice survey is available in [1] and [2].

Notations: We write $[m]$ for set $\{1, 2, \cdots, m\}$. For any subset $\mathcal{J} \subseteq [d]$ with ordered elements $\{j_1, j_2, \cdots, j_k\}$, the vectors $(X_{j_1}, X_{j_2}, \cdots, X_{j_k})$, and $(x_{j_1}, x_{j_2}, \cdots, x_{j_k})$ are denoted, respectively, by $\mathbf{X}^{\mathcal{J}}$ and $\mathbf{x}^{\mathcal{J}}$.

II. Fourier for Correlated Random Variables

In this section, we propose a novel Fourier expansion for functions of *correlated* binary features.

We start with a brief overview of the well-known Fourier expansion on Boolean cube [5]. Let $\mathbf{X} = (X_1, X_2, ..., X_d)$ be a vector of mutually independent random variables taking values from a $\{-1, 1\}$. Let μ_j and σ_j be the mean and standard-deviation of $X_j, j \in [d]$. Suppose that these random variables are non-trivial, that is $\sigma_j > 0$ for all $j \in [d]$. The Fourier expansion is defined via a set of basis functions called *parities*. The *parity* for a subset $\mathcal{S} \subseteq [d]$ is defined as

$$\phi_{\mathcal{S}}(\mathbf{x}) \triangleq \prod_{i \in \mathcal{S}} \frac{x_i - \mu_i}{\sigma_i}, \qquad \text{for all } \mathbf{x} \in \mathbb{R}^d.$$

Since X_i's are mutually independent, the parities are orthonormal, that is $\mathbb{E}[\phi_{\mathcal{S}}(\mathbf{X})^2] = 1$ for any subset $\mathcal{S}$, and $\mathbb{E}[\phi_{\mathcal{S}}(\mathbf{X})\ \phi_{\mathcal{T}}(\mathbf{X})] = 0$ when $\mathcal{T} \neq \mathcal{S}$ (that is $\exists x \in \mathcal{T} \bigcup \mathcal{S}$ such that $x \notin \mathcal{T} \bigcap \mathcal{S}$). Under the assumption that $\mathcal{X} = \{-1, 1\}^d$, the parities form an orthonormal basis for the space of bounded function $f : \{-1, 1\}^d \mapsto \mathbb{R}$ [5]. That is, any bounded function $f : \{-1, 1\}^d \mapsto \mathbb{R}$ can be written as a linear combination of the form

$$f(\mathbf{x}) = \sum_{\mathcal{S} \subseteq [d]} \mathtt{f}_{\mathcal{S}}\ \phi_{\mathcal{S}}(\mathbf{x}),$$

for all $\mathbf{x} \in \{-1, 1\}^d$, where $\mathtt{f}_{\mathcal{S}} \in \mathbb{R}$ are called the *Fourier coefficients* of f with respect to $P_{\mathbf{X}}$, the distribution of $\mathbf{X}$. Further, the Fourier coefficients can be computed as $\mathtt{f}_{\mathcal{S}} = \mathbb{E}[f(\mathbf{X})\phi_{\mathcal{S}}(\mathbf{X})]$, for all subsets $\mathcal{S} \subseteq [d]$.

With this overview, we are ready to construct our Fourier expansion. Note that, in a general probability space with correlated features, the standard Fourier expansion is no longer well-defined. Because, the parities $\phi_{\mathcal{S}}$ are not necessarily orthogonal. That said, we construct our Fourier expansion by adopting a Gram-Schmidt-type procedure to make the parities *orthogonal*. Then, we use this basis to develop our Fourier expansion for function of correlated random variables. The orthogonalization process is explained in the following.

A. Orthogonalization process:

Fix the following ordering for subsets of $[d]$:

$$\emptyset, \{1\}, \{2\}, \{1, 2\}, \{3\}, \{1, 3\}, \{2, 3\}, \cdots, \{1, 2, ..., d\}. \quad (1)$$

For any pair of functions g_1, g_2 denote $\langle g_1, g_2 \rangle = \mathbb{E}[g_1(\mathbf{X})g_2(\mathbf{X})]$. We apply the Gram-Schmidt process on the parities $\phi_{\mathcal{S}_i}$ with the above ordering and $\langle g_1, g_2 \rangle$ as the inner product. With this method, the orthogonalized parity corresponding to the ith subset is obtained from the following equations

$$\tilde{\psi}_{\mathcal{S}_i} = \phi_{\mathcal{S}_i} - \sum_{j=1}^{i-1} \langle \psi_{\mathcal{S}_j}, \phi_{\mathcal{S}_i} \rangle \psi_{\mathcal{S}_j} \quad (2)$$

$$\psi_{\mathcal{S}_i} = \begin{cases} \frac{\tilde{\psi}_{\mathcal{S}_i}}{\|\tilde{\psi}_{\mathcal{S}_i}\|_2} & \text{if } \|\tilde{\psi}_{\mathcal{S}_i}\|_2 > 0 \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

where $\|\tilde{\psi}_{\mathcal{S}_i}\|_2 = \sqrt{\langle \tilde{\psi}_{\mathcal{S}_i}, \tilde{\psi}_{\mathcal{S}_i} \rangle}$. Note that the first orthogonalized parity is given by $\psi_{\emptyset}(\mathbf{x}) = 1$ for all $\mathbf{x} \in \mathbb{R}^d$. By construction, the resulted nontrivial parities $\psi_{\mathcal{S}_i}$'s are orthonormal, that is $\langle \psi_{\mathcal{S}_i}, \psi_{\mathcal{S}_j} \rangle = 0$ for $i \neq j$ and $\langle \psi_{\mathcal{S}_i}, \psi_{\mathcal{S}_i} \rangle = 1$ if $\psi_{\mathcal{S}_i}$ is not trivial.

Depending on the statistics of the features, the number of non-trivial parities ranges from 1 to 2^d. On one extreme, if the features are mutually independent, then $\psi_{\mathcal{S}_i} = \phi_{\mathcal{S}_i}$. On the other extreme, if the features are trivial, then $\psi_{\mathcal{S}_i} = 0$ for $i > 1$, and hence there is only one non-trivial parity. Note also that different orderings for the subsets of $[d]$ result in different orthogonalized parities. We can show that ordering (1) is beneficial to remove "redundant" features. Hence, unless otherwise stated, we use the ordering in (1).

In the next proposition we establish our Fourier expansion for functions of correlated binary random variables.

Proposition 1 (Correlated Fourier Expansion). *Let $P_{\mathbf{X}}$ be any probability distribution on $\{-1, 1\}^d$ and $f : \{-1, 1\}^d \mapsto$*

$\mathbb{R}$ *be a bounded function. Let* $\psi_{\mathcal{S}}$*'s be the orthogonalized parities as defined in* (2)*. Then, for all* $\mathbf{x} \in \{-1,1\}^d$ *except a measure-zero subset,* $f(\mathbf{x})$ *is decomposed as*

$$f(\mathbf{x}) = \sum_{\mathcal{S}\subseteq[d]} f_{\mathcal{S}}\psi_{\mathcal{S}}(\mathbf{x}),$$

where the summation is taken over all $\mathcal{S} \subseteq [d]$ *for which* $\psi_{\mathcal{S}}$ *is not trivial. Further, the coefficients* $f_{\mathcal{S}}$ *are unique and obtained from* $f_{\mathcal{S}} = \mathbb{E}[f(\mathbf{X})\psi_{\mathcal{S}}(\mathbf{X})]$.

As discussed before, depending on $P_{\mathbf{X}}$, some of the parities $\psi_{\mathcal{S}}$ are trivial. Hence, the corresponding coefficients $f_{\mathcal{S}}$ are made to be zero.

We view our binary Fourier as a framework that captures a special class of nonlinearities — those characterized via orthogonalized parities. Our numerical experiments presented in Section V verifies that such a special class is sufficient for many data sets (see Table I).

III. Information Sufficiency

We build upon our orthogonalization process in (2) and develop our UFFS algorithm (see Algorithm 1) to capture non-linear redundancies in the features. For this purpose, we first define a measure to identify the features as "sufficiently informative" and "redundant". Intuitively, the former group contains all the *information* accessible from the features. The later consists of the features that are a function of the "informative" features, and hence, can be removed from the data set.

Suppose that there are d features denoted by the random vector $\mathbf{X} = (X_1, X_2, ..., X_d)$ taking values from a discrete subset $\mathcal{X} \subset \mathbb{R}^d$. We say $\mathcal{J} \subseteq [d]$ is a "sufficiently informative" feature subset, if $H(\mathbf{X}) = H(X^{\mathcal{J}})$, where H is the Shannon entropy. This definition is related to the notion of Markov Blanket [28], as $\mathcal{J}$ is a Markov blanket for any feature in $\mathcal{J}^c$. Also, $\mathcal{J}$ being sufficiently informative immediately leads to $\mathcal{J}^c$ being redundant. Because, the condition $H(\mathbf{X}) = H(X^{\mathcal{J}})$ implies that there exists a mapping T, such that $X^{\mathcal{J}^c} = T(X^{\mathcal{J}})$, with probability one [34]. Hence, all the features not included in $\mathcal{J}$ can be removed. With this elimination, the dimension is reduced from d to $|\mathcal{J}|$. As there are multiple such $\mathcal{J}$'s, the objective is to find the smallest one[1]. Tolerating small amounts of imperfections, we formalize the above notion in the following.

Definition 1 (Sufficiently Informative). *For discrete features and* $0 \leq \epsilon \leq 1$*, a feature subset* $\mathcal{J}$ *is said to be* ϵ*-sufficiently informative, if* $H(\mathbf{X}|X^{\mathcal{J}}) \leq \epsilon$*. The feature subset* $\mathcal{J}$ *is sufficiently informative, if* $H(\mathbf{X}|X^{\mathcal{J}}) = 0$*. Such* $\mathcal{J}$ *is called minimal, if it has the minimum cardinality among all sufficiently informative feature subsets.*

Next, we make a connection between the above definition and the orthogonalization process in (2). We employ this process to extract a sufficiently informative feature subset. Fix the standard ordering as in (1), and generate the orthogonalized parities $\psi_{\mathcal{S}_i}$.

Theorem 1. *Let* $\mathcal{J}_\epsilon \subseteq [d]$ *be the set of all* i*'s such that* $\|\tilde{\psi}_{\{i\}}\|_2 > \epsilon$*. Then, for sufficiently small* $\epsilon > 0$*,* $H(\mathbf{X}|X^{\mathcal{J}_\epsilon}) = 0$*. Further, if the features take values from* $\{-1,1\}^d$*, then there exists a permutation of the features so that* $\mathcal{J}_\epsilon$ *with* $\epsilon = 0$ *is a sufficiently informative subset that is minimal.*

Proof. We start by deriving an upper-bound on $H(\mathbf{X}|X^{\mathcal{J}_\epsilon})$ in terms of the orthogonalized parities in (2). Note that $H(\mathbf{X}|X^{\mathcal{J}_\epsilon}) = H(X^{\mathcal{J}_\epsilon^c}|X^{\mathcal{J}_\epsilon})$, where $\mathcal{J}_\epsilon^c$ is the complement of $\mathcal{J}_\epsilon$. Thus, from the chain rule [34], this quantity equals to $\sum_{i\in\mathcal{J}_\epsilon^c} H(X_i|X^{\mathcal{J}_\epsilon}, X^{i-1})$. As X_i is a discrete random variable and $\phi_{\{i\}}(\mathbf{x}) = (x_i - \mu_i)/\sigma_j$, then

$$H(X_i|X^{\mathcal{J}_\epsilon}, X^{i-1}) = H\big(\phi_{\{i\}}(\mathbf{X})|X^{\mathcal{J}_\epsilon}, X^{i-1}\big),$$

Since $\phi_{\{i\}}$ is the standard parity as in Section II, then, from the orthogonalization process in (2), we can write

$$\phi_{\{i\}} = \tilde{\psi}_{\{i\}} + \sum_{\mathcal{S}\subseteq[i-1]} \alpha_{\mathcal{S}}\psi_{\mathcal{S}}, \tag{4}$$

where $\alpha_{\mathcal{S}} = \langle\phi_{\{i\}}, \psi_{\mathcal{S}}\rangle$. In this decomposition, the terms in the summation depend only on X^{i-1}. This is due to the particular ordering in (1). Therefore, we get the following upper-bound

$$H(\phi_{\{i\}}|X^{\mathcal{J}_\epsilon}, X^{i-1}) = H(\tilde{\psi}_{\{i\}}|X^{\mathcal{J}_\epsilon}, X^{i-1}) \leq H(\tilde{\psi}_{\{i\}}),$$

where the last inequality follows by removing the conditioning in the entropy. Lastly, adapting this bound for all $i \in \mathcal{J}_\epsilon^c$, we get the following upper-bound

$$H(X^d|X^{\mathcal{J}_\epsilon}) \leq \sum_{i\in\mathcal{J}_\epsilon^c} H(\tilde{\psi}_{\{i\}}). \tag{5}$$

Now set $\epsilon = \min\{\|\tilde{\psi}_{\{i\}}\|_2 : i \in [d], \|\tilde{\psi}_{\{i\}}\|_2 > 0\}$. Then, for any $i \notin \mathcal{J}_\epsilon$, we have that $\|\tilde{\psi}_{\{i\}}\|_2 = 0$. Therefore, $H(\tilde{\psi}_{\{i\}}) = 0$ for all $i \in \mathcal{J}_\epsilon^c$ and, from (5), we get that $H(X^d|X^{\mathcal{J}_\epsilon}) = 0$. This completes the proof for the first statement of the theorem.

Next, we prove the second statement: "if the features take values from $\{-1,1\}^d$, then there exist a permutation of the features so that $\mathcal{J}_\epsilon$ with $\epsilon = 0$ is a *sufficiently informative* subset with minimum cardinality." Note that, from Definition 1, the subset $\mathcal{J}_0$ is sufficiently informative. This is because for any $j \notin \mathcal{J}_0$ the parity $\tilde{\psi}_{\{j\}}(\mathbf{X}) = 0$ with probability one. Therefore, from (2), the standard parity $\phi_{\{j\}}$ is a function of $(X_1, X_2, ..., X_{j-1})$. Implying that X_j is a function of $(X_1, X_2, ..., X_{j-1})$. Hence, $H(X^d|X^{\mathcal{J}_0}) = 0$. It remains to prove $\mathcal{J}_0$ is minimal when the features take values from $\{-1,1\}^d$ and are permuted appropriately.

Let $\mathcal{A} \subseteq [d]$ be a sufficiently informative subset with minimum cardinality as in Definition 1. Consider a permutation of the features such that the first $|\mathcal{A}|$ features are from $\mathcal{A}$. We perform the orthogonalization process on the permuted features. Let $\mathcal{J}_0$ be the subset for which $\|\tilde{\psi}_{\{i\}}\|_2 > 0$. Since, $\mathcal{A}$ is sufficiently informative with minimal cardinality, then $\mathcal{A} \subseteq \mathcal{J}_0$. We show that in fact $\mathcal{J}_0 \subseteq \mathcal{A}$, implying that $\mathcal{J}_0 = \mathcal{A}$ and, hence, $\mathcal{J}_0$ is minimal. By contradiction, suppose

[1]The set of all features is a trivial example of a sufficiently informative feature subset.

that $\mathcal{J}_0 \backslash \mathcal{A}$ is not empty. Then, there exists $j \notin \mathcal{A}$ such that $\|\tilde{\psi}_{\{j\}}\|_2 > 0$. As a result, $\psi_{\{j\}}$ is orthogonal to all $\psi_{\mathcal{S}}$ with $\mathcal{S} \subseteq A$ and, hence, cannot be written as a linear combination of $\psi_{\mathcal{S}}$ with $\mathcal{S} \subseteq \mathcal{A}$. This is a contradiction because subset $\mathcal{A}$ being sufficiently informative implies that any function $f(\mathbf{x}^d)$ can be written as $g(\mathbf{x}^{\mathcal{A}})$ for some function g. Thus, the Fourier expansion of $f(\mathbf{x}^d)$ must involve only $\psi_{\mathcal{S}}$, for $\mathcal{S} \subseteq \mathcal{A}$. But as explained above, $\psi_{\{j\}}$ is a function that contradicts this property. Therefore, $\mathcal{J}_0 \backslash \mathcal{A} = \emptyset$, and hence, $\mathcal{J}_0 = \mathcal{A}$ and is minimal. □

IV. Unsupervised Learning Algorithm

As a result of Theorem 1, $\|\tilde{\psi}_{\{i\}}\|_2$ can be viewed as a measure of the *redundancy* of each feature and that the orthogonalization procedure can remove them. We use this measure for unsupervised feature selection, where n independent and identically distributed (i.i.d.) instances $\{\mathbf{x}(i), i \in [n]\}$, with possible correlations across feature dimension, are available.

The idea is to perform the orthogonalization process as in (2) and find the features j for which $\|\tilde{\psi}_{\{j\}}\|_2$ is smaller than a threshold ϵ. These features are declared as redundant. As for the algorithm, two issues need to be addressed: 1) the orthogonalization takes exponential time, as there are 2^d feature subsets, and 2) estimation of $\|\tilde{\psi}_{\{j\}}\|_2$ from the training instances. In what follows, we address these issues. Our UFFS algorithm is presented in Algorithm 1.

a) **Fixed-depth search:** We propose to address the first issue using a *fixed-depth* search method. Given a parameter $t \leq d$, the orthogonalization is performed only on feature subsets of size at most t. For that we use the standard ordering as in (1), but restricted to subsets of size at most t.

b) **Empirical orthogonalization:** We propose a recursive formula to perform the orthogonalization and estimate $\|\tilde{\psi}_{\{j\}}\|_2$. Let $b_{j,i} = \langle \phi_{\mathcal{S}_j}, \phi_{\mathcal{S}_i} \rangle$, and define $a_{j,i} = \langle \psi_{\mathcal{S}_j}, \phi_{\mathcal{S}_i} \rangle$. Therefore, (2) can be written as that

$$\tilde{\psi}_{\mathcal{S}_i} = \phi_{\mathcal{S}_i} - \sum_{j<i} a_{j,i} \psi_{\mathcal{S}_j}.$$

Due to the orthonormality of $\psi_{\mathcal{S}_i}$'s, we obtain that $\|\tilde{\psi}_{\mathcal{S}_i}\|_2^2 = b_{i,i} - \sum_{j<i} a_{j,i}^2$. Further, the coefficients $a_{j,i}$ can be calculated recursively as

$$a_{j,i} = \frac{1}{\sqrt{b_{j,j} - \sum_{r<j} a_{r,j}^2}} \Big(b_{j,i} - \sum_{\ell<j} a_{\ell,j} a_{\ell,i} \Big). \tag{6}$$

With this formulas, we first compute an empirical estimate of $b_{j,i}$'s, denoted by $\hat{b}_{j,i}$. Then, we compute an estimation of $a_{j,i}$'s (denoted by $\hat{a}_{j,i}$) by calculating (6) with $b_{j,i}$ and $a_{j,i}$ replaced by $\hat{b}_{j,i}$ and $\hat{a}_{j,i}$, receptively. Lastly, we obtain an empirical estimate of $\|\tilde{\psi}_{\mathcal{S}_i}\|_2$ by computing $\sqrt{\hat{b}_{i,i} - \sum_{j<i} \hat{a}_{j,i}^2}$.

c) **Clustering the features:** The above two processes are implemented in Algorithm 1. For large dimensional data sets, we can group the features into multiple clusters of approximately equal size (say m features). Then, we perform Algorithm 1 on each cluster, and remove the redundant features within it.

With this approach, the computational complexity of UFFS algorithm with depth parameter t and cluster size m is $O(n \frac{d}{m} m^{2t})$. The parameters m and t are chosen independently of (n, d). For instance, we choose $t = 3$ and $m = 40$. As a result, we obtain a complexity linear in the size of the data set.

Algorithm 1 Unsupervised Fourier Feature Selection (UFFS)

Input: n training samples $\mathbf{x}_i \in \mathbb{R}^d$, depth parameter $t \leq d$, and redundancy threshold $\epsilon \in (0, 1)$

Output: Features' measures $\mathsf{norm}(j), j = 1, 2, ...d$

Compute the empirical mean $\hat{\mu}_j$ and standard deviation $\hat{\sigma}_j$ of each feature.

Generate all subsets $\mathcal{S}_i \subseteq [d]$ with size at most t and with the standard ordering as in (1). Compute the matrix $\hat{\mathbf{B}}$ with elements:

$$\hat{b}_{j,i} \leftarrow \frac{1}{n} \sum_{l=1}^{n} \Big[\prod_{u \in \mathcal{S}_j} \frac{x_{lu} - \hat{\mu}_u}{\hat{\sigma}_u} \Big] \Big[\prod_{v \in \mathcal{S}_i} \frac{x_{lv} - \hat{\mu}_v}{\hat{\sigma}_v} \Big].$$

Set $\hat{\mathbf{A}} \leftarrow \hat{\mathbf{B}}$

for row j of $\hat{\mathbf{A}}$ **do**

  update the jth row: $\hat{\mathbf{A}}_{j,*} \leftarrow \hat{\mathbf{A}}_{j,*} - \sum_{\ell<j} \hat{a}_{\ell,j} \hat{\mathbf{A}}_{\ell,*}$

  Compute $\mathsf{norm}(\mathcal{S}_j) \leftarrow \sqrt{[\hat{b}_{j,j} - \sum_{r<j} \hat{a}_{r,j}^2]^+}$

  if $\mathsf{norm}(\mathcal{S}_j) \leq \epsilon$ **then**

    Set the jth row of $\hat{\mathbf{A}}$ zero: $\hat{\mathbf{A}}_{j,*} \leftarrow \mathbf{0}$

  else

    Normalize the jth row: $\hat{\mathbf{A}}_{j,*} \leftarrow \frac{\hat{\mathbf{A}}_{j,*}}{\mathsf{norm}(\mathcal{S}_j)}$

Declare all $\ell \in [d]$ with $\mathsf{norm}(\{\ell\}) \geq \epsilon$ as non-redundant.

We present our experimental results next. We provide a consistency analysis on asymptotic performance of the algorithm.

Theorem 2. *Let $\hat{\mathcal{J}}_n$ be the set of features declared by Algorithm 1 with parameter $t \leq k$ when executed on n discrete i.i.d. samples. Then, there exists a function λ such that $\hat{\mathcal{J}}_n$ is a $\lambda(\epsilon, n)$-sufficiently informative. Further, $\lim_{n \mapsto \infty} \lim_{\epsilon \mapsto 0} \lambda(\epsilon, n) = 0$*

Proof sketch. Let $\hat{D}_n$ denote the empirical distribution of the training samples. That is $\hat{D}_n(\mathbf{x}) = \frac{1}{n}$ if $\mathbf{x}$ is in the training set; otherwise $\hat{D}_n(\mathbf{x}) = 0$. Note that, even with the partial fixed-depth orthogonalization, we can still apply the first part of Theorem 1. The reason is that (4) holds with the summation ranging over all $\mathcal{S} \subseteq [i-1]$ with $|\mathcal{S}| \leq t$. That said, we use Theorem 1 with $\hat{D}_n$ as the distribution of the random variables in the statement. As a result, $\hat{H}_n(\mathbf{X}|\mathbf{X}^{\hat{\mathcal{J}}_n}) = 0$, where $\hat{H}_n$ is the conditional entropy calculated over $\hat{D}_n$ as the distribution. The rest of the argument is a concentration analysis. In particular, from McDiarmid's inequality and the continuity of entropy, we can show that $\hat{H}_n$ converges to the true conditional entropy. □

V. Numerical Experiments

We now compare the performance our UFFS algorithm with a number of well-known methods for unsupervised feature

TABLE I
COMPARISON OF UNSUPERVISED ALGORITHMS.

	S1	S2	S3	USPS	Covertype	Australian	Musk	ALL AML	Lung
No FS	77.9	75.0	87.0	97.3	75.6	84.9	92.2	94.3	94.6
UFFS k	11	12	11	93	34	12	35	39	114
UFFS	**80.3**	**76.8**	**86.2**	**97.0**	**76.9**	**85.1**	**85.7**	**97.1**	**94.6**
LS	55.1	61.2	71.0	95.6	72.8	85.4	84.5	97.2	93.6
MCFS	56.6	59.0	65.8	93.9	72.3	84.8	84.2	95.9	94.1
UDFS	64.0	60.6	64.3	80.8	72.0	84.9	80	86.2	92.6

selection. We tested the algorithms on several real-world data sets as given in Table II. These data sets are benchmarks and taken from [2] and the UCI repository [35].

In addition, we generated three data sets, denoted by S1, S2, and S3. Each data set has 1000 samples and 30 features: 10 informative denoted by $(X_1, X_2, ..., X_{10})$, 10 nonlinear redundant $(X_{11}, X_{12}, ..., X_{20})$, and 10 linearly redundant $(X_{21}, X_{12}, ..., X_{30})$. The informative features are generated according to three distributions, one for each data set. The distribution for S1 is $N(0, \mathbf{I}_{10})$, for S2 is uniform distribution over $[-1, 1]^{10}$, and for S3 is uniform distribution over $\{-1, 1\}^{10}$.

Each nonlinear redundant feature is generated from $X_j = 3X_{i_1}X_{i_2}X_{i_3}$, where $j = 11, 12, ..., 20$, and i_1, i_2, i_3 are randomly and uniformly selected from $\{1, 2, ..., 10\}$. The linearly redundant features are generated from $X_j = \sum_{l=1}^{5} a_{j,l}X_{i_l}$, where i_l's are selected randomly from $\{1, 2, ..., 10\}$ and $a_{j,l} \sim \text{Unif}(0, 1)$. We use the above redundancy model for each data set. For the sake of performance comparison, we add a labeling to the above data sets. However, the labels are not revealed to the algorithms. We generate a fixed but randomly generated labeling function $f(\mathbf{X})$ on $\mathbb{R}^{10}$. This function is the sign of the following randomly generated polynomial in $\mathbb{R}^{10}$:

$$f(\mathbf{x}) = \text{sign}\Big[\prod_{1\le j\le 3}\big(b_{0,j} + \sum_{1\le i\le 10} b_{i,j}x_i\big)\Big],$$

where $b_{i,j} \sim \text{Unif}(0, 1)$ and mutually independent.

TABLE II
PROPERTIES OF THE REAL-WORLD DATA SETS.

Data set	USPS	Lung	Covertype	Australian	Musk	ALL AML
Features	256	3312	54	14	166	7128
Samples	9298	203	581	690	467	72

We compare the performance of UFFS with Laplacian Score (LS) [25], MCFS [26], and UDFS [22] on the real and the synthetic data sets. The labels are not revealed to the algorithms, but used for measuring the performances. Features are randomly ordered, so that the initial ordering would not affect the experiments' outcomes. Contrary to other algorithms, UFFS does not rank the feature; instead it outputs a set of indices as the non-redundant features.

We run UFFS three times: first with $t = 1, m = d$, second, with $t = 2, m = 50$ but on the selected features from the first run, and third, with $t = 3, m = 30$ but on the selected features from the second run. For each experiment, let k denote the number of the selected features by UFFS at the third run. For comparing the performance to the ranking algorithms, we select only the k features with the highest rank. Once the features are selected by each unsupervised algorithm, we reveal the samples of the selects features with the labels to a classifier and compute its prediction accuracy. A support vector machine (SVM) classifier with radial basis function as kernel is employed for all the studies. We perform a 5-fold cross validation using this classifier and on the entire data set.

Table I shows the average of the resulted classification accuracies for each algorithm. The second row is the resulted accuracy without any feature selection. The third row is k which is the number of non-redundant features declared by the UFFS. Observe that, in synthetic data sets, k is very close to 10 which is the actual number of non-redundant features. The resulted accuracy by the UFFS is very close or greater than the accuracy without feature selection which verifies that the removed features were redundant. Further, it significantly outperforms other algorithms in the synthetic and many real data sets. This result shows that the UFFS performs well on data sets with nonlinear redundancies.

A. Running Time Comparison

We numerically compared the running time of the algorithms. The results (in seconds) are reported in Table III. For the existing algorithms, the implementations are taken from [2] and correspond to the original implementations[2]. As it shows, the running time of our algorithm (UFFS) is comparable to other algorithms even for high-dimensional datasets such as ALL AML with $d \approx 7000$.

TABLE III
COMPARISON OF RUNNING TIMES (IN SECONDS).

	S1	S2	S3	USPS	Cov.	Aust.	Musk	ALLAML	Lung
UFFS	2.6	2.85	1.1	248	2	3	2.1	280	96
UDFS	11.1	22.79	16.9	17875	3	4.1	2.37	28305	780
MCFS	2.45	2.37	2.55	389	1.2	1.43	1.7	75.4	98.2
LS	1.22	1.19	1.2	266	0.62	0.75	0.49	8.38	4.4

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[2]All the experiments were performed on 48-CPU workstation, with Intel(R) Xeon(R) CPU E7-8857 v2 @ 3.00GHz and 256GB RAM.

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