STOCHASTIC FUNCTIONAL ANALYSIS WITH APPLICATIONS TO ROBUST MACHINE LEARNING

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ABSTRACT. It is well-known that machine learning protocols typically under-utilize information on the probability distributions of feature vectors and related data, and instead directly compute regression or classification functions of feature vectors. In this paper we introduce a set of novel features for identifying underlying stochastic behavior of input data using the Karhunen-Loève (KL) expansion, where classification is treated as detection of anomalies from a (nominal) signal class. These features are constructed from the recent Functional Data Analysis (FDA) theory for anomaly detection. The related signal decomposition is an exact hierarchical tensor product expansion with known optimality properties for approximating stochastic processes (random fields) with finite dimensional function spaces. In principle these primary low dimensional spaces can capture most of the stochastic behavior of ‘underlying signals’ in a given nominal class, and can reject signals in alternative classes as stochastic anomalies. Using a hierarchical finite dimensional KL expansion of the nominal class, a series of orthogonal nested subspaces is constructed for detecting anomalous signal components. Projection coefficients of input data in these subspaces are then used to train an ML classifier. However, due to the split of the signal into nominal and anomalous projection components, clearer separation surfaces of the classes arise. In fact we show that with a sufficiently accurate estimation of the covariance structure of the nominal class, a sharp classification can be obtained. We carefully formulate this concept and demonstrate it on a number of high-dimensional datasets in cancer diagnostics. This approach yields improved accuracies over the current benchmarks. In particular, this method leads to a significant increase in precision and accuracy over the current top benchmarks for the Global Cancer Map (GCM) gene expression network dataset.

Keywords: Functional Data Analysis, Support Vector Machine, Machine Learning

1. INTRODUCTION

We introduce a systematic approach for the construction of machine learning (ML) feature vectors that improves class separations, using techniques in probability theory and functional analysis. Our implementations involve techniques from computational applied mathematics and computer science. The approach will be applied within a framework of high dimensional noisy gene expression data for cancer diagnostics, and lead to significant increases in predictive accuracy over benchmarks. Due to its foundation on functional analysis and tensor product expansions our approach can be easily applied to classification problems on complex topologies, including gene expression networks.

A fundamental issue in Machine Learning (ML) predictive modeling is robustness and sensitivity to data quality. Machine learning involving complex noisy observations involves a host of difficulties, including the problem of overfitting, which can give rise to highly unstable and inaccurate decision boundaries. This problem is particularly difficult for data with high dimension ($p$) and low sample size ($N$), (i.e. $p \gg N$), for example gene expression arrays in which genes number in the tens of thousands while available tissue samples are limited by high biopsy costs. However, this can also present itself in high dimension with even larger large sample sizes (i.e. $p \ll N$), with noisy inputs again leading to high decision boundary oscillations. Such oscillations generally arise from fitting noise, and can lead to poor machine performance. Our overarching goals in this work are to: i) To develop stochastic functional analysis approaches for significantly improving accuracy and robustness of machine learning methods on high dimensional noisy datasets that can be based on
complex topologies. ii) To motivate and develop high performance computing algorithms based on these approaches.

Our approach identifies underlying distributions of data using Karhunen-Loève expansions, with classification treated detection of anomalies to a (nominal) signal class.

2. Mathematical preliminaries

We demonstrate our approach on the ML classification problem. A novel strategy for classification will here consist of construction of a series of subspaces orthogonal to a stochastic representation of data belonging to one of the classes. For two class classification, the second class is treated as a change or anomaly with respect to the first. The constructed subspaces allow detection of such ‘anomalies’ with high accuracy from data and projection coefficients, and are used to train an ML classifier.

More precisely, data are viewed as a realization of a random field, and the Karhunen-Loève expansion is an important tool for representing such fields as spatial-stochastic tensor expansions. This decomposition has been shown to be optimal in several ways, making it attractive for analysis of such random fields. Let \((\Omega, \mathcal{F}, \mathbb{P})\) be a complete probability space, with \(\Omega\) a set of outcomes, and \(\mathcal{F}\) a \(\sigma\)-algebra of events equipped with the probability measure \(\mathbb{P}\). Let \(U\) be a domain of \(\mathbb{R}^d\) and \(L^2(U)\) be the Hilbert space of all square integrable functions \(v : U \to \mathbb{R}\) equipped with the standard inner product \(\langle u, v \rangle = \int_U u v \, dx\), for all \(u(x), v(x) \in L^2(U)\). In addition, let \(L^2_p(\Omega; L^2(U))\) be the space of all functions \(v : \Omega \to L^2(U)\) equipped with the inner product \(\langle u, v \rangle_{L^2_p(\Omega; L^2(U))} = \int_\Omega \langle u, v \rangle \, d\mathbb{P}\), for all \(u, v \in L^2_p(\Omega; L^2(U))\). We point out that our approach is applicable to complex topologies on \(\mathbb{R}^d\), networks, spatio-temporal domains, etc.

**Definition 1.** Suppose that \(v \in L^2_p(\Omega; L^2(U))\).

i) Denote

\[ E_v := \mathbb{E}[v] := \int_\Omega v(x, \omega) \, d\mathbb{P} \]

as the mean of \(v\).

ii) Define the covariance function

\[ \text{Cov}(v(x, \omega), v(y, \omega)) := \mathbb{E}[(v(x, \omega) - \mathbb{E}[v(x, \omega)])(v(y, \omega) - \mathbb{E}[v(y, \omega)])]. \]

iii) Define the linear operator \(T : L^2(U) \to L^2(U)\) by

\[ T(u)(x) := \int_U \text{Cov}(x, y)u(y) \, dy \]

for all \(u \in L^2(U)\).

The above covariance structure will be critical for an accurate stochastic representation of the random field \(v\). In particular, the eigenstructure of the linear operator \(T : L^2(U) \to L^2(U)\) plays a major role. From Lemma 2 and Theorem 1 in [4], there exists a set eigenfunctions \(\{\phi_k\}_{k \in \mathbb{N}}\), with \(\langle \phi_k, \phi_l \rangle = \delta[k - l]\) and a sequence of eigenvalues \(\lambda_1 \geq \lambda_2 \geq \cdots > 0\) such that \(T\phi_k = \lambda_k\phi_k\) for all \(k \in \mathbb{N}\). From this eigenstructure the following is proved in Proposition 2.8 in [6].

**Theorem 1.** If \(v \in L^2(\Omega; L^2(U))\), then the random field \(v\) can be represented in terms of the Karhunen-Loève (KL) tensor product expansion as

\[ v(x, \omega) = E_v + \sum_{k \in \mathbb{N}} \lambda_k^2 \phi_k(x)Y_k(\omega), \]

where \(\mathbb{E}[Y_k Y_l] = \delta_{kl}\) and \(\mathbb{E}[Y_k] = 0\) for all \(k, l \in \mathbb{N}\).

From orthogonality properties of the tensor expansion it is not hard to show that
\[ \|v - E_v\|_{L^2(\Omega; L^2(U))}^2 = \sum_{k \in \mathbb{N}} \lambda_k^2. \]
Thus the eigenvalue magnitudes control the contribution to the variance of each term of the tensor product expansion.

Suppose we are interested in forming the optimal $M$ dimensional approximation. We can conclude the optimal choice with respect to the Bochner norm $\| \cdot \|_{L^2(\Omega; L^2(U))}$ is formed from the first $M$ expansion terms, giving the truncated KL expansion:

\[ v_M(x, \omega) = E_v + \sum_{k=1}^M \lambda_k^2 \phi_k(x)Y_k(\omega), \]

with
\[ \|v - v_M\|_{L^2(\Omega; L^2(U))}^2 = \sum_{k=M+1}^{\infty} \lambda_k^2. \]

In fact it can be shown this is the optimal expansion i.e. no other orthogonal expansion has smaller residuals than these.

From tensor product theory the space $L^2(\Omega; L^2(U))$ is isomorphic to $L^2(\Omega) \otimes L^2(U)$. Let $H_M \subset L^2(U)$ such that $\dim H_M = M$ and $P_{H_M \otimes L^2(\Omega)} : L^2(U) \otimes L^2(\Omega) \to H_M \otimes L^2(\Omega)$ is an orthogonal projection operator. The following theorem is a direct extension of Theorem 2.7 in [6], showing optimality of KL expansions.

**Theorem 2.** Suppose $f \in L^2(U) \otimes L^2(\Omega)$, with $E_f = 0$. Then

\[ \inf_{H_M \subset L^2(U), \dim H_M = M} \|f - P_{H_M \otimes L^2(\Omega)}f\|_{L^2(\Omega) \otimes L^2(U)}^2 = \left( \sum_{k=M+1}^{\infty} \lambda_k \right)^{\frac{1}{2}}. \]

**Remark 1.** We conclude that the infimum above is achieved when $H_M = \text{span}\{\phi_1, \ldots, \phi_M\}$ i.e., for the truncated KL expansion.

**Remark 2.** The KL expansion is largely a theoretical tool for signal analysis. The main difficulty in its construction arises in estimation of the random variables $Y_1(\omega), \ldots, Y_M(\omega)$. Although these are mutually uncorrelated, in general they are not independent, leading to a high dimensional joint distribution estimation problem. Even for moderate dimension $M$, the number of realizations of $v(x, \omega)$ needed to construct a joint pdf becomes impractical. However, for purposes of detecting anomalous signals and building a classifier, only the eigenpairs $\{\lambda_k, \phi_k\}_{k=1}^M$ are needed, a significantly easier problem. This can be achieved by constructing a covariance matrix from realizations of $v(x, \omega)$ and computing the eigenvalues and eigenvectors (See the method of snapshots, [1]).

### 3. Approach

Our approach to machine learning classification is to detect signals defined on the domain $U$ that do not belong to the family of finite dimensional truncated KL expansions $v_M(x, \omega) - E_v = \sum_{k=1}^M \lambda_k^2 \phi_k(x)Y_k(\omega)$. To be more precise, we seek to detect signals orthogonal to the eigenspace spanned by $\{\phi_1, \ldots, \phi_M\}$. The proofs of theorems presented in this section can be found in [2].

**Assumption 1.** Without loss of generality assume that $E_v = 0$, and consider a sequence of nested subspaces $P_0 \subset P_1 \subset \cdots \subset L^2(U)$ such that $\bigcup_{k \in \mathbb{N}_0} P_k = L^2(U)$ and $P_0 := \text{span}\{\phi_1, \phi_2, \ldots, \phi_M\}$. Furthermore, let the subspaces $S_k \subset L^2(U)$, for $k = 0, 1, 2, \ldots$, be defined by $P_{k+1} = P_k \oplus S_k$, so that $P_0 \bigoplus_{k \in \mathbb{N}_0} S_k = L^2(U)$. 
Assumption 2. For all $l \in \mathbb{N}_0$ let $\{\psi_k^l\}_{k=1}^{M_l} \subseteq \mathcal{A}$ be a collection of orthonormal functions with $S_l = \text{span}\{\psi_1^l, \ldots, \psi_{M_l}^l\}$ and $M_l := \dim S_l$.

Remark 3. In practice the basis functions for the finite dimensional spaces $P_n = P_0 \oplus S_0 \oplus \ldots \oplus S_{n-1}$ will be constructed by using a series of local Singular Value Decompositions (SVDs). The space $P_n$ is assumed to be formed from the span of $N$ characteristic functions, where the maximum level $n$ will be determined algorithmically. The construction of the basis for these spaces is intricate and are described in detail in the publication from [2].

Remark 4. Since the basis of $\bigoplus_{k \in \mathbb{N}_0} S_k$ is orthonormal, for any function $u \in L^2(U)$ the orthogonal projection coefficient onto the function $\psi_k^l \in W_l$ is

$$d_k^l := \int_U u \psi_k^l \, dx.$$ 

Given that $d_k^l$ are the orthogonal projection coefficients (from $S_k$) of a novel signal $u(x, \omega) \in L_P^2(\Omega; L^2(U))$, they provide a mechanism to detect the magnitude of the novel part of the signal orthogonal to eigenspace $P_0$. In more colloquial terms, we desire to detect the components of $u(x, \omega)$ via stochastic properties different from those of the eigenspace. Suppose that $u(x, \omega) = v(x, \omega) + w(x, \omega)$ i.e. the signal $u(x, \omega)$ is formed from components $v(x, \omega)$ and $w(x, \omega) \in P_0^\perp$. The goal then is to detect the component $w(x, \omega)$ orthogonal to eigenspace $P_0$. Thus $v(x, \omega)$ can represent a signal from the nominal class and $u(x, \omega)$ the second class. However, in practice we can only build the eigenspace for the truncated KL expansion $v_M(x, \omega)$. The following theorem is stated from [2] and provides a mechanism relating strengths of the classes with their coefficient magnitudes.

Theorem 3. Let $t_M := \sum_{j \geq M+1} \lambda_j$ and suppose that $u(x, \omega) = v(x, \omega)+w(x, \omega)$ for some $w(x, \omega) \in L_P^2(\Omega; L^2(U))$, with $w(x, \omega) \perp V_0$ almost surely. Then

$$\|w(x, \omega)\|_{L_P^2(\Omega; L^2(U))}^2(1 - 2t_M) + t_M \leq \sum_{l \in \mathbb{N}_0} \sum_{k=1}^{M_l} \mathbb{E}[(d_k^l)^2] \leq \|w(x, \omega)\|_{L_P^2(\Omega; L^2(U))}^2(1 + 2t_M) + t_M.$$ 

![Figure 1](image-url)

**Figure 1.** Illustrative example of the separation between small and large anomalous norms $\|w(x, \omega)\|_{L_P^2(\Omega; L^2(U))}^2$ based on the coefficients $d_k^l$. The blue dots correspond to coefficients $d_k^l$ when $\|w(x, \omega)\|_{L_P^2(\Omega; L^2(U))}^2$ is small. Conversely, a large norm for $\|w(x, \omega)\|_{L_P^2(\Omega; L^2(U))}^2$ leads to coefficients $d_k^l$ that are likely to be large.
If \( \|w(x, \omega)\|_{L^2(\Omega; L^2(U))}^2 \) is small, then from Theorem 3 the coefficients \( d_k^l \) are more likely to be concentrated around the origin. Conversely, if \( \|w(x, \omega)\|_{L^2(\Omega; L^2(U))}^2 \) is large then \( d_k^l \) are likely to be large (See Figure 1), (though there is an unlikely possibility that some of them could be small).

We can now separate the coefficients with a surface from an SVM optimization.

The separations between signals depend on several factors: i) The number of eigenfunctions \( M \); ii) The accuracy of the computation of the eigenspace (dependent on availability of data); iii) The presence of noise in both signals. In many practical applications such as for gene expression data, \( p \) will be large and \( m \) relatively small. Thus, generally, if we extract \( N_T \) samples from class \( A \) to construct the multilevel filter, there is no guarantee that applying this filter to the remainder of the data we will yield near-zero values for coefficients. However, in general it is expected that the multilevel coefficients for class \( A \) will be smaller than those for class \( B \). In Figure 2 the classification training framework with respect to two classes of data is shown. Note the approach is general and can also apply to data from more novel data arising from complex topologies.

**Figure 2.** Multilevel KL orthogonal training framework for binary classification using SVM. With a slight abuse of notation the map \( \Phi : L^2(U) \to \bigoplus_{k \in \mathbb{N}_0} S_k \) corresponds to the transformation of the signal \( u(x, \omega) \) into the spaces \( \bigoplus_{k \in \mathbb{N}_0} S_k \) and so provides the projection coefficients. The multilevel spaces are built from the classes where more data is available, in this case from the data of class \( A \); \( N_T < m_1 \) samples are chosen ( \( m_1^A, \ldots, m_{N_T}^A \) ) to estimate the covariance function (matrix) and thus the \( M \) eigenvalues and eigenfunctions. The multilevel filter for \( \bigoplus_{k \in \mathbb{N}_0} S_k \) is built from these eigenfunctions and the map \( \Phi \) is applied to the data \( m_1^A, \ldots, m_{m_1}^A \) and \( m_1^B, \ldots, m_{m_2}^B \), and the SVM classifier is trained.
4. Results

Remark 5. The code was executed on an Intel i7-3770 CPU (4 cores) @ 3.40GHz with 32Gb memory. Each crossvalidation leave-one-out training and testing step requires a few seconds. The code and instructions on how to run the tests in this paper will be available in GitHub.

In Figure 3 a comparison is shown between benchmark SVM performance on raw gene expression data (from the GCM cancer dataset from [5] (see also the work from [8]), and performance of multilevel coefficients. The data consist of 190 tumour ($m_1 = 190$ class A) and $m_2 = 90$ normal (class B) tissue data with $p = 16,063$ gene expression levels. The multilevel filter is built from $N_T = 100$ tumour samples and the number of KL expansion terms is set to $M = 39$. From the construction of the multilevel filter we obtain a basis for the spaces $S_0 \oplus S_1 \oplus \cdots \oplus S_8$. Notice that the for the raw dataset it is hard to distinguish the normal compared to the tumour gene expression levels. However, for the multilevel coefficients we can clearly see that the tumour levels are small compared with the normal tissue. This is expected as the tumour dataset is closer to the eigenspace.

The multilevel filter is now applied to the remaining $m_1 - N_T = 90$ tumour samples and $m_2 = 90$ normal samples and the projection coefficients for the spaces $S_0 \oplus S_1 \oplus \cdots \oplus S_8$ are obtained. A linear SVM classifier is trained using 89 tumour and normal tissue samples and and 1 tumour and normal tissue test. Using a leave-one-out cross-validation approach we have a total of $89^2 = 7,921$ cases. The multilevel method is compared with the direct SVM approach, where the leave-one-out cross validation is done over the entire dataset i.e. $189 \times 89 = 17,010$ cases. The method is tested on raw and standardized (normalized to zero mean, unit variance) data. For the raw data only the projection coefficients for the space $S_0$ are used. For the standardized (normalized) data all the projection coefficients for the spaces $S_0, \ldots, S_{n-1}$ are used. In Table 1 the accuracy and precision results are shown. Observe that for raw data the Multilevel linear SVM accuracy and precision increase more than 20%. For standardized data the increase is more than 2%, which is significantly higher since the baseline accuracy is more than 90%. From [8] Table 3, the highest benchmark accuracy is 93.21\%.

Remark 6. The choice of parameter $M$ can affect accuracy. The best avenue is a cross-validation for selecting this parameter; this will be explored in detail in another publication.

Remark 7. Note that standardization/normalization does not always lead to higher performance. For the case of Neural Networks it can be detrimental to computational performance ([7]).

For the lung cancer dataset from [3], $m_1 = 150$ (Mesothelioma tissue, class A) and $m_2 = 31$ (ADCA tissue, class B). The multilevel filter is constructed with $M = 20$ eigenfunctions from $N_T = 119$ Mesothelioma class A tissue samples and applied to the rest of the samples. Using a linear SVM leave-one-out cross-validation approach, leading to 900 cases, the accuracy and precision is 100% for both the linear SVM and the multilinear method for standardized data. For raw data there is a significant improvement using the multilevel linear SVM method. Notice that from Table 3 in [8] the accuracy for the lung data set is 99.45%.

Remark 8. The main limitation of this approach to machine learning is accurate estimation of the covariance structure. This is directly related to the the number of samples $m$ of the data. For a small number of samples the eigenfunctions cannot be estimated with sufficient accuracy and the performance degrades. For example, we tested our approach of the Colon cancer dataset from [8], with 22 normal and 40 cancerous gene expressions signals. The performance was inferior to the benchmark.
Figure 3. Multilevel gene expression from the GCM cancerous dataset. (a) Gene expression original data for normal and tumour tissue. (b) Multilevel projection coefficients of normal and tumor gene expression levels on orthogonal eigenspace. Notice that projection coefficients have a sharper distinction.

Table 1. Performance comparison between linear SVM and Multilevel linear SVM for GCM and Lung cancer data set.

| Method                      | Raw Data | Standardized Data |
|-----------------------------|----------|-------------------|
|                             | Acc. (%) | Prec. (%)         | Acc. (%) | Prec. (%) |
| Linear SVM (GCM)            | 49.74    | 49.47             | 92.95    | 95.56     |
| **Multilevel Linear SVM (GCM)** | **73.46** | **75.51**        | **95.27** | **97.93** |
| Linear SVM (Lung)           | 86.69    | 91.63             | 100.00   | 100.00    |
| **Multilevel Linear SVM (Lung)** | **96.10** | **95.67**        | **100.00** | **100.00** |

5. Conclusions

In this paper we introduce a novel approach for creating features for machine learning based on stochastic functional analysis. From the covariance structure of a singular class of signals the problem is posed as a detection of an anomalous signal i.e. an unlikely realization of the baseline structure. A multilevel orthogonal basis is constructed to detect the magnitude and location of these anomalies. Signals from different classes that are hard to distinguish are mapped to small and to large coefficients with significantly greater separation. An SVM classifier can then more easily construct the separation boundary.

The performance of the multilevel filter and the classifier depend on the availability of a rich dataset for construction of the truncated eigenspace. For signals that belong to a finite dimensional eigenspace and with sufficient data it can be shown that our approach leads to perfect classification (Theorem 3). Moreover, for the case of limited data availability the approach still outperforms the benchmarks as shown in the application to cancer diagnostics from gene expression data. The performance is expected to improve as more data is obtained.
Future work:

- The effects of estimating the covariance structure on the accuracy of the prediction will be studied theoretically and in practice.
- Since the multilevel filter leads to projection coefficients with greater distinguishability, this approach should be effective for ameliorating the problem of overfitting. We will study this topic in more detail in a future publication.
- A battery of tests will be performed to measure the performance of the multilevel method on semi-synthetic data. For example, from a set of gene expression data belonging to the same class the Karhunen Loeve expansion can be used as a bootstrap method to generate large numbers of realizations that have the same covariance structure as the covariance matrix estimated from the data. From these realizations the effects of estimating the covariance matrix on the performance of the multilevel method can be studied.
- The performance of radial SVM and Deep Neural Networks coupled with the multilevel filter will be studied.
- The multilevel method will be tested on more complex domains under different application contexts, e.g., in models of electric power grids.

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