Marginal Fisher Analysis With Polynomial Matrix Function

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ABSTRACT Marginal fisher analysis (MFA) is a dimensionality reduction method based on a graph embedding framework. In contrast to traditional linear discriminant analysis (LDA), which requires the data to follow a Gaussian distribution, MFA is suitable for non-Gaussian data, and it has better pattern classification ability. However, MFA has the small-sample-size (SSS) problem. This paper aims to solve the small-sample-size problem while increasing the classification performance of MFA. Based on a matrix function dimensionality reduction framework, the criterion of the MFA method is reconstructed by using the polynomials matrix function transformation, and then a new MFA method is proposed, named PMFA (polynomial marginal fisher analysis). The major contributions of the proposed PMFA method are that it solves the small-sample-size problem of MFA, and it can enlarge the distance between marginal sample points of inter-class, so that it can get better pattern classification performance. Experiments on the public face datasets show that PMFA can get a better classification ability than MFA and its improved methods.

INDEX TERMS Dimensionality reduction, manifold learning, marginal fisher analysis, matrix function, the small-sample-size (SSS) problem.

I. INTRODUCTION

In some fields, such as data visualization and face recognition, features are usually represented as high-dimensional data. The original high-dimensional data contains redundant and noisy information, which can easily cause errors in practical applications, and the direct processing of high-dimensional data may cause considerable computational consumption. To better analyze and process data, it is necessary to find low-dimensional features that effectively represent high-dimensional data.

Many dimensionality reduction methods have been proposed. Principal component analysis (PCA) [1] and LDA [2] are widely used linear subspace algorithms. As an unsupervised learning algorithm, the principle of PCA is to maximize the covariance of reduced dimension samples. As a supervised learning algorithm, the principle of LDA is to make different classes as far as possible and the same classes as close as possible after dimensionality reduction.

There are many dimensionality reduction methods based on manifold, such as ISOMAP [3], LLE [4], LE [5], MVU [6], t-SNE [7], LPP [8], and NPE [9]. What they have in common is to find a neighborhood in each sample point, and retain the local structure information of the sample points while mapping the high-dimensional data into low-dimensional data. With the emergence of these classical manifold learning algorithms one after another, some researchers have hoped to unify manifold learning algorithms using a framework.
Bengio et al. unified ISOMAP, LLE, and LE into kernel functions [10]. Yan et al. proposed a unified graph embedding framework [11]. This framework can explain the existing dimensionality reduction algorithms with a linear, kernel, tensor extension of a certain intrinsic graph, or direct graph embedding.

In the graph embedding framework, the marginal fisher analysis method (MFA) is proposed. The main idea behind MFA is that it describes intra-class compactness by constructing an intrinsic graph and inter-class separability by constructing a penalty graph. Based on the design of the two graphs, it is also suitable for data of non-Gaussian distribution; therefore, there is no need for a priori knowledge of data distribution. However, the classical LDA method requires the data to follow a Gaussian distribution. Compared with LDA, MFA can find a more discriminative direction. However, the dimensions of the samples are usually much larger than the number of samples, resulting in the intra-class compactness matrix of the MFA being singular, and the generalized eigenvalue problem of MFA is difficult to solve. This may be called the small-sample-size (SSS) problem of MFA.

In recent years, much research has been conducted on MFA. Based on the separability criterion of MFA, Yu et al. proposed the orthogonal MFA (OMFA) and uncorrelated MFA (UMFA) method, in which orthogonal and irrelevant constraints are added to the base vector [12]. Siena proposed a coupled MFA (CMFA) method, which considers the nearest neighbor of each data sample and uses different rules to construct the penalty graph of the MFA [13]. Huang et al. proposed the multiple MFA (MMFA) method that uses edge data points and manifold structures and considers multiple marginal data pairs when constructing a penalty graph [14]. For the SSS problem of MFA, MFA uses PCA to reduce the dimensionality of the samples and then avoids the singularity of the intra-class compactness matrix, but this will lose some useful information about the original samples [11]. In addition, some methods have been proposed to solve the SSS problem of MFA. For example, Wang et al. proposed a general matrix exponential framework, the SSS problem of MFA [15] can be solved by an exponential MFA (EMFA) method which is based on this framework. Huang proposed a regularized MFA (RMFA) [16], which multiplies a unit matrix by a small number to construct a regular term into the inner-class compactness matrix of the MFA so that the resulting matrix is invertible. The graph embedding framework is reformulated in [17], as a special case of the GEU framework formula, the MFA technique is extended as GEU-MFA. Recently, there are many algorithms based on manifold learning, such as GDE [18], CR-DLPP [19] and LMGE-DDR [20].

In [21], a general framework for dimensionality reduction based on the manifold was proposed. The main idea of the framework is to use two scalar functions to map the scatter matrices into the corresponding matrix functions, and then to make dimensionality reduction and feature extraction. However, in real life, it is difficult to choose such two functions. In mathematics, any function can be approximated by a polynomial, so we can use the polynomial to uniformly represent the above optional and various forms of functions. Then, this framework is easier to use.

This paper aims to solve the SSS problem and improve the classification ability of MFA. So, based on the above idea, i.e., combining the polynomial function and the framework in [21], we proposed a new MFA method, named PMFA (polynomial marginal fisher analysis). Specially, we use two appropriate polynomials to map the scattering matrices of MFA to the new space, which can avoid the SSS problem and get better pattern classification performance. We also discuss the design of the two polynomial functions, and provide a theoretical analysis of the proposed method. Experiments are conducted on synthetic data set and some public face datasets, which show that the proposed PMFA is an effective method. As an effective feature extraction method, like MFA and its variants, PMFA can be applied in many fields, such as face recognition [13], [16], facial expression recognition [22], autism trait classification [23], image representation [24], etc.

The remainder of this paper is organized as follows. The Section II summarizes MFA and the matrix function dimensionality reduction framework. Section III presents polynomial marginal fisher analysis (PMFA). Section IV verifies PMFA with experiments. Finally, Section V summarizes the study and future directions.

| Symbol | Explanation |
|--------|-------------|
| $X = \{x_1, x_2, \ldots, x_m\}$ | the $m$-dimensional data in $\mathbb{R}^n$ space |
| $x_i$ | the original sample |
| $m$ | the dimensionality of training samples |
| $n$ | the number of training samples |
| $c_i$ | the category label of the $i$th category |
| $c_i \in \{1, 2, L, m\}$ | and $c_i \in \{1, 2, L, m\}$ |
| $m_c$ | the number of categories of the samples |
| $y_i$ | the projected sample |
| $L$ | the Laplace matrix |
| $L^r$ | the Laplace matrix |
| $rank\{g\}$ | the rank of the matrix |

II. RELATED WORK

A. MARGINAL FISHER ANALYSIS

MFA first constructs an intrinsic graph $G^c = \{X, W\}$ and penalty graph $G^p = \{X, W^p\}$, which are used to describe inter-class separability and intra-class compactness, respectively. Then, MFA tries to find an optimal projection matrix $U$ and makes a projection $y_i = U^T x_i$, so that the dimension of $y_i$ is smaller than that of $x_i$. To clarify the method, Table 1 summarizes the frequently used notations.
The intra-class compactness of the projected sample is defined as:
\[
S_c = \sum_{i \in N_{k1}} \sum_{j \in N_{k1}(i)} \|y_i - y_j\|^2 = 2tr \left\{ U^T XLX^TU \right\}
\]
where \( L = D - W \); \( D \) is a diagonal matrix composed of the sum of the rows of \( W \), i.e., \( D_{ii} = \sum_j W_{ij} \). \( W \) is defined as:
\[
W_{ij} = \begin{cases} 
1, & \text{if } i \in N_{k1}(j) \text{ or } j \in N_{k1}(i) \\
0, & \text{else}.
\end{cases}
\]
where \( N_{k1}(i) \) represents an index set of the \( k_1 \) nearest neighbors of the sample \( x_i \) in the intrinsic graph \( G^c \).

The projected inter-class data separation is defined as:
\[
S_p = \sum_{i \in N_{k2}} \sum_{j \in N_{k2}(c_j)} \|y_i - y_j\|^2 = 2tr \left\{ U^T XL^P X^TU \right\}
\]
where \( L^P = D^P - W^P \); \( D^P \) is a diagonal matrix composed of the row sum of the matrix \( W^P \), i.e., \( D^P_{ii} = \sum_j W^P_{ij} \). \( W^P \) is defined as:
\[
W^P_{ij} = \begin{cases} 
1, & \text{if } i \in N_{k2}(c_j) \text{ or } j \in N_{k2}(c_i) \\
0, & \text{else},
\end{cases}
\]
where \( N_{k2}(c_j) \) represents an index set of the \( k_2 \) nearest pairs for the class \( c_j \) in the penalty graph \( G^P \).

The marginal fisher criterion is defined as:
\[
J(U) = \max_U \frac{tr \left( U^T XL^P X^TU \right)}{tr \left( U^T XLX^TU \right)}.
\]
Let the matrix \( Z_p = XL^P X^T \), matrix \( Z = XLX^T \), and upper Eq. (5) can be solved using the generalized eigenvectors problem:
\[
Z_p u = \lambda Zu.
\]

The basic MFA algorithm is given in Algorithm 1.

For the above Eq. (6), the rank of matrix \( Z \) has an inequality:
\[
\text{rank} (Z) = \text{rank} \left( XLX^T \right) \leq \text{rank} (X) \leq \min (m, n).
\]

Usually, the dimension of training samples is much larger than the number of training samples, that is \( m \ll n \), so \( \text{rank} (Z) < n \) and \( Z = XLX^T \) is an \( n \)-order matrix, i.e., \( Z \) is a singular matrix, so Eq. (6) is difficult to solve directly, which is the SSS problem of MFA.

Algorithm 1 MFA
1) Input a dataset \( X \)
2) PCA projection: project the data set into the PCA subspace, let \( X_{PCA} \) denote the transformation matrix of PCA
3) Constructing the intra-class compactness and inter-class separability matrices:
   Adjacency matrix: \( W_{ij} = W_{ji} = 1 \) if \( x_j \) is among the \( k_1 \) nearest neighbors of \( x_i \) in the same class
   Similarity matrix: \( W^p_{ij} = W^p_{ji} = 1 \) if the pair \((i, j)\) is among the \( k_2 \) nearest pairs
4) Marginal fisher criterion
   \[
   J(U) = \max_U \frac{tr \left( U^T XL^P X^TU \right)}{tr \left( U^T XLX^TU \right)}
   \]
5) Compute the eigenvalues and eigenvectors as:
   \[
   X(D^p - W^p)X^TU = \lambda X(D - W)X^TU
   \]
6) Output the final linear projection direction as:
   \[
   Y = U^TX_{PCA}
   \]

B. MATRIX FUNCTION AND ITS EIGEN-SYSTEM
The definition of the matrix function and the corresponding properties are presented, which is used in the paper.

Definition 1 [25]: Let \( A \) be a square matrix and \( f(x) \) be a scalar function. If one replaces the variable \( x \) in \( f(x) \) with the square matrix \( A \), the resulting matrix \( f(A) \) is called the matrix function of the matrix \( A \).

Theorem 1 [26]: Let \( A \) be a real symmetric square matrix of \( n \)-order, \( f(x) \) be a scalar function, \( \lambda_i \) be the eigenvalue of the matrix \( A \) and \( \upsilon_i \) be the eigenvector belonging to the eigenvalue \( \lambda_i \), i.e., \( Av_i = \lambda_i v_i (i = 1, 2, \cdots, n) \). For the matrix function \( f(A) \), one has:
\[
f(A)v_i = f(\lambda_i)v_i (i = 1, 2, \cdots, n),
\]
where \( f(\lambda_i) \) are the eigenvalues of \( f(A) \), and \( v_i \) are the eigenvectors corresponding to \( f(A) \).

Theorem 2 (Weierstrass Approximation Theorem [27]):
Continuous functions on closed intervals can be approximated uniformly using a polynomial series.

C. MATRIX FUNCTION DIMENSIONALITY REDUCTION FRAMEWORK
In [21], a general matrix function dimensionality reduction framework is proposed for the dimensionality reduction method in manifold learning.

The criterion function of the manifold-based dimensionality reduction method is expressed as:
\[
J(U) = \max_U \frac{\left\| U^T S_1 U \right\|}{\left\| U^T S_2 U \right\|},
\]
where the matrices \( S_1 \) and \( S_2 \) have different forms for the different methods and \( U \) is the desired optimal projection matrix.
The main concept of the matrix function framework in [21] is to map the matrices $S_1$ and $S_2$ in Eq. (8) into the matrix functions $f(S_1)$ and $g(S_2)$ with the scalar functions $f(x)$ and $g(x)$, so that the criterion Eq. (8) becomes:

$$J(U) = \arg \max_U \frac{\|U^T f(S_1) U\|}{\|U^T g(S_2) U\|}. \quad (9)$$

Eq. (9) can be reduced the generalized eigenvectors problem:

$$f(S_1) u = \lambda g(S_2) u. \quad (10)$$

Notice that the matrices $S_1$ and $S_2$ are composed of the original sample, and the above mapping $f(\cdot)$ and $g(\cdot)$ transform the matrices $S_1$ and $S_2$ from the original sample space to a new sample space.

The functions $f(x)$ and $g(x)$ in Eq. (9) are configurable. If selects different functions, the matrix function dimensionality reduction framework can construct a series of methods for dimensionality reduction. How to select the two functions is discussed in [21]. In conclusion, the two functions should satisfy the two conditions: (1) for any $x$, the function $g(x)$ should be $g(x) \neq 0$ and then the matrix function $g(S_2)$ is non-singular so that the SSS problem can be avoided by the new dimensionality reduction method; (2) for better classification after mapping, the function $f(x)$ should be a monotonically increasing function and $f(x) > x$, at the same time, $g(x) \approx x$ (org(x) $< x$).

### III. THE PROPOSED NEW METHOD

#### A. MARGINAL FISHER ANALYSIS WITH POLYNOMIAL MATRIX FUNCTION

In the criterion of MFA, i.e., Eq. (5), denote the matrix $Z_p = XLX^T$ and the matrix $Z = XLX^T$, then Eq. (5) can be expressed as:

$$J(U) = \max_U \frac{\text{tr}(U^T Z_p U)}{\text{tr}(U^T Z U)}. \quad (11)$$

According to section II.C, we can solve the small-sample-size problem and improve the classification performance of MFA by selecting two suitable functions to map the matrices $Z_p$ and $Z$ to the corresponding matrix functions, that is:

$$Z_p \rightarrow f(Z_p), \quad Z \rightarrow g(Z). \quad (12)$$

After mapping, we get a new criterion function:

$$J_p(U) = \max_U \frac{\text{tr}(U^T f(Z_p) U)}{\text{tr}(U^T g(Z) U)} \quad (13).$$

According to section II.C, if $f(x)$ and $g(x)$ have satisfied the two conditions, the new method of Eq. (13) can avoid the small-sample-size problem of MFA and improve the classification ability of MFA. Although there are several functions to choose from, there are two problems. One is that although many functions meet the conditions, it is difficult to give a specific function form. Another problem is that among all the functions that meet the conditions, some are good, some are poor, so is there a standard form of the function?

Theorem 2, the polynomial can approximate any function, that is, any function can be formulated by a polynomial. So, inspired by Theorem 2, we use polynomial functions to implement the above objectives.

We choose an $n$-order polynomial $f(x) = \sum_{k=0}^{n} a_k x^k$ to map the matrix $Z_p$, thus the gotten matrix function is $f(Z_p) = a_0 I + a_1 Z_p + \cdots + a_n Z^n_p$. Simultaneously, we use a simple linear function $g(x) = b + x (b > 0)$ to map the matrix $Z$, the gotten matrix function is $g(Z) = b I + Z$. Thus, the Eq. (13) becomes:

$$J_p(U) = \max_U \frac{\text{tr}(U^T f(X(D^p - W)p^p) X^T U)}{\text{tr}(U^T (b I + Z) U)}. \quad (14)$$

It can be reduced the generalized eigenvectors problem:

$$\left(\sum_{k=0}^{n} a_k Z_p^k\right) u = \lambda (b I + Z) u. \quad (15)$$

Thus, a new MFA method has been presented. Since the polynomial is used to reconstruct the criterion of MFA, this new method is named polynomial marginal fisher analysis (PMFA). The PMFA algorithm is given below:

**Algorithm 2 PMFA**

1. **Input** a dataset $X$
2. **Constructing the in-class compactness and inter-class separability matrices:**
   - Adjacency matrix: $W_{ij} = W_{ji} = 1$ if $x_j$ is among the $k_1$ nearest neighbors of $x_i$ in the same class
   - Similarity matrix: $W_{ij} = W_{ji} = 1$ if the pair $(i, j)$ is among the $k_2$ shortest pairs
3. **New criterion:** select two suitable functions $f(x)$ and $g(x)$ to map the matrices $X(D^p - W)p^p X^T$ and $(X(D - W))X^T$ to the corresponding matrix functions, get a new criterion function:
   $$J(U) = \max_U \frac{\text{tr}(U^T f(X(D^p - W)p^p X^T U))}{\text{tr}(U^T g(X(D - W))X^T U)}.$$
4. **Compute the eigenvalues and eigenvectors as:**
   $$f(X(D^p - W)p^p X^T) u = \lambda g(X(D - W))X^T u$$
5. **Output** the final linear projection direction as:
   $$Y = U^T X$$

### B. THEORETICALLY ANALYSIS

In this section, we theoretically discuss why we chose $f(x) = a_0 + a_1 x + \cdots + a_n x^n (a_k > 0 (k = 0, 1, \ldots, n))$ and $g(x) = b + x (b > 0)$ to map matrices $Z_p$ and $Z$.

1. **Avoid the small-sample-size problem**
   - After mapping the matrix $Z$ with the linear function $g(x) = b + x (b > 0)$, the gotten matrix function is $g(Z) = b I + Z$.
   - Let $\lambda_{\text{rel}}$ be the eigenvalues of the matrix $Z$. We know that the matrix $Z$ is semidefinite according to Section II. A, and so
\( \lambda_{wi} \geq 0 \). According to Theorem 1, \( b + \lambda_{wi} \) are the eigenvalues of the matrix function \( g(Z) = bI + Z \). Since \( b > 0 \), we have \( b + \lambda_{wi} > 0 \) then the matrix function \( g(Z) = bI + Z \) will not have zero eigenvalues and will be nonsingular. Thus, Eq. (15) is solvable. Therefore, the small-sample-size problem of PMFA is avoided.

2) IMPROVE CLASSIFICATION PERFORMANCE
In the MFA method, \( W_{ij} \) is the correlation coefficient between the sample pairs \( x_i \) and \( x_j \) from the different classes, \( W_{ij} \) is the correlation coefficient between the samples \( x_i \) and \( x_j \) of the same class. The inter-class distance \( d_b \) and the intra-class distance \( d_w \) in the sample space can be expressed as:

\[
d_b = \frac{1}{2} \sum_{i,j} \| x_i - x_j \|^2 W_{ij} = \text{tr} (XLX^T) = \text{tr} (Z_p),
\]

\[
d_w = \frac{1}{2} \sum_{i,j} \| x_i - x_j \|^2 W_{ij} = \text{tr} (XLX^T) = \text{tr} (Z).
\]

Let \( \lambda_{bi} \) and \( \lambda_{wi} \) be the eigenvalues of \( Z_p \) and \( Z \) respectively, the two distances can be written as:

\[
d_b = \text{tr} (Z_p) = \lambda_{b1} + \lambda_{b2} + \cdots + \lambda_{bn},
\]

\[
d_w = \text{tr} (Z) = \lambda_{w1} + \lambda_{w2} + \cdots + \lambda_{wn}.
\]

For the PMFA method, the matrix \( Z_p \) is mapped into the matrix function \( f(Z_p) = \sum_{k=0}^{n} a_k Z_p^k \) by the polynomial \( f(x) = \sum_{k=0}^{n} a_k x^k \), and the matrix \( Z \) is mapped into the matrix function \( g(Z) = bI + Z \) by \( g(x) = b + x \). According to Theorem 1, \( f(\lambda_{bi}) = \sum_{k=0}^{n} a_k \lambda_{bi}^k \) are the eigenvalues of matrix function \( f(Z_p) = \sum_{k=0}^{n} a_k Z_p^k \), and \( g(\lambda_{wi}) = b + \lambda_{wi} \) are the eigenvalues of the matrix function \( g(Z) = bI + Z \). After mapping, the new inter-class distance \( d'_b \) and the intra-class distance \( d'_w \) are:

\[
d'_b = \text{tr} (f(Z_p)) = \left( \sum_{k=0}^{n} a_k \lambda_{b1}^k \right) + \left( \sum_{k=0}^{n} a_k \lambda_{b2}^k \right)
\]

\[
d'_w = \text{tr} (g(Z)) = (b + \lambda_{w1}) + (b + \lambda_{w2}) + \cdots + (b + \lambda_{wn}).
\]

Usually, the eigenvalues of the matrix \( Z_p, \lambda_{bi} \), take a larger value, so we have \( f(\lambda_{bi}) = \sum_{k=0}^{n} a_k \lambda_{bi}^k \gg \lambda_{bi} \) and \( g(\lambda_{wi}) = b + \lambda_{wi} \approx \lambda_{wi} \). Then, we have \( d'_b \gg d_b \) and \( d'_w \approx d_w \).

In this way, with the mapping of polynomial, the PMFA method keeps almost the intra-class distance while greatly enlarging the marginal space between the inter-class samples, which is beneficial to pattern classification.

To illustrate the main idea of the PMFA method visually, we present a geometric interpretation of PMFA in Fig. 1. For convenience, two class examples are used for illustration. The red circle and the blue circle represent two different classes respectively, the red square and the blue square represent the centers of the two different classes. In Fig. 1, orange lines represent the intra-class distance, and green lines represent the inter-class margin distance. Fig. 1(a) shows the initial samples space. In Fig. 1(b), PMFA uses the polynomial function to map the initial samples to the new space where the inter-class distance is almost unchanged, and the inter-class edge distance is enlarged. Fig. 1(c) shows a new space after the projection of the samples.

3) COMPUTATIONAL COMPLEXITY ANALYSIS
The computational complexity of the MFA and PMFA is evaluated in this section. For a given dataset \( X \in \mathbb{R}^{m \times n} \), \( m \) is the dimensionality of training samples, \( n \) is the number of the training samples. Both methods need to perform the following two steps:

1. Construct an intrinsic graph and a penalty graph in \( O((k_1 + k_2)n^2) \).
2. Solve the eigenvalue problem in \( O(m^3) \) [14].

\[FIGURE 1. Geometric interpretation of PMFA.\]
For MFA, the covariance matrix needs to be calculated in $O(m^2 n)$ and its eigenvalue decomposition is $O(m^3)$, thus, the complexity is $O((k_1 + k_2)n^2 + m^3 + m^2n + m^3)$.

For PMFA, it requires the use of the polynomial matrix function transformation in $O(4m^3)$, thus computation complexity is $O((k_1 + k_2)n^2 + m^3 + 4m^3)$.

Usually, one has $n \gg m$, so there is little difference in computational complexity between MFA and PMFA.

### C. THE DESIGN OF THE POLYNOMIAL

In this Section, we discuss how to select the polynomial $f(x)$ and $g(x)$ in Section III A. For $f(x) = b + x (b > 0)$, the constant $b$ takes usually a little value, empirically, let $b = 0.01$, i.e., $g(x) = 0.01 + x$. The design of the polynomial $f(x)$ is discussed as follows.

It is well-known that, for any function $p(x)$, it has Taylor's expansion

$$p(x) = \frac{p(x_0)}{0!} + \frac{p'(x_0)}{1!}(x-x_0) + \cdots + \frac{p^{(n)}(x_0)}{n!}(x-x_0)^n + o \left[(x-x_0)^n \right]$$

When $x_0 = 0$, it is reduced to McLaughlin's expansion

$$p(x) = \frac{p(0)}{0!} + \frac{p'(0)}{1!}x + \cdots + \frac{p^{(n)}(0)}{n!}x^n + o \left[x^n \right]. \tag{22}$$

In real application, the coefficients in Eq. (22) can be simplified to a certain constant $c$, so Eq. (22) can be rewritten as $p(x) = c \left(1 + x + \frac{x^2}{2} + \cdots + \frac{x^n}{n!} \right)$. According to the previous Section, the smaller the denominator of the polynomial, the larger the eigenvalue obtained by the polynomial $p(x)$ mapping, so the polynomial $p(x)$ can be simplified to $p(x) = 1 + x + \frac{x^2}{2} + \cdots + \frac{x^n}{n!}$.

Let's review EMFA [15], which uses exponential function $y = e^x$ to map eigenvalues, and then to enlarge the distance of samples. In this paper, the designed polynomial should be stronger than the exponential function when the distance is extended.

For the polynomial $p(x)$, the larger the $n$ value, the larger the eigenvalue after mapping. The smaller the $n$, the smaller the influence on the eigenvalues. Thus, we try to let $n = 3, 5, 7$, then the polynomial $p(x)$ becomes

$$s(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3},$$

$$h(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4} + \frac{x^5}{5}, \text{ and}$$

$$f(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4} + \frac{x^5}{5} + \frac{x^6}{6} + \frac{x^7}{7}.$$  

In order to study the mapping ability of the functions $y = e^x$, $s(x)$, $h(x)$, and $f(x)$ to eigenvalues, we give their geometric illustration in Fig. 2. As can be seen that when $n = 7$, the value $f(\lambda)$ is the largest, so the ability to enlarge the distance is the strongest. However, the greater the $n$ value, the greater the computational complexity of computing the $n$-order polynomial matrix function. We set $n = 7$, i.e., the seventh-order polynomial $f(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4} + \frac{x^5}{5} + \frac{x^6}{6} + \frac{x^7}{7}$ is chosen.

Now, we have

$$f(\lambda_0) = \sum_{k=0}^{7} \frac{\lambda_0^k}{k} \text{ and } g(\lambda) = 0.01 + x, \text{ when mapping eigenvalues, we have } f (\lambda_{bi}) = \sum_{k=0}^{7} \frac{\lambda_{bi}^k}{k} > e^{\lambda_{bi}}.$$  

Then, we have

$$\frac{f(\lambda_{bi})}{g(\lambda_{wi})} = \frac{\sum_{k=0}^{7} \frac{\lambda_{bi}^k}{k}}{0.01 + \lambda_{wi}} > \frac{e^{\lambda_{bi}}}{e^{\lambda_{wi}}} > \frac{\lambda_{bi}}{\lambda_{wi}}. \tag{23}$$

According to this analysis, the classification ability of PMFA should be better than that of EMFA, and much better than that of MFA.

### D. AN EXPERIMENT OF THE DISTANCE DIFFUSION

After selecting the polynomial $f(x)$ and $g(x)$, we provide an experiment to illustrate the distance diffusion effect of PMFA in four face datasets: AR [28], ORL [29], FERET [30], and PIE [31]. In the experiment, for each data set, the original samples are normalized to avoid the large value, and $k_1 = 3$, $k_2 = 8$. The inter-class distance $d_o$ and the intra-class distance $d_w$ of MFA are calculated by Eq. (18) and (19), and the inter-class distance $d'_o$ and the intra-class distance $d'_w$ of PMFA are calculated by Eq. (20) and (21), where the first ten largest eigenvalues are used. Table 2 shows the comparisons of the results of the MFA and PMFA methods on four face datasets. As can be seen, compared with MFA, PMFA increases the inter-class distance and maintains the intra-class distance.

|          | AR     | ORL    | FERET  | PIE    |
|----------|--------|--------|--------|--------|
| $d_o$    | 367.59 | 8.27   | 159.91 | 143.68 |
| $d'_o$   | 858.38 | 20.81  | 489.50 | 392.60 |
| $d_w$    | 70.91  | 8.15   | 37.07  | 85.33  |
| $d'_w$   | 71.72  | 8.29   | 37.22  | 83.93  |

**FIGURE 2.** Geometric illustration of the functions.

**TABLE 2.** The comparisons of distance of MFA and PMFA.
IV. EXPERIMENTAL RESULTS
A. EXPERIMENTAL SETUP
In the experiments, to verify the validity of the proposed PMFA method, the classical LDA [2], the original MFA [11], and the latest improvement of MFA: MMFA (Multiple MFA) [14], and two methods that solved the SSS problem of MFA: EMFA (Exponential MFA) [15] and RMFA (Regularized MFA) [16] are compared with the proposed PMFA method.

For the proposed PMFA method, according to section III C, two polynomial functions are selected to map the matrices $Z_p$ and $Z$ to the corresponding matrix functions:

\[
f(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4} + \frac{x^5}{5} + \frac{x^6}{6} + \frac{x^7}{7} \quad \text{and} \quad g(x) = 0.01 + x.
\]

In the further experiment, the PMFA method is also compared with the latest proposed manifold-based learning algorithms, including GDE [18], CR-DLPP [19], LMGE-DDR [20], GEU-MFA-U, and GEU-MFA-S [17].

B. DATA VISUALIZATION
To illustrate the classification performance of PMFA, we conduct data visualization experiments on the synthetic data set (Gaussian and non-Gaussian distribution) and the real face data set.

The synthetic data of Gaussian distribution is a 3-dimensional dataset in Fig. 3(a). This three-class set contains 600 points. Each class is generated using a single Gaussian.

Fig. 3(b) shows the projection in a 1-D subspace using LDA, Fig. 3(c), (d) is the 2-D projection of MFA and PMFA, respectively. Fig. 3(e) shows the projection using PMFA in a 3-D subspace. As we can see, that both MFA and PMFA provide prediction data with good distinction capabilities. We can also see that, compared with MFA, PMFA makes the intra-class samples more compact, and the marginal distance of the inter-class samples larger.

In Fig. 3(f), a binary classification problem shows the classification ability of LDA, MFA, and PMFA in the case of non-Gaussian distribution. Where, the red solid circles and blue solid circles are two different classes of synthetic data, which do not follow the Gaussian distribution. The solid lines represent optimal classification lines and the dotted lines represent the optimal projection directions learned from LDA, MFA, and PMFA, respectively. The results show that: (1) in the case of non-Gaussian distribution, LDA does not work well, but MFA and PMFA can still find the best projection directions; (2) the best projection direction learned by PMFA is better than that of MFA, because PMFA not only considers the edge points but also enlarges the distance of the inter-class samples.

Fig. 4 shows the 2-D projection on the Georgia Tech face database using the MFA, RMFA, EMFA, and PMFA methods. It can be observed that PMFA is more effective than MFA, RMFA, and EMFA.
C. FACE RECOGNITION

In this part, we conduct experiments on four face databases: ORL, Yale, AR, and Georgia Tech [32]. Fig. 5 shows some of the sample pictures from the datasets. It showed the details of the datasets used in the experiment in Table 3.

In the experiment, the matrix $Z_p$ and $Z$ are normalized to their norm, then mapping $Z_p$ with $f(x)$, and adds 0.01 to the diagonal element of $Z$. For each class in all the datasets, we select $p$ samples as the training samples and the rest as the test samples. For the $p$ training samples, to get stable results, the experiment is repeated three times and the $p$ samples are randomly selected for each time. In each experiment, for the $p$ training sample, the dimension of subspace range between 10 and 100 with the step size being 5. The recognition rate corresponding to the optimal subspace dimension is the optimal recognition rate. Therefore, for the three experiments, there are three optimal recognition rates. Finally, the average

### FIGURE 4. The two-dimension projection of Georgia Tech face database. (a) MFA. (b) RMFA (c) EMFA. (d) PMFA.

### TABLE 3. Details of the datasets.

| Dataset          | Number of classes | Sample number of each class | Image size | Data dimension |
|------------------|-------------------|-----------------------------|------------|----------------|
| ORL              | 40                | 10                          | 32×32      | 1024           |
| Yale             | 15                | 11                          | 24×24      | 576            |
| Georgia Tech     | 126               | 14                          | 32×32      | 1024           |
| AR               | 50                | 15                          | 40×50      | 2000           |

### TABLE 4. The recognition accuracy, standard deviation and optimal dimensions of the ORL dataset.

| Method   | 4 trains | 5 trains | 6 trains |
|----------|----------|----------|----------|
| LDA      | 91.67±1.21(30) | 93.33±1.64(35) | 95.23±1.98(39) |
| MFA      | 92.78±1.97(55) | 95.83±2.02(65) | 97.92±1.44(60) |
| RMFA     | 95.39±1.03(55) | 96.83±1.61(55) | 97.86±1.30(85) |
| EMFA     | 95.97±1.88(55) | 97.00±1.73(40) | 98.13±0.98(65) |
| MMFA     | 94.41±1.61(55) | 97.24±1.46(95) | 98.09±2.01(60) |
| PMFA     | 96.25±0.42(100) | 98.00±0.50(70) | 98.54±1.57(60) |
value is used as the recognition rate when the training sample is \( p \). Tables 4-7 show the recognition results (recognition accuracy (%) ± standard deviation and optimal dimension) of these methods.

We also evaluate the performance of these methods when the subspace dimension takes different values. In each experiment, for a training sample \( p \) and a subspace dimension, there is a recognition rate. When the subspace dimension is between 10 and 100, the recognition rate of each method in each dimension can be got, Figs. 6-9 show how the recognition rate varies with the dimension.

FIGURE 5. The sample pictures taken from the datasets in the experiment. The first line is from the ORL face dataset, the second line is from the Yale face dataset, the third line is from the Georgia Tech face dataset, and the last line is from the AR face dataset.

TABLE 5. The recognition accuracy, standard deviation and optimal dimensions of the Yale dataset.

| Method | 4 trains | 5 trains | 6 trains |
|--------|----------|----------|----------|
| LDA    | 67.30±6.56(100) | 75.30±7.81(35) | 81.00±7.19(35) |
| MFA    | 79.36±2.40(75)  | 81.48±3.80(50) | 86.66±5.81(25) |
| RMFA   | 80.90±1.96(35)  | 81.56±1.44(20) | 88.67±3.34(65) |
| EMFA   | 79.56±0.55(20)  | 80.74±1.24(50) | 83.11±6.01(25) |
| MMFA   | 79.92±0.84(75)  | 81.76±2.97(65) | 87.96±5.36(40) |
| PMFA   | 82.54±2.20(75)  | 82.96±3.71(50) | 90.22±6.84(25) |

FIGURE 6. Comparison of performance and dimension on ORL dataset (training sample \( p = 4 \)).

FIGURE 7. Comparison of performance and dimension of the Yale dataset (training sample \( p = 4 \)).
The results show that the recognition rate of the PMFA method is better than the latest methods.

V. CONCLUSION AND FUTURE DIRECTIONS

In this paper, based on the framework of matrix function dimensionality reduction, when the polynomial matrix function transformation is used in the MFA method, PMFA (Polynomial Marginal Fisher Analysis) is proposed. The proposed PMFA method has two advantages: one is that it solves the small-sample-size problem of MFA, and the other is that it can enlarge the distance of the inter-class sample, then have a good ability for pattern classification. However, the computational complexity and classification ability are closely related to the selected polynomial function, so enough research is needed when choosing an appropriate polynomial. In the future, the design of the polynomial functions can be improved, and the idea of the polynomial matrix function transformation can also be used to some other dimensionality reduction methods.

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D. THE FURTHER EXPERIMENTS

In this section, we also compare the PMFA method and other latest proposed manifold-based learning algorithms on PIE, AR, Yale, FERET and Yale B [33] datasets in Table 8. These including GDE [18], CR-DLPP [19], LMGE-DDR [20], GEU-MFA-U, and GEU-MFA-S [17]. Where GEU-MFA-U and GEU-MFA-S are the latest methods of MFA. We use the recognition rates reported in the literature for comparison, because the source code of these methods is not available.
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