

## Article

# On the Extremal Trace Problem on Sets Homeomorphic to the Stiefel Manifold and Its Application to Multi-Omics Data Integration

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## Abstract

In this paper, we consider the extremal trace problem for the coupled Laplacian on the sets homeomorphic to the Stiefel manifold defined on the complex Euclidean space. The study is implemented via various mathematical methods, including topological and probabilistic approaches. A detailed, comprehensive classification of the stationary points is given, which itself deserves to be considered as a general method in the framework of the optimization theory. Finally, an application to biologically meaningful integration of heterogeneous datasets, in which the structure of molecular interactions serves as a significant constraint for the mathematical model, is proposed. The main advantage of the elaborated method in comparison with the previously used ones is the absence of any conditions on the structure of the initial heterogeneous datasets. This paper is a continuation of a series of papers by our research group devoted to the development of new mathematical methods for integrating multi-omics data.

**Keywords:** manifold alignment; unsupervised topological alignment for single-cell multi-omics integration; graph Laplacian; single-cell RNA-seq; single-cell epigenomics

**MSC:** 47B15; 47A10; 47S10; 47B12; 47A75; 47B32



Academic Editors: Myriam Cilla Hernandez and Carlos Borau Zamora

Received: 25 May 2026

Revised: 24 June 2026

Accepted: 1 July 2026

Published: 3 July 2026

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## 1. Introduction

### 1.1. Challenges and Limitations in Multi-Omics Integration

Modern biomedicine is experiencing an era of accumulation of molecular data. The development of high-performance sequencing, mass spectrometry, and chromatography technologies has made it possible to simultaneously measure thousands of molecular features at several levels of the organization of a living system—genomic, transcriptomic, proteomic, metabolomic, and lipidomic. The totality of such data is commonly referred to as multi-omics data, and its integrative analysis opens up fundamentally new opportunities for understanding the molecular mechanisms of diseases, identifying biomarkers, and developing therapeutic targets. Nevertheless, despite the rapid progress in the field of generating such data, the problem of their meaningful biological interpretation remains unresolved. A living cell is a complex dynamic system in which molecular processes at different levels are interconnected in a non-linear manner, regulated by numerous feedbacks

and unfolding on different time scales. An attempt to describe this system exclusively using statistical methods of correlation analysis inevitably runs into a fundamental contradiction between mathematical formalization and biological reality.

Nowadays, a number of tools have been developed for integrating multi-omics data: mixOmics [1] represents a specialized package developed for multivariate analysis of biological data with emphasis on data exploration, MultiVI [2] represents a deep generative model for probabilistic analysis of multimodal single-cell data, designed to integrate different molecular modalities into a unified representation, PolarBear [3] represents a semi-supervised machine learning model for predicting missing modalities and aligning single-cell data between different types of omic measurements, sciCAN [4] represents a method for integrating single-cell chromatin accessibility and gene expression data using cycle-consistent adversarial networks, Pamona [5] represents a modification of the manifold alignment method based on the Gromov–Wasserstein distance and others, such as MUON [6], MOFA [7], etc. With all the variety of mathematical approaches, from the principal component method and canonical correlation analysis to variational autoencoders and alignment of manifolds, they are all united by a number of fundamental limitations.

First, most of them are based on the search for statistical correlations between datasets. This approach allows us to identify jointly varying features, but does not answer the question of the nature of the detected relationships: whether they are causal, indirect or accidental. The results of such an analysis are often difficult to interpret in biological terms, since the mathematical correlation between the levels of gene expression and the concentrations of metabolites is not equivalent to establishing a biological regulatory relationship between them.

Second, the existing tools mostly rely on the linear conceptual scheme of the central dogma of molecular biology: genome  $\rightarrow$  transcriptome  $\rightarrow$  proteome. This scheme is justified for describing the flow of genetic information, but it is fundamentally incomplete in relation to the metabolome and lipidome. Metabolites and lipids are not direct products of translation: their synthesis, transformation and degradation are carried out by enzymes, that is, they are determined by the activity and quantitative composition of the proteome. Moreover, the metabolites and lipids themselves are actively involved in the regulation of gene expression, enzyme activity, and the state of cell membranes, forming complex feedback loops. Ignoring this regulatory logic when integrating data means fundamentally simplifying the biological picture.

Third, most of the tools were developed with a focus on single-cell transcriptomic and epigenomic data (scRNA-seq, scATAC-seq), which limits their applicability in a situation where data on small non-coding RNAs, lipidomes and metabolomes measured at the level of cell populations or tissues are included in the analysis.

Fourth, many methods reduce data to low-dimensional latent representations optimized for visualization or clustering, but not for biological interpretation. The components of such representations, as a rule, do not correspond to any biologically significant axes of variation and cannot be directly compared with known molecular pathways or regulatory programs.

The described limitations indicate the need for a qualitative rethink of the very approach to integrating multi-omics data. Instead of considering it as a problem of finding mathematical correspondences between data matrices, we should turn to the conceptual framework of systems biology, which considers the cell as a dynamic network of interacting molecular components. At the same time, we use the most harmonious mathematical approach of coupling data matrices independent of any artificial constructions and techniques, which justifies its relevance. Our research group has analyzed genomic data to identify damaging mutations [8], scRNA-seq transcriptomic data of cell lines [9], proteomic

data [10], small non-coding RNA data [11], as well as metabolomic profiles. The accumulated experience of working with various types of omics data creates a foundation for developing methods for their integration.

The following papers consider a method of coupling several types of measurements of observed data in a single cell [5,12–15]. Apparently, the stated results are not based upon the interdisciplinary approach, for the abstract concept reflecting the relationship between the mathematical technique used and the special aspects of the concrete application is not clearly presented. The relationship between heterogeneous datasets is mostly determined by the technicalities of the optimization theory methods. The latter involve artificial penalty functions, which do not fully reveal the inherent structure of the datasets.

In the paper [16], the authors consider a new algorithm for unsupervised topological alignment of multi-omics data for a single cell. The method does not require any information on the correspondence between cells or measurements.

First, the internal low-dimensional structure of each dataset of a single cell is embedded into a matrix, the elements of which indicate the pairwise distances corresponding to cells within the same dataset, and then the cell images are aligned by comparison of distance matrices using the matrix optimization method.

Second, separate non-comparable measurements corresponding to single-cell datasets are mapped into a latent embedding space to provide comparability of measurements by virtue of the aligned cell images.

In the paper [17], the authors study the topological alignment method formulated for two modalities. The modality is understood as a set of features for a sample of cells. The information on the features is given in a matrix, the columns of which represent cells, and the rows represent features. Apparently, the given experimental concept admitting two modalities requires an additional technical tool ensuring uniformity of the quantitative data. In this regard, the so-called transition matrix projecting one dataset onto the space corresponding to another dataset is involved. Generally, the elements of the transition matrix correspond to the biological characteristics, for instance profiles of scATAC-seq [18–21].

However, the variety of the approaches devoted to coupling the heterogeneous datasets and their mapping into a common latent space ought to be classified and systematized in order to find the most general mathematical structure that is invariant with respect to several classical methods of the coupled manifold alignment.

### *1.2. Aims and Main Contributions of the Study*

In the paper [22], we studied natural methods of the coupled manifold alignment such as the coupled graph Laplacian method and the kernel-based method. We consider the field of complex numbers as a natural algebraic structure coupling heterogeneous datasets where the real and imaginary parts of the complex number correspond to the datasets, respectively. The main achievement is an attempt to construct an abstract qualitative theory creating an opportunity to consider a number of heterogeneous datasets endowed with the most general—and, at the same time, natural—coupling structure. However, the main disadvantage of the coupled graph Laplacian method is the special condition imposed upon the complex coupled matrix corresponding to the datasets in order to obtain a complete system of the generalized eigenvectors of the coupled graph Laplacian operator. Although the idea to involve a natural algebraic structure coupling heterogeneous datasets seems to be interesting and promising, the conditions imposed upon the coupled matrix are restrictive and may influence the framework of the applications. Thus, we were highly motivated to avoid restrictions of any kind related to the coupled matrix, which led us to the problem related to the absence of the complete system of the generalized eigenvectors. Apparently, this statement of the problem is technically inconvenient, which motivated us

to study the issue from the mathematically various points of view and, as a result, to write this paper.

In this paper, we continue to elaborate the coupled graph Laplacian method for the alignment of topological structures in Euclidean spaces, the central idea of which is to create a mapping of various sets onto a space in which images can be comparable in some sense. The problem can be considered in the context of the analysis of heterogeneous data, regardless of any assumptions on the coupled matrix corresponding to the heterogeneous datasets. Moreover, we provide a qualitative theory of the extremal trace problem on the sets homeomorphic to the Stiefel manifold for the coupled graph Laplacian operator, which is of interest in itself. Generally, the main scientific gap that is supposed to be eliminated is the absence of a unified feature space for analyzing data of different natures and, as a result, lying on various low-dimensional manifolds in their corresponding high-dimensional initial spaces [23]. The central hypothesis of the study is that, for a set of such data, a common latent space can be constructed in which the geometric relationships between the elements of the set (for example, pairwise distances or angles) will reflect the relationships between the corresponding objects from different data sources. This will allow information transfer between sets when solving various application problems. The relevance of the issues under consideration arises from the established background of the problem of the coupled manifold alignment; in turn, the latter appeals to specific problems of biology that are of vital importance to humanity.

The paper is organized as follows: in Section 2, we present notations and some well-known facts, and introduce the concept of the coupled unsupervised manifold alignment; in Section 3, we state the main extremal problem in terms of the Stiefel manifold; in Section 3.1, we present the main idea of the Lagrangian method and prove auxiliary propositions; in Section 3.2, we establish the classification of the stationary points via the Hessian and prove the main theorem that provides a complete description of the extremal problem; and in Section 4, we observe the biological part of the investigation and discuss prospective mathematical generalizations.

## 2. Preliminaries

Throughout the paper, we consider finite dimensional matrices  $\mathbb{C}^{n \times m}$ ,  $n, m \in \mathbb{N}$  over the field of the complex numbers and use the following notation  $A = \{a_{sj}\} \in \mathbb{C}^{n \times m}$ ,  $s = 1, 2, \dots, n$ ,  $j = 1, 2, \dots, m$  for a matrix. We use the following standard notation for the transpose operation  $A^T = \{a_{js}\}$ . Consider a matrix  $A = \{a_{sj}\} \in \mathbb{C}^{n \times m}$ ,  $a_{sj} \in \mathbb{C}$ , and denote

$$\mathbf{a}_s := (a_{s1}, a_{s2}, \dots, a_{sm})^T, \mathbf{a}_j = (a_{1j}, a_{2j}, \dots, a_{nj})^T.$$

We consider a complex linear vector space  $\mathbb{C}^n$  consisting of the set of column matrices whose elements are complex numbers  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ ,  $x_j \in \mathbb{C}$ ,  $j = 1, 2, \dots, n$ . Analogously, we define the real linear vector space  $\mathbb{R}^n$ . A complex linear vector space supplied with the given below structure of the inner (scalar) product operation is called a complex Euclidean space

$$(\mathbf{x}, \mathbf{y})_{\mathbb{C}^n} := \sum_{j=1}^n x_j \bar{y}_j, \mathbf{x}, \mathbf{y} \in \mathbb{C}^n.$$

Note that the complex Euclidean space represents a particular case of the unitary space, i.e., a linear space over the field of the complex numbers endowed with the inner product operation. Define the norm in the general sense in a space with the inner product as follows

$\|\mathbf{x}\| = \sqrt{(\mathbf{x}, \mathbf{x})}$ . Consider a matrix  $A = \{a_{sj}\} \in \mathbb{C}^{n \times m}$ , and denote  $\bar{A} = \{\bar{a}_{sj}\}$ . In accordance with the orthogonal decomposition theorem, we have

$$\mathbb{C}^n = \mathbb{C}^m \oplus \mathbb{C}^{n-m}, \quad n > m,$$

i.e., for an arbitrary element  $\mathbf{x} \in \mathbb{C}^n$ , there exists a unique pair  $\mathbf{x}_1 \in \mathbb{C}^m$ ,  $\mathbf{x}_2 \in \mathbb{C}^{n-m}$  of elements so that the following representation holds  $\mathbf{x} = \mathbf{x}_1 + \mathbf{x}_2$ . In this way, we can put the element  $\mathbf{x}_1$  into correspondence with the element  $\mathbf{x}$ , which is called the orthogonal projection of the space  $\mathbb{C}^n$  onto the subspace  $\mathbb{C}^m$ . Given an arbitrary set  $X$ , a totally ordered set  $Y$ , and a function  $f : X \rightarrow Y$ , the *argmin* over some subset  $\Omega \subseteq X$  is defined by the following expression

$$\operatorname{argmin}_{x \in \Omega} f(x) := \{y \in \Omega : f(y) \leq f(x), x \in \Omega\}.$$

Note  $A : \mathbb{C}^m \rightarrow \mathbb{C}^n$ . We use the following notations for the Hermitian components of the operator

$$\Re A = \frac{A + A^*}{2}, \quad \Im A = \frac{A - A^*}{2i}, \quad \bar{A} := \{\bar{a}_{sj}\}, \quad \Re(A) := \{\Re a_{sj}\}, \quad \Im(A) := \{\Im a_{sj}\}.$$

The latter matrices are called the real and imaginary parts of the matrix  $A$ , respectively. The detailed information on the properties of the Hermitian components is given in the paper [24]. Denote by  $D(A)$ ,  $R(A)$ ,  $N(A)$  the domain of definition, the range, and the kernel or null space of the operator  $A$ , respectively. Define matrix trace in the ordinary way  $\operatorname{tr} A = a_{11} + a_{22} + \dots + a_{nn}$ , where  $A \in \mathbb{C}^{n \times n}$ . Let a matrix  $A \in \mathbb{C}^{n \times n}$  have a set of the eigenvalues  $\mu_j$ ,  $j = 1, 2, \dots, n$ , and denote by  $\nu(\mu_j)$  the algebraic multiplicity of the eigenvalue  $\mu_j$ .

Consider a function  $f : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}$ , and define a derivative of a scalar function  $f(X)$ ,  $X \in \mathbb{C}^{n \times n}$  by a matrix  $X$  as follows

$$\frac{\partial f}{\partial X} = \left\{ \frac{\partial f}{\partial x_{sj}} \right\}_{s,j=1}^n.$$

Taking into account  $X = \{x_{sj}\}_{s,j=1}^n \Rightarrow X^* = \{\bar{x}_{js}\}_{s,j=1}^n$ , we come to the following definition that is in the framework of the formal theory

$$\frac{\partial f}{\partial X^*} := \left( \frac{\partial f}{\partial X} \right)^T.$$

Consider a differential

$$df = \sum_{s,j=1}^n \frac{\partial f}{\partial x_{sj}} dx_{sj} = \operatorname{tr} \left\{ \left( \frac{\partial f}{\partial X} \right)^T dX \right\}.$$

The following properties of the matrix differential can be deduced directly from the properties of the differential  $d(XY) = dXY + XdY$ ,  $d(X + Y) = dX + dY$ . The following implication is based upon the arbitrariness of the differential, i.e.,  $\operatorname{tr}(CdX) = 0, \Rightarrow C = 0$ . Consider the so-called Wirtinger derivatives

$$\frac{df}{dX} := \frac{1}{2} \left( \frac{\partial f}{\partial A} - i \frac{\partial f}{\partial B} \right), \quad \frac{df}{d\bar{X}} := \frac{1}{2} \left( \frac{\partial f}{\partial A} + i \frac{\partial f}{\partial B} \right), \quad A := \Re(X), \quad B := \Im(X).$$

Separating the real and imaginary parts of the complex matrix variable  $X \in \mathbb{C}^{n \times n}$ , we can consider the differential of the function of real variables

$$\begin{aligned} df &= \sum_{s,j=1}^n \frac{\partial f}{\partial a_{sj}} da_{sj} + \frac{\partial f}{\partial b_{sj}} db_{sj} = \text{tr} \left\{ \left( \frac{\partial f}{\partial A} \right)^T dA + \left( \frac{\partial f}{\partial B} \right)^T dB \right\} = \\ &= \text{tr} \left\{ \left( \frac{df}{dX} \right)^T dX + \frac{df}{d\bar{X}} d\bar{X} \right\}, \end{aligned} \quad (1)$$

where the second equality can be established by direct substitution and subsequent calculation.

1. Consider a set of elements  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  belonging to a normed space. Generally, in terms of applications, each vector  $\mathbf{x}_j$  represents measurements corresponding to a concrete object. In particular, if we consider a problem of biological integration, we assume that  $\mathbf{x}_j \in \mathbb{R}^q$ ,  $q \in \mathbb{N}$ , where each coordinate reflects a concrete measurement. Let us construct a weighted graph  $G$  having  $n$  vertices, where one vertex corresponds to one element, and a set of edges connecting the adjacent vertices of the graph. We numerate the vertices according to the given order, i.e.,  $j$ -th vertex corresponds to  $\mathbf{x}_j$ . We suppose that the  $s$ -th and  $j$ -th vertices are adjacent to each other if the elements  $\mathbf{x}_s$  and  $\mathbf{x}_j$  are related, for instance close in some sense. The main challenge consists in defining the rather vague notion of closeness in a more concrete way [25].

Here, we consider two variants; the first one is the so-called  $\varepsilon$ —neighborhood method which postulates the following sense of closeness. Suppose that the vertices  $s$  and  $j$  are adjacent to each other if

$$\|\mathbf{x}_s - \mathbf{x}_j\| < \varepsilon,$$

where the norm is understood in the abstract sense. However, the Euclidean norm is typically used in applications. Note that this type of closeness is geometrically motivated, and the relationship is naturally symmetric. However, it often leads to a graph with several connected components and it is difficult to choose the convenient value of  $\varepsilon$  to avoid the unconnected graph.

The second variant is the so-called  $n$ —nearest neighbors method, which postulates the following sense of closeness. Suppose that the  $s$ -th and  $j$ -th vertices are adjacent to each other if  $\mathbf{x}_s$  belongs to the set of  $n$  nearest neighbors (in the sense of the norm) of the element  $\mathbf{x}_j$ , or  $\mathbf{x}_j$  belongs to the set of  $n$  nearest neighbors of the element  $\mathbf{x}_s$ .

Having constructed the graph in accordance with the one of the methods given above, we can choose weights to form the weight matrix. The first one relates to the heat kernel; we assume that, if the  $s$ -th and  $j$ -th are connected, in symbol  $s \sim j$ , then the weight matrix is formed from the elements

$$A_{sj} = e^{-t^{-1}\|\mathbf{x}_s - \mathbf{x}_j\|^2}, \quad t \in \mathbb{R} \setminus \{0\}, \quad s, j = 1, 2, \dots, n,$$

in the contrary case, we assume that  $A_{sj} = 0$ . Thus, we have

$$A_{sj} = \begin{cases} e^{-t^{-1}\|\mathbf{x}_s - \mathbf{x}_j\|^2}, & s \sim j \\ 0, & s \not\sim j \end{cases}.$$

In accordance with this definition, we obtain the adjacency matrix of the weighted graph  $A = \{A_{sj}\} \in \mathbb{R}^{n \times n}$ . The substantiation on choosing this weight is represented in the papers [26,27]. The second one is the so-called simple weight; we assume that  $A_{sj} = 1$

if the  $s$ -th and  $j$ -th vertices are connected and  $A_{sj} = 0$  if the  $s$ -th and  $j$ -th vertices are disconnected, i.e.,

$$A_{sj} = \begin{cases} 1, & s \sim j \\ 0, & s \not\sim j \end{cases}.$$

This kind of simplicity gives the opportunity to avoid choosing the value of the parameter  $t$ . Consider heterogeneous datasets

$$\{\mathbf{x}_1^{(1)}, \mathbf{x}_2^{(1)}, \dots, \mathbf{x}_n^{(1)}\}, \{\mathbf{x}_1^{(2)}, \mathbf{x}_2^{(2)}, \dots, \mathbf{x}_n^{(2)}\}.$$

The fact of the heterogeneity can be described by the choice of the norm. In other words, the freedom of the choice of the norm allows us to create a suitable mathematical model when the phenomenon of heterogeneity appears. In accordance with the above, we can construct two adjacency matrices corresponding to the datasets  $A^{(1)}, A^{(2)}$ .

Generally, if we want to apply an abstract operation to the datasets, for instance topological alignment, we can implement it separately considering each dataset. Otherwise, we can create a connecting structure and apply the operation to the datasets coupled with the structure. Thus, we can apply the graph Laplacian method to the datasets separately, where in this concrete case the operation is a mapping  $\mathbb{E}^q \rightarrow \mathbb{E}^m$ , ( $m \ll q$ ), heuristically called topological or manifold alignment. However, the situation is rather different if we want to consider the second scenario related to coupling the heterogeneous datasets. Since in this case, if we want to generalize the graph Laplacian method directly, having involved the field of the complex numbers, we would face classical technical difficulties based on peculiarities related to the algebraic structure, for instance, non-selfadjointness of a symmetric operator.

Motivated by the problems described above and prospective advantages, throughout the paper, we consider a symmetric matrix  $W \in \mathbb{C}^{n \times n}$ ,  $\operatorname{Re} W_{sj}, \operatorname{Im} W_{sj} > 0$ , where from the applied point of view, we are able to put in correspondence  $\operatorname{Re} W_{sj} = A^{(1)}, \operatorname{Im} W_{sj} = A^{(2)}$ . Here, the coupled structure mentioned above is represented in its most general form being an algebraic structure—the field of the complex numbers.

Define a diagonal matrix

$$D = \{D_{sj}\}, D_{sj} = \begin{cases} \sum_{k=1}^n W_{kj}, & s = j \\ 0, & s \neq j \end{cases}.$$

Further, we assume that  $D_{jj} \neq 0$ ,  $j = 1, 2, \dots, n$ , which does not restrict the appropriate class of matrices due to the given sense of the elements. Consider an operator  $L := D - W$ . It is clear that  $\operatorname{Re}(L), \operatorname{Im}(L)$  are the graph Laplacian operators and the fact is that  $L$  is not selfadjoint. The verification is left to the reader; however, the corresponding matrix is symmetric, i.e.,  $L^* = \bar{L}$ . The operator  $L$  is called the coupled graph Laplacian operator. Consider the following formula deduced by direct calculation (see Lemma 1 [22])

$$(L\mathbf{x}, \mathbf{x})_{\mathbb{C}^n} = \frac{1}{2} \sum_{s,j=1}^n |x_s - x_j|^2 W_{sj}. \quad (2)$$

This gives us a technically significant fact  $\arg(L\mathbf{x}, \mathbf{x})_{\mathbb{C}^n} \in (0, \pi/2)$ ,  $\mathbf{x} \in \mathbb{C}^n$ . Note that relation (2) shows that the kernel of the coupled graph Laplacian is a one-dimensional subspace of  $\mathbb{C}^n$  defined as follows

$$N(L) = \{\mathbf{x} \in \mathbb{C}^n : x_j = a, a \in \mathbb{C}, j = 1, 2, \dots, n\}.$$

Therefore, taking into account the fact  $N(L) = N(L^*)$ , we obtain

$$\mathbb{C}^n = N(L) \oplus R(L).$$

Since  $N(L)$  is an invariant subspace of the operator  $L$ ,  $R(L)$  is the invariant subspace of the operator  $L$  having the dimension  $n - 1$ . Apparently, to avoid the trivial solution of the optimization problem involving the operator  $L$ , we should consider the subspace  $R(L)$ . Consider the so-called connection condition

$$X^* T_\zeta X = I_m, \quad X \in \mathbb{C}^{n \times m}, \quad m \leq n, \quad (3)$$

where

$$T_\zeta := \Re \left( D \operatorname{diag} \{ e^{i\zeta_1}, e^{i\zeta_2}, \dots, e^{i\zeta_n} \} \right), \quad \zeta_j \in (0, \pi/2).$$

Define the sets

$$R^m(L) := \{ X \in \mathbb{C}^{n \times m} : x_j \in R(L), j = 1, 2, \dots, m \}, \quad \mathfrak{M}_m^n := \{ X \in R^m(L) : X^* T_\zeta X = I_m \},$$

Let us show that  $\mathfrak{M}_m^n$  is a compact connected manifold without boundary. Assume that  $X \in R^m(L)$ ; it is clear that, since  $R(L)$  is a Euclidean space of the dimension  $n - 1$ , we can produce a unitary transform  $U \in \mathbb{C}^{n \times (n-1)}$  such that  $X = U\tilde{X}$ ,  $\tilde{X} \in \mathbb{C}^{(n-1) \times m}$ . Substituting to the connection condition, i.e.,  $X^* T_\zeta X = I_m$ , we get  $\tilde{X}^* \tilde{T}_\zeta \tilde{X} = I_m$ ,  $\tilde{T}_\zeta := U^* T_\zeta U$ . It is clear that  $T_\zeta \succ 0 \Rightarrow \tilde{T}_\zeta \succ 0$ ; the proof is left to the reader. Thus, the obtained relation can be rewritten in the form  $\tilde{Y}^* \tilde{Y} = I_m$ ,  $\tilde{Y} = \tilde{T}_\zeta^{-1/2} \tilde{X}$ . It is clear that the latter relation can be extended to  $\tilde{Y} \in \mathbb{C}^{(n-1) \times m}$  and we obtain the Stiefel manifold  $V_m(\mathbb{C}^{n-1}) := \{ Y \in \mathbb{C}^{(n-1) \times m} : Y^* Y = I_m \}$ . It is a well-known fact that the Stiefel manifold is a compact connected manifold without boundary. Since the operator  $\tilde{T}_\zeta^{-1/2}$  is defined and the following mapping is injective and continuous

$$\tilde{T}_\zeta^{-1/2} : V_m(\mathbb{C}^{n-1}) \rightarrow \mathfrak{M}_m^n,$$

using Brouwer's theorem on the invariance of domain, we conclude that  $\tilde{T}_\zeta^{-1/2}$  is a homeomorphism (it can be established directly). Therefore,  $\mathfrak{M}_m^n$  is a compact connected manifold without boundary in the sense of the Frobenius norm or in the sense of any other norm due to the norm equivalence in the Euclidean space.

2. In this paragraph, we formulate the Lagrange multipliers method in terms of the matrix calculus. Consider a real matrix function  $F(X, X^*)$ ,  $X \in \mathbb{C}^{n \times m}$  and the complex restriction condition  $G(X, X^*) = 0$  given by the matrix  $G \in \mathbb{C}^{m \times m}$ , i.e.,

$$F : \mathbb{C}^{n \times m} \rightarrow \mathbb{R}, \quad \operatorname{Re} G_{sj}(X, X^*) = \operatorname{Im} G_{sj}(X, X^*) = 0, \quad s, j = 1, 2, \dots, m.$$

Taking into account the fact  $x_{sj} = \operatorname{Re} x_{sj} + i \operatorname{Im} x_{sj}$ , we can reformulate the conditional extremum problem in classical terms corresponding to real functions of  $2nm$  real variables. In accordance with the classical theory, the Lagrangian is represented by the following expression

$$\mathcal{L} = F - \sum_{s,j=1}^m \{ \mu_{sj} \operatorname{Re} G_{sj} + \eta_{sj} \operatorname{Im} G_{sj} \}, \quad \mu_{sj}, \eta_{sj} \in \mathbb{R}.$$

This expression can be rewritten in the form

$$\mathcal{L} = F - \sum_{s,j=1}^m \operatorname{Re} \{ \bar{\lambda}_{sj} G_{sj} \}, \quad \lambda_{sj} := \mu_{sj} + i \eta_{sj}.$$

Note that

$$\sum_{s,j=1}^m \operatorname{Re}\{\bar{\lambda}_{sj}G_{sj}\} = \operatorname{Re} \operatorname{tr}\{\Lambda^*G\}, \quad \Lambda := \{\lambda_{js}\} \in \mathbb{C}^{m \times m}.$$

Therefore

$$\mathcal{L}(X, \Lambda) = F(X, X^*) - \operatorname{Re} \operatorname{tr}\{\Lambda^*G(X, X^*)\}. \quad (4)$$

Let us show that the restriction  $\Lambda = \Lambda^*$  does not influence the general statement of the problem. It is a well-known fact that an arbitrary matrix can be decomposed into the sum of the Hermitian and skew-Hermitian parts; we have  $\Lambda = \Lambda_H + \Lambda_S$ , where  $\Lambda_H^* = \Lambda_H$ ,  $\Lambda_S^* = -\Lambda_S$ . Therefore

$$\operatorname{tr}\{\Lambda^*G\} = \operatorname{tr}\{(\Lambda_H + \Lambda_S)^*G\} = \operatorname{tr}\{\Lambda_H G\} - \operatorname{tr}\{\Lambda_S G\}.$$

Taking into account the fact  $\overline{\operatorname{tr}\{\Lambda_S G\}} = \operatorname{tr}\{\Lambda_S^* G\} = -\operatorname{tr}\{\Lambda_S G\}$ , we conclude that  $\operatorname{Re} \operatorname{tr}\{\Lambda_S G\} = 0$ . Substituting this relation into the Equation (4), we obtain the desired result, i.e., without loss of generality, we can assume  $\Lambda = \Lambda^*$ .

### 3. Main Results

Consider the following problems

$$\text{PI)} \quad \mathfrak{A}_m := \arg \min_{X \in \mathfrak{M}_m^n} |\operatorname{tr}\{X^* L X\}|, \quad \text{PII)} \quad \mathfrak{B}_m := \arg \max_{X \in \mathfrak{M}_m^n} |\operatorname{tr}\{X^* L X\}|.$$

Problems PI and PII are called the minimum and maximum trace problems, respectively. The connection condition (3) evidently corresponds to the so-called  $T_\zeta$ —orthogonality property of the columns of the matrix  $X$ . Note that the connection condition originates from the case corresponding to the Laplace matrix having real elements. In this case, if the diagonal matrix multiplier is the identity matrix, we obtain the very condition of  $D$ -orthogonality of the columns of the matrix  $X$ . The latter construction admits a convenient, from the theoretical point of view, description in terms of the generalized eigenvalue problem for the graph Laplacian operator [22], since in this case, due to the properties of the Hermitian matrices, it is not hard to prove that the generalized eigenvalue problem has a set of solutions forming a  $D$ -orthogonal basis in  $\mathbb{C}^n$ . However, we will see that the situation corresponding to the formulated problems is rather complicated in the complex case for the Hermitian nature of the connection condition contradicts the symmetric nature of the coupled graph Laplacian. The latter fact technically influences the opportunity to consider the problems in terms of the generalized eigenvalue problem.

Consider the following relation (see Lemma 1 [22])

$$\operatorname{tr}\{X^* L X\} = \sum_{j=1}^m (L \mathbf{x}_j, \mathbf{x}_j)_{\mathbb{C}^n} = \frac{1}{2} \sum_{s,j=1}^n \|\mathbf{x}_s - \mathbf{x}_j\|_{\mathbb{C}^m}^2 W_{sj}. \quad (5)$$

It is remarkable that, from the applied point of view, the main concept of PI (PII) is to select some compact manifold to minimize or maximize the absolute value of functional (5) reflecting how the images of the elements  $W$  relate to each other under the mapping constructed by  $\mathfrak{A}_m$  or  $\mathfrak{B}_m$  correspondence, in this regard, the choice of the compact manifold is mostly dictated by the technical peculiarities. More precisely, we have a concrete correspondence satisfying biologically determined conditions revealed in mathematical construction (5), i.e.,

$$\mathfrak{A}_m^T : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{m \times n}, \quad \mathfrak{B}_m^T : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{m \times n}.$$

This correspondence allows us to reduce the dimension of the initial high-dimensional space by mapping the data into the compressed transposed representations, taking into account their mutual nature reflected by the involved complex structure. Consequently, the codomain of the operators corresponds to the planned low-dimensional feature space, where  $m$  explicitly denotes the target reduced dimensionality. A matrix belonging to the set  $\mathbb{C}^{m \times n}$  is uniquely decomposed into its real and imaginary parts, the columns of which represent the low-dimensional images of the high-dimensional elements of the initial datasets.

### 3.1. Stationary Points

As a main technical tool in solving the trace problems, we consider the Lagrange multiplier method. Let us use the following notations

$$\psi(X) := \operatorname{tr}(X^* LX), \quad F(X, X^*) := |\operatorname{tr}(X^* LX)|^2, \quad G(X, X^*) := X^* T_\zeta X - I_m, \quad H := \bar{\psi} L + \psi L^*.$$

For the reader's convenience, we recall that

$$W \in \mathbb{C}^{n \times n}, \operatorname{Re} W_{sj}, \operatorname{Im} W_{sj} > 0, \quad D := \operatorname{diag}\{D_{11}, D_{22}, \dots, D_{nn}\}, \quad D_{jj} = \sum_{k=1}^n W_{kj}, \quad L := D - W,$$

$$T_\zeta := \Re \left( D \operatorname{diag}\{e^{i\zeta_1}, e^{i\zeta_2}, \dots, e^{i\zeta_n}\} \right), \quad \zeta_j \in (0, \pi/2).$$

**Theorem 1.** *There exists a solution of the problem PI (PII); moreover, if  $X$  is a solution, then*

$$\exists \Lambda = \operatorname{diag}\{\lambda_1, \lambda_2, \dots, \lambda_m\}, \quad \lambda_j \in \mathbb{R} : \quad HX - T_\zeta X \Lambda = 0.$$

**Proof.** Note that the image of the Stiefel manifold  $\mathfrak{M}_m^n$  is a compact connected manifold without boundary (see the preliminary section); the following functions are continuous

$$X^* LX : \mathbb{C}^{n \times m} \rightarrow \mathbb{C}^{m \times m}, \quad \operatorname{tr}\{X\} : \mathbb{C}^{m \times m} \rightarrow \mathbb{C}.$$

Thus, applying the Weierstrass theorem, we conclude that there exists a solution of the problem PI (PII). Observe the differentials  $d(X^* LX) = dX^* LX + X^* L dX$ ,  $dF = \bar{\psi} d\psi + \psi d\bar{\psi}$ . Using the trace properties, we can rewrite the latter relation as follows:  $dF = \operatorname{tr}\{X^* H dX\} + \operatorname{tr}\{H X dX^*\}$ . Consider the Lagrange multiplier method in terms of the previous paragraph. Applying Formula (4), we get

$$\mathcal{L}(X, \Lambda) = |\operatorname{tr}(X^* LX)|^2 - \operatorname{tr}\{\Lambda(X^* T_\zeta X - I)\}, \quad \Lambda = \Lambda^*,$$

where we used the obvious relation  $\operatorname{Re} \operatorname{tr}\{\Lambda(X^* T_\zeta X - I)\} = \operatorname{tr}\{\Lambda(X^* T_\zeta X - I)\}$ . In accordance with the above, we have

$$d\mathcal{L}(X, \Lambda) = \operatorname{tr}\{(X^* H - \Lambda X^* T_\zeta) dX\} + \operatorname{tr}\{(H X - T_\zeta X \Lambda) dX^*\},$$

where we have taken into account the connection condition, which yields  $d\Lambda(X^* T_\zeta X - I) = 0$ . Using simple reasoning based upon arbitrariness in choosing differential, we can prove the following relation

$$\frac{d\mathcal{L}(X, \Lambda)}{d\bar{X}} = HX - T_\zeta X \Lambda. \quad (6)$$

For this purpose, it is sufficient to establish the following implication

$$df = \operatorname{tr}\{C_1 dX\} + \operatorname{tr}\{C_2 dX^*\}, \quad C_1 \in \mathbb{C}^{m \times n}, C_2 \in \mathbb{C}^{n \times m}, \implies C_1 = \left( \frac{df}{d\bar{X}} \right)^T, \quad C_2 = \left( \frac{df}{dX} \right).$$

Consider the following reasoning based on the properties of the trace

$$df = \text{tr}\{C_1 dX + C_2^T d\bar{X}\} = \text{tr}\left\{(C_1 + C_2^T)dA + i(C_1 - C_2^T)dB\right\},$$

where we used the representation  $X = A + iB$ . On the other hand, using Formula (2), we have

$$\text{tr}\left\{\left(C_1^T + C_2 - \frac{\partial f}{\partial A}\right)^T dA + \left(iC_1^T - iC_2 - \frac{\partial f}{\partial B}\right)^T dB\right\} = 0.$$

By virtue of the arbitrariness of the differentials  $dA$  and  $dB$  of the independent real matrix variables, we have

$$\text{tr}\left\{\left(C_1^T + C_2 - \frac{\partial f}{\partial A}\right)^T dA\right\} = 0, \quad \text{tr}\left\{\left(iC_1^T - iC_2 - \frac{\partial f}{\partial B}\right)^T dB\right\} = 0.$$

Due to the same reason (see the preliminary section), we obtain

$$C_1^T + C_2 = \frac{\partial f}{\partial A}, \quad i(C_1^T - C_2) = \frac{\partial f}{\partial B}.$$

Solving the system, we obtain the desired result. Note that relation (6), in accordance with the notations given in the preliminary section, can be rewritten in the form

$$\frac{d\mathcal{L}(X, \Lambda)}{dA} = \text{Re}\{HX - T_\zeta X\Lambda\}, \quad \frac{d\mathcal{L}(X, \Lambda)}{dB} = \text{Im}\{HX - T_\zeta X\Lambda\}.$$

The derivative with respect to the matrix of the multipliers gives us

$$\frac{d\mathcal{L}(X, \Lambda)}{d\Lambda} = X^* T_\zeta X - I.$$

Apparently, the above equations define stationary points and can be written in the form

$$HX - T_\zeta X\Lambda = 0, \quad X^* T_\zeta X - I = 0. \quad (7)$$

Therefore

$$X^* HX = X^* T_\zeta X\Lambda = \Lambda \in \mathbb{C}^{m \times m}.$$

Since the matrix  $\Lambda$  is Hermitian, there exists a unitary transform  $U$  such that

$$U^* \Lambda U = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_m\},$$

where  $\lambda_j$  are real parameters. Taking into account the fact that the unitary transform preserves the orbit and the connection condition, i.e.,

$$\text{tr}\{X^* HX\} = \text{tr}\{U^* X^* HXU\}, \quad U^* X T_\zeta XU = U^* I_m U = I_m,$$

we conclude that, without loss of generality, the parameter can be chosen in the form  $\Lambda = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_m\}$ . On the other hand, if the point  $X$  is a solution of the problem PI (PII), then it belongs to the open set  $\mathcal{U} \subset \mathfrak{M}_m^n$  in the sense of the topology induced by the topology of  $\mathbb{C}^n$ . Applying the classical theorems of differential calculus, we conclude that it is a stationary point.  $\square$

The theorem proved above establishes the necessary condition related to the solution of the problem PI (PII), which motivates us to study solutions of the stationary system (7). Having classified the points, we can find the global minimum and the global maximum,

i.e., the solutions of the problems PI and PII. Let us rewrite the stationary system (7) in the following form

$$H\mathbf{x}_j = \lambda_j T_\zeta \mathbf{x}_j, (T_\zeta \mathbf{x}_j, \mathbf{x}_k)_{\mathbb{C}^n} = \delta_{jk}, j, k = 1, 2, \dots, m, \quad (8)$$

that can be understood as the eigenvalue problem. Apparently, we can claim that the solutions of the stationary system (7) are the solutions of the generalized eigenvalue problem (8). Note that  $T_\zeta \succ 0$ ; indeed, if we assume that  $\zeta_j \in (0, \pi/2)$ , then taking into account the assumptions  $\arg W_{sj} \in (0, \pi/2)$ , we get  $\arg\{D_{ss}\} - \zeta_s \in (-\pi/2, \pi/2)$  and therefore

$$(T_\zeta \mathbf{x}, \mathbf{x})_{\mathbb{C}^n} = \sum_{s=1}^n \operatorname{Re}\{e^{-i\zeta_s} D_{ss}\} |x_s|^2 > 0, \mathbf{x} \neq \mathbf{0}.$$

It follows that the system of the eigenvectors of the following generalized eigenvalue problem is complete

$$H(X)\mathbf{e}_j = \phi_j T_\zeta \mathbf{e}_j, (T_\zeta \mathbf{e}_j, \mathbf{e}_k)_{\mathbb{C}^n} = \delta_{jk}, j, k = 1, 2, \dots, n,$$

where  $X$  is a parameter, the eigenvalues are arranged in increasing order; we assume that zero eigenvalues correspond to the vectors belonging to  $N(H)$ . Indeed, we can easily prove this fact if we consider a selfadjoint operator  $T_\zeta^{-1/2} H T_\zeta^{-1/2}$  having a complete system of the eigenvectors.

Motivated by the formula  $H = |\psi| \{e^{-i\theta} L + e^{i\theta} L^*\}$ ,  $\theta := \arg \psi$ , we have come to the following generalized eigenvalue problem

$$\Psi(\theta)\mathbf{e}_j = \mu_j T_\zeta \mathbf{e}_j, (T_\zeta \mathbf{e}_j, \mathbf{e}_k)_{\mathbb{C}^n} = \delta_{jk}, j, k = 1, 2, \dots, n, \quad (9)$$

where  $\Psi(\theta) = e^{-i\theta} L + e^{i\theta} L^*$ ,  $\theta \in \mathbb{R}$ . Since the operator  $\Psi(\theta)$  depends upon the parameter  $\theta$ , only then  $\mu_j := \mu_j(\theta)$ ,  $\mathbf{e}_j := \mathbf{e}_j(\theta)$ . Note that the system of the eigenvectors is complete. Define the matrices

$$E_p(\theta) := (\mathbf{e}_{p_1}(\theta), \mathbf{e}_{p_2}(\theta), \dots, \mathbf{e}_{p_m}(\theta)) \in \mathbb{C}^{n \times m}, p_j \in \{1, 2, \dots, n\}, p_j \neq p_q, j \neq q.$$

It is clear that we have  $C_n^m$  matrices formed from the various  $m$ —element subsets of the eigenvectors, i.e., we can enumerate the indices of the groups as follows:  $p = 1, 2, \dots, C_n^m$ , where we put  $E_1(\theta) := (\mathbf{e}_1(\theta), \mathbf{e}_2(\theta), \dots, \mathbf{e}_m(\theta))$ ,  $E_2(\theta) := (\mathbf{e}_{n-m+1}(\theta), \mathbf{e}_{n-m+2}(\theta), \dots, \mathbf{e}_n(\theta))$ . Here, we assume that the matrices corresponding to other values of the index  $p$  are formed from the element-columns without any special structure. Further, we use the notation  $\mathfrak{P}_p := \{p_1, p_2, \dots, p_m\}$  for the set of numbers corresponding to the concrete index  $p$ . Since  $\arg W_{sj} \in (0, \pi/2)$ , using relation (5), we deduce  $\arg\{\psi(X)\} \in (0, \pi/2)$ . Note that the following functions are continuous

$$X^* L X : \mathbb{C}^{n \times m} \rightarrow \mathbb{C}^{m \times m}, \operatorname{tr}\{\cdot\} : \mathbb{C}^{m \times m} \rightarrow \mathbb{C}, \arg : \mathbb{C} \setminus \{0\} \rightarrow [0, 2\pi).$$

Therefore, the mapping  $\arg\{\psi(X)\} : \mathfrak{M}_m^n \rightarrow (0, \pi/2)$  is continuous; thus, the image of the connected compact  $\mathfrak{M}_m^n$  under the mapping is a connected compact, i.e., the segment  $\mathbb{J} := [a, b] \subset (0, \pi/2)$ . Thus, we have

$$\arg\{\psi(X)\} : \mathfrak{M}_m^n \rightarrow \mathbb{J}. \quad (10)$$

Consider the following equations

$$\arg\psi\{E_p(\theta)\} = \theta, \theta \in \mathbb{J}, p = 1, 2, \dots, C_n^m. \quad (11)$$

Denote by  $\mathbb{S}_p$  a set of the solutions of the equation with the corresponding index, i.e.,

$$\mathbb{S}_p := \{\theta \in \mathbb{J} : \arg \psi\{E_p(\theta)\} = \theta\}, \quad p = 1, 2, \dots, C_n^m.$$

Note that, generally, the question regarding the existence of a solution is open. This fact indicates that, in general,  $E_p(\theta)$  are not solutions of the problem (8); however, the issue ought to be considered comprehensively. Denote

$$\rho_p(\theta) := \sum_{j=1}^m \mu_{p_j}(\theta), \quad \theta \in \mathbb{R}.$$

Consider the generalized eigenvalue problem (9), which can be rewritten in the form

$$T_\zeta^{-1}\Psi(\theta)\mathbf{e}_j = \mu_j(\theta)\mathbf{e}_j, \quad j = 1, 2, \dots, n.$$

Note that the operator  $T_\zeta^{-1}\Psi(\theta)$  does not have root vectors but has the eigenvectors only.

The proof is based on the fact that the operator  $T_\zeta^{-\frac{1}{2}}\Psi(\theta)T_\zeta^{-\frac{1}{2}}$  corresponding to the equivalent eigenvalue problem is selfadjoint. Therefore, the geometric multiplicities of the eigenvalues are equal to the algebraic multiplicities; see [28] for more details. Consider a corresponding Riesz projector

$$\mathcal{P}(\theta) = -\frac{1}{2\pi i} \oint_{\Gamma} (T_\zeta^{-1}\Psi(\theta) - \lambda I)^{-1} d\lambda = -\frac{1}{2\pi i} \oint_{\Gamma} (\Psi(\theta) - \lambda T_\zeta)^{-1} T_\zeta d\lambda,$$

where  $\Gamma$  is a closed contour bounding a domain containing the eigenvalue  $\mu(\theta)$ ; the eigenvalues do not belong to the contour. Note that the operator function

$$\Re\{e^{-iz}L\} = e^{-iz}L + e^{iz}L^*, \quad z \in \mathbb{C}$$

is holomorphic with respect to the parameter  $z$  and therefore its restriction to the real half-axis is analytic. Thus, we can apply results by Kato related to the perturbation of the finite dimensional operator (Chapter II, §1.3, §1.4) [29]. In order to avoid misunderstanding, which may happen while using terminology, we want to show an obvious representation that holds in the sufficiently small  $\varepsilon$ -neighborhood of the arbitrary chosen point  $\theta_0 \in \mathbb{R}$ ; we have

$$\Re\{e^{-i\theta}L\} = \Re\{e^{-i\theta_0}L\} + (\theta - \theta_0)\Re^{(1)}\{e^{-i\theta_0}L\} + \dots + \frac{(\theta - \theta_0)^q}{q!}\Re^{(q)}\{e^{-i\theta_0}L\} + \dots,$$

where

$$\Re^{(q)}\{e^{-i\theta_0}L\} = \begin{cases} (-i)^k \Im\{e^{-i\theta_0}L\}, & q = 2k + 1, \\ (-1)^k \Re\{e^{-i\theta_0}L\}, & q = 2k, \quad k \in \mathbb{N}_0. \end{cases}$$

Therefore, in accordance with [29] (p. 67), the eigenvalues  $\mu_j(\theta)$ ,  $\theta \in \mathbb{R}$ ,  $j = 1, 2, \dots, n$  have constant geometric multiplicities except for a set of the *exceptional points* that is finite on any compact segment. Denote the set of the exceptional points by  $\mathbb{D}$  and let  $\mathbb{R}_0 := \mathbb{R} \setminus \mathbb{D}$ ; then the given description means  $\nu\{\mu_j(\theta)\} = \text{const}$ ,  $\theta \in \mathbb{R}_0$ ,  $j = 1, 2, \dots, n$ . In accordance with the results represented in Chapter II, §1.3, §1.4 [29], we can claim that, in the sufficiently small  $\varepsilon$ -neighborhood of the point  $\theta_0 \in \mathbb{R}_0$ , we have

$$\mu_j(\theta) \notin \Gamma_j, \quad j = 1, 2, \dots, n,$$

where  $\Gamma_j$  is a closed contour bounding a domain containing the eigenvalue  $\mu_j(\theta_0)$  only. The corresponding Riesz projectors are analytic operator functions

$$\mathcal{P}_j(\theta) = -\frac{1}{2\pi i} \oint_{\Gamma_j} (\Psi(\theta) - \lambda T_\zeta)^{-1} T_\zeta d\lambda, \quad \theta \in (\theta_0 - \varepsilon, \theta_0 + \varepsilon).$$

Throughout the paper, unless otherwise stated, we assume that  $\theta \in \mathbb{R}_0$ .

**Theorem 2.** Assume that  $\mu_{p_j} \neq \mu_k$ ,  $j = 1, 2, \dots, m$ ,  $k \notin \mathfrak{P}_p$ ; then the following relation holds

$$\rho'_p(\theta) = \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) \Psi'(\theta) \mathbf{e}_{p_j}(\theta), \quad \theta \in \mathbb{R}_0.$$

**Proof.** For the sake of simplicity in notation, we present the proof for the case  $p = 1$ , since the other cases are identical. Consider the Riesz projector corresponding to the group of eigenvalues  $\mu_1(\theta), \mu_2(\theta), \dots, \mu_m(\theta)$ ,  $\theta \in \mathbb{R}_0$ . In accordance with the above, we can arrange the contours so that the following sum is an analytic operator function

$$\mathcal{P}_{\bar{m}}(\theta) := -\sum_{j=1}^m \frac{1}{2\pi i} \oint_{\Gamma_j} (\Psi(\theta) - \lambda T_\zeta)^{-1} T_\zeta d\lambda, \quad \theta \in \mathbb{R}_0.$$

It is clear that  $\mathcal{P}_{\bar{m}}$  is a projector, i.e.,

$$\mathcal{P}_{\bar{m}} : \mathbb{C}^n \rightarrow \mathfrak{X}, \quad \mathfrak{X} := \text{span}\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_m\}.$$

Let us establish the following representation  $\mathcal{P}_{\bar{m}} = E_1 E_1^* T_\zeta$ . Note that, for an arbitrary  $\mathbf{v} \in \mathfrak{X}$ , we have the following representation  $\mathbf{v} = E_1 \mathbf{c}$ , where the vector  $\mathbf{c}$  represents the coordinates of the vector  $\mathbf{v}$  in the basis  $\{\mathbf{e}_j\}_1^m$ . Thus, we have  $E_1 E_1^* T_\zeta \mathbf{v} = E_1 E_1^* T_\zeta E_1 \mathbf{c} = E_1 \mathbf{c} = \mathbf{v} = \mathcal{P}_{\bar{m}} \mathbf{v}$ . Note that

$$\mathbb{C}^n = \mathfrak{X} \oplus_{T_\zeta} \mathfrak{X}^\perp,$$

where the orthogonality is understood in the  $T_\zeta$ -weighted sense. If  $\mathbf{z} \in \mathfrak{X}^\perp$ , then we have

$$E_1^* T_\zeta \mathbf{z} = 0, \Rightarrow E_1 E_1^* T_\zeta \mathbf{z} = 0,$$

therefore,  $\mathcal{P}_{\bar{m}} \mathbf{x} = E_1 E_1^* T_\zeta \mathbf{x}$ ,  $\mathbf{x} \in \mathbb{C}^n$ , which yields the desired result. Using this fact, we have

$$\begin{aligned} \sum_{j=1}^m \mu_j(\theta) &= \sum_{j=1}^m \mathbf{e}_j^*(\theta) \Psi(\theta) \mathbf{e}_j(\theta) = \text{tr}\{E_1^*(\theta) \Psi(\theta) E_1(\theta)\} = \\ &= \text{tr}\{T_\zeta^{-1} \Psi(\theta) E_1(\theta) E_1^*(\theta) T_\zeta\} = \text{tr}\{A(\theta) \mathcal{P}_{\bar{m}}(\theta)\}, \end{aligned}$$

where  $A(\theta) := T_\zeta^{-1} \Psi(\theta)$ . Therefore

$$\sum_{j=1}^m \mu'_j(\theta) = \text{tr}\{A'(\theta) \mathcal{P}_{\bar{m}}(\theta)\} + \text{tr}\{A(\theta) \mathcal{P}'_{\bar{m}}(\theta)\}.$$

Let us show that  $\text{tr}\{A(\theta) \mathcal{P}'_{\bar{m}}(\theta)\} = 0$ . Using the property  $\mathcal{P}_{\bar{m}}^2 = \mathcal{P}_{\bar{m}}$  of the projector, we have  $\mathcal{P}'_{\bar{m}} = \mathcal{P}'_{\bar{m}} \mathcal{P}_{\bar{m}} + \mathcal{P}_{\bar{m}} \mathcal{P}'_{\bar{m}}$ . It follows that  $\mathcal{P}'_{\bar{m}} \mathcal{P}_{\bar{m}} = \mathcal{P}'_{\bar{m}} \mathcal{P}_{\bar{m}}^2 + \mathcal{P}_{\bar{m}} \mathcal{P}'_{\bar{m}} \mathcal{P}_{\bar{m}}$ . Thus, we obtain

$\mathcal{P}_{\tilde{m}}\mathcal{P}'_{\tilde{m}}\mathcal{P}_{\tilde{m}} = 0$ . Note that the matrix of the operator  $\mathcal{P}_{\tilde{m}}$  has a block representation in the basis  $\{\mathbf{e}_j\}_1^n$ , i.e.,

$$\mathcal{P}_{\tilde{m}} = \begin{pmatrix} I_m & 0 \\ 0 & 0 \end{pmatrix}.$$

In the matrix form, we have

$$\mathcal{P}_{\tilde{m}}\mathcal{P}'_{\tilde{m}}\mathcal{P}_{\tilde{m}} = \begin{pmatrix} I_m & 0 \\ 0 & 0 \end{pmatrix} \times \begin{pmatrix} \mathcal{P}'_{11} & \mathcal{P}'_{12} \\ \mathcal{P}'_{21} & \mathcal{P}'_{22} \end{pmatrix} \times \begin{pmatrix} I_m & 0 \\ 0 & 0 \end{pmatrix} = 0.$$

This implies that  $\mathcal{P}'_{11} = 0$ . On the other hand, we have the following implication

$$\mathcal{P}_{\tilde{m}}\mathcal{P}'_{\tilde{m}}\mathcal{P}_{\tilde{m}} = 0, \Rightarrow \{I - \mathcal{P}_{\tilde{m}}\}\mathcal{P}'_{\tilde{m}}\{I - \mathcal{P}_{\tilde{m}}\} = 0.$$

The verification is by direct calculation and left to the reader. It follows that  $\mathcal{P}'_{22} = 0$ . Since the subspace generated by the first  $m$  eigenvectors is an invariant subspace of the operator  $A$ ,  $\mathcal{P}_{\tilde{m}}A = A\mathcal{P}_{\tilde{m}}$ . Therefore, by direct calculation, we get

$$A = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}.$$

Eventually, we have come to the representation

$$A\mathcal{P}'_{\tilde{m}} = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \times \begin{pmatrix} 0 & \mathcal{P}'_{12} \\ \mathcal{P}'_{21} & 0 \end{pmatrix},$$

from which it follows that  $\text{tr}\{A\mathcal{P}'_{\tilde{m}}\} = 0$ . Therefore

$$\begin{aligned} \rho'_1(\theta) &= \sum_{j=1}^m \mu'_j(\theta) = \text{tr}\{A'(\theta)\mathcal{P}_{\tilde{m}}(\theta)\} = \text{tr}\{T_{\zeta}^{-1}\Psi'(\theta)E_1(\theta)E_1^*(\theta)T_{\zeta}\} = \\ &= \sum_{j=1}^m \mathbf{e}_j^*(\theta)\Psi'(\theta)\mathbf{e}_j(\theta), \theta \in \mathbb{R}_0. \end{aligned}$$

The proof is complete.  $\square$

Note that the normalized eigenvectors are unique up to a phase factor; we use this fact in the following lemma to establish analytic properties of the eigenvectors.

**Lemma 1.** *The phase factors can be chosen so that the generalized eigenvectors corresponding to simple eigenvalues are analytic. There exists a  $T_{\zeta}$ —orthonormal basis of the analytic eigenvectors in the subspace corresponding to the multiple eigenvalues.*

**Proof.** First, consider the case corresponding to the eigenvalue whose geometrical multiplicity equals one. Note that, at the point  $\theta \in \mathbb{R}$ , the eigenvectors of the problem are defined up to a phase factor, i.e.,  $e^{i\zeta_j(\theta)}\mathbf{e}_j(\theta)$  is an eigenvector, where  $\zeta_j(\theta)$  is unknown function. In accordance with the definition, we have

$$\Psi(\theta_0)\mathbf{e}_j(\theta_0) = \mu_j(\theta_0)T_{\zeta}\mathbf{e}_j(\theta_0), \theta_0 \in \mathbb{R}_0, j = 1, 2, \dots, n.$$

Denote  $\mathbf{u}_j(\theta) = \mathcal{P}_j(\theta)\mathbf{e}_j(\theta_0) = \alpha_j(\theta)\mathbf{e}_j(\theta)$ , where  $\theta$  belongs to a sufficiently small neighborhood of the point  $\theta_0$ . It is clear that  $\alpha_j(\theta_0) = 1$ . Since the matrix of the Riesz projector is analytic, we have

$$\mathbf{u}(\theta) = \sum_{k=0}^{\infty} \mathbf{a}_k(\theta - \theta_0)^k, \quad \mathbf{u}^*(\theta) = \sum_{k=0}^{\infty} \mathbf{a}_k^*(\theta - \theta_0)^k.$$

Consider  $\mathbf{z}_j(\theta) := \mathbf{u}_j(\theta)|\alpha_j(\theta)|^{-1}$ ; we have

$$|\alpha_j(\theta)|^2 = \mathbf{u}^*(\theta)T_{\zeta}\mathbf{u}(\theta) = \sum_{s=1}^n |u_s(\theta)|^2 D_{ss} e^{i\zeta_s}.$$

Note that

$$\bar{u}_s(\theta) = \sum_{k=0}^{\infty} \bar{a}_{sk}(\theta - \theta_0)^k,$$

therefore, the function  $|\alpha_j(\theta)|^2$  is analytic and there exists an  $\varepsilon$ -neighborhood  $(\theta_0 - \varepsilon, \theta_0 + \varepsilon)$  where  $\alpha_j(\theta) \neq 0$  inside the interval, since  $\alpha_j(\theta_0) = 1$ . Thus, it is clear that the vector functions  $\mathbf{z}_j(\theta)$ ,  $\theta \in \mathbb{R}_0$  are analytic. Applying the operator, we get

$$\Psi(\theta)\mathbf{z}_j(\theta) = \mu_j(\theta)T_{\zeta}\mathbf{z}_j(\theta), \quad \mathbf{z}_j^*(\theta)T_{\zeta}\mathbf{z}_k(\theta) = \delta_{jk}, \quad j, k = 1, 2, \dots, n.$$

Thus, we obtain the desired result. Consider the case corresponding to a multiple eigenvalue  $\mu_j(\theta)$ , i.e.,  $\nu\{\mu_j(\theta)\} > 1$ ,  $\theta \in \mathbb{R}_0$ . In this case, we have the corresponding invariant subspace of the eigenvectors

$$\mathfrak{N}_j(\theta), \quad \dim \mathfrak{N}_j(\theta) = \nu\{\mu_j(\theta)\}, \quad \theta \in \mathbb{R}_0.$$

Note that, if we have a set  $\{\mathbf{e}_{jk}(\theta_0)\}_{k=1}^{\nu}$ ,  $\theta_0 \in \mathbb{R}_0$  of  $T_{\zeta}$ -orthonormal eigenvectors, their analytic images  $\mathbf{u}_{jk}(\theta) := \mathcal{P}_j(\theta)\mathbf{e}_{jk}(\theta_0)$  may not be  $T_{\zeta}$ -orthonormal; however, as it can be proved easily, they are linearly independent. For this purpose, it is sufficient to apply the Riesz projector to an arbitrary linear combination of the vectors  $\{\mathbf{e}_{jk}(\theta_0)\}_1^{\nu}$ .

Apparently, we can apply the Gram–Schmidt process in order to obtain the  $T_{\zeta}$ -orthonormal basis in  $\mathfrak{N}_j(\theta)$ . The question is whether the coefficients that appear in the Gram–Schmidt process are analytic; however, using the reasoning analogous to the ones corresponding to  $\alpha_j(\theta)$ , we can easily establish the fact. Let us describe the first step in the Gram–Schmidt process; we have

$$\tilde{\mathbf{u}}_{j1}(\theta) = \mathbf{u}_{j1}(\theta), \quad \tilde{\mathbf{u}}_{j2}(\theta) = \mathbf{u}_{j2}(\theta) - \gamma_{1,2}(\theta)\tilde{\mathbf{u}}_{j1}(\theta),$$

where  $\gamma_{1,2}(\theta) := \mathbf{u}_{j1}^*(\theta)T_{\zeta}\mathbf{u}_{j2}(\theta) \|\sqrt{T_{\zeta}}\mathbf{u}_{j1}(\theta)\|_{\mathbb{C}^n}^{-2}$ . Since  $\mathbf{u}_{j1}(\theta)$  is continuous in the  $\varepsilon$ -neighborhood of the point  $\theta_0$  and  $\mathbf{u}_{j1}(\theta_0) = \mathbf{e}_{j1}(\theta_0) \neq \mathbf{0}$ , we conclude that  $\gamma_{1,2}(\theta)$  is analytic in the  $\varepsilon$ -neighborhood of the point  $\theta_0$ . Consider

$$\tilde{\mathbf{e}}_{jk}(\theta) = \tilde{\mathbf{u}}_{jk}(\theta) \|\sqrt{T_{\zeta}}\tilde{\mathbf{u}}_{jk}(\theta)\|_{\mathbb{C}^n}^{-1}, \quad k = 1, 2,$$

since  $\gamma_{1,2}(\theta_0) = 0$ , we have  $\tilde{\mathbf{u}}_{jk}(\theta_0) = \mathbf{e}_{jk}(\theta_0) \neq \mathbf{0}$ ,  $k = 1, 2$ . Therefore,  $\tilde{\mathbf{e}}_{jk}(\theta)$  is analytic in the  $\varepsilon$ -neighborhood of the point  $\theta_0$ . The proof corresponding to the indices  $k = 2, 3, \dots, \nu$  is absolutely analogous. The proof is complete.  $\square$

**Lemma 2.** The following equality holds

$$\rho'_p(\theta) = \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) \Psi'(\theta) \mathbf{e}_{p_j}(\theta), \theta \in \mathbb{R}_0.$$

**Proof.** In accordance with Lemma 1, we can consider a set of analytic eigenvectors  $\mathbf{e}_j(\theta)$ ,  $\theta \in \mathbb{R}_0$ ,  $j = 1, 2, \dots, n$ . Therefore

$$\rho'_p(\theta) = \sum_{j=1}^m \left( \mathbf{e}_{p_j}^*(\theta) \Psi(\theta) \mathbf{e}'_{p_j}(\theta) \right)^* + \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) \Psi'(\theta) \mathbf{e}_{p_j}(\theta) + \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) \Psi(\theta) \mathbf{e}'_{p_j}(\theta) = I_1 + I_2 + I_3.$$

Since  $\Psi(\theta) \mathbf{e}_{p_j} = \mu_{p_j} T_\zeta \mathbf{e}_{p_j}$ , taking into account the fact

$$\mathbf{e}_{p_j}^*(\theta) \Psi(\theta) = \left\{ \Psi(\theta) \mathbf{e}_{p_j}(\theta) \right\}^* = \left\{ \mu_{p_j}(\theta) T_\zeta \mathbf{e}_{p_j}(\theta) \right\}^* = \mu_{p_j}(\theta) \mathbf{e}_{p_j}^*(\theta) T_\zeta,$$

and the connection condition, we obtain

$$I_1 + I_3 = \sum_{j=1}^m \mu_{p_j}(\theta) \left( \mathbf{e}_{p_j}^*(\theta) T_\zeta \mathbf{e}_{p_j}(\theta) \right)' = 0.$$

The proof is complete.  $\square$

**Lemma 3.** The following relation holds

$$\rho''_p(\theta) = \operatorname{Re} \sum_{j=1}^m \sum_{k=m+1}^n \frac{|\mathbf{e}_k^*(\theta) \Psi'(\theta) \mathbf{e}_j(\theta)|^2}{\mu_j(\theta) - \mu_k(\theta)} - \rho_p(\theta), \theta \in \mathbb{R}_0.$$

**Proof.** In accordance with Lemma 1, we can assume that the eigenvectors of the following eigenvalue problem are analytic

$$\Psi(\theta) \mathbf{e}_j(\theta) = \mu_j(\theta) T_\zeta \mathbf{e}_j(\theta), \mathbf{e}_j^*(\theta) T_\zeta \mathbf{e}_k(\theta) = \delta_{jk}, \theta \in \mathbb{R}_0, j, k = 1, 2, \dots, n.$$

Differentiating the left-hand side and the right-hand side, we get

$$\Psi'(\theta) \mathbf{e}_j(\theta) + \Psi(\theta) \mathbf{e}'_j(\theta) = \mu'_j(\theta) T_\zeta \mathbf{e}_j(\theta) + \mu_j(\theta) T_\zeta \mathbf{e}'_j(\theta).$$

The latter relation can be rewritten in the form

$$\{\mu'_j(\theta) T_\zeta - \Psi'(\theta)\} \mathbf{e}_j(\theta) = \{\Psi(\theta) - \mu_j(\theta) T_\zeta\} \mathbf{e}'_j(\theta).$$

Substituting

$$\mathbf{e}'_j(\theta) = \sum_{k=1}^n \alpha_{kj}(\theta) \mathbf{e}_k(\theta),$$

we get

$$\begin{aligned} \{\mu'_j(\theta) T_\zeta - \Psi'(\theta)\} \mathbf{e}_j(\theta) &= \{\Psi(\theta) - \mu_j(\theta) T_\zeta\} \left( \sum_{k=1}^n \alpha_{kj}(\theta) \mathbf{e}_k(\theta) \right) = \\ &= \sum_{k=1}^n \alpha_{kj}(\theta) \{\Psi(\theta) \mathbf{e}_k(\theta) - \mu_j(\theta) T_\zeta \mathbf{e}_k(\theta)\} = \sum_{k=1}^n \alpha_{kj}(\theta) \{\mu_k(\theta) - \mu_j(\theta)\} T_\zeta \mathbf{e}_k(\theta). \end{aligned}$$

Using  $T_\zeta$ -orthogonal property, we obtain

$$\alpha_{mj}(\theta) \{\mu_m(\theta) - \mu_j(\theta)\} = \sum_{k=1}^n \alpha_{kj}(\theta) \{\mu_k(\theta) - \mu_j(\theta)\} \mathbf{e}_m^*(\theta) T_\zeta \mathbf{e}_k(\theta) =$$

$$= \mathbf{e}_m^* \{ \mu_j'(\theta) T_\zeta - \Psi'(\theta) \} \mathbf{e}_j(\theta) = -\mathbf{e}_m^*(\theta) \Psi'(\theta) \mathbf{e}_j(\theta), \quad m \neq j.$$

Therefore

$$\alpha_{mj}(\theta) = \frac{\mathbf{e}_m^*(\theta) \Psi'(\theta) \mathbf{e}_j(\theta)}{\mu_j(\theta) - \mu_m(\theta)}, \quad \mu_j(\theta) \neq \mu_m(\theta); \quad \mathbf{e}_m^*(\theta) \Psi'(\theta) \mathbf{e}_j(\theta) = 0, \quad \mu_j(\theta) = \mu_m(\theta).$$

In order to express  $\alpha_{jj}(\theta)$ , let us notice the following obvious implication

$$\mathbf{e}_j^*(\theta) T_\zeta \mathbf{e}_j(\theta) = 1, \implies \operatorname{Re} \{ \mathbf{e}_j^*(\theta) T_\zeta \mathbf{e}_j'(\theta) \} = 0.$$

On the other hand, we have

$$\alpha_{jj}(\theta) = \mathbf{e}_j^*(\theta) T_\zeta \left( \sum_{k=1}^n \alpha_{kj}(\theta) \mathbf{e}_k(\theta) \right) = \mathbf{e}_j^*(\theta) T_\zeta \mathbf{e}_j'(\theta).$$

It follows that  $\alpha_{jj}(\theta)$  is an analytic function and  $\alpha_{jj}(\theta) = i\beta_j(\theta)$ , where  $\beta_j$  denotes an unknown real analytic function. Further, we want to use arbitrariness in choosing a phase factor and suppose  $\tilde{\mathbf{e}}_j(\theta) = e^{i\psi_j(\theta)} \mathbf{e}_j(\theta)$ , where  $\psi_j(\theta)$  is some unknown (at this stage of reasoning) analytic function. Using the technique analogous to the one related to eliminating the Berry connection, let us show that we can choose  $\psi_j$  so that  $\alpha_{jj} = 0$ . We have

$$\tilde{\mathbf{e}}_j'(\theta) = i\psi_j'(\theta) e^{i\psi_j(\theta)} \mathbf{e}_j(\theta) + e^{i\psi_j(\theta)} \mathbf{e}_j'(\theta).$$

In accordance with the above, we get

$$\tilde{\alpha}_{jj}(\theta) = \tilde{\mathbf{e}}_j^*(\theta) T_\zeta \tilde{\mathbf{e}}_j'(\theta) = e^{-i\psi_j(\theta)} \mathbf{e}_j^*(\theta) T_\zeta \left\{ i\psi_j'(\theta) e^{i\psi_j(\theta)} \mathbf{e}_j(\theta) + e^{i\psi_j(\theta)} \mathbf{e}_j'(\theta) \right\} = i(\psi_j'(\theta) + \beta_j(\theta)).$$

Substituting

$$\psi_j(\theta) = -\int \beta_j(\theta) d\theta + C,$$

we conclude that the analytic eigenvectors can be chosen so that  $\alpha_{jj}(\theta) = 0$ . Applying Lemma 1 and Lemma 2, we get

$$\rho_p''(\theta) = \frac{1}{2} \sum_{j=1}^m \mathbf{e}_j^*(\theta) \Psi''(\theta) \mathbf{e}_j(\theta) + \operatorname{Re} \sum_{j=1}^m \mathbf{e}_j^*(\theta) \Psi'(\theta) \mathbf{e}_j'(\theta) = I_1 + I_2.$$

By direct calculation, we get  $\Psi''(\theta) = -\Psi(\theta)$ ; therefore,  $I_1 = -\rho_p(\theta)$ . On the other hand,

$$\begin{aligned} I_2 &= \operatorname{Re} \sum_{j=1}^m \sum_{k=1}^n \mathbf{e}_j^*(\theta) \Psi'(\theta) \mathbf{e}_k(\theta) \alpha_{kj}(\theta) = \operatorname{Re} \sum_{j=1}^m \mathbf{e}_j^*(\theta) \Psi'(\theta) \sum_{\substack{k=1 \\ \mu_k \neq \mu_j}}^n \frac{\mathbf{e}_k^*(\theta) \Psi'(\theta) \mathbf{e}_j(\theta)}{\mu_j(\theta) - \mu_k(\theta)} \mathbf{e}_k(\theta) = \\ &= \operatorname{Re} \sum_{j=1}^m \sum_{\substack{k=1 \\ \mu_k \neq \mu_j}}^n \frac{|\mathbf{e}_k^* \Psi'(\theta) \mathbf{e}_j(\theta)|^2}{\mu_j(\theta) - \mu_k(\theta)} = \operatorname{Re} \sum_{j=1}^m \sum_{k=m+1}^n \frac{|\mathbf{e}_k^*(\theta) \Psi'(\theta) \mathbf{e}_j(\theta)|^2}{\mu_j(\theta) - \mu_k(\theta)}. \end{aligned}$$

The proof is complete.  $\square$

**Lemma 4.** The following inequality holds

$$0 < \operatorname{card} \mathbb{S}_p \leq \operatorname{card} (\mathbb{D} \cap \mathbb{J}) + 1, \quad p = 1, 2, \dots, C_n^m.$$

**Proof.** Consider a function  $Y_p(\theta) = \arg \operatorname{tr} \{ E_p^*(\theta) L E_p(\theta) \}$ ,  $\theta \in \mathbb{R}$ . Applying Lemma 1, we conclude that the matrix functions  $E_p(\theta)$  are continuous on the set  $\mathbb{R}_0$  with respect

to the Frobenius norm and therefore with respect to an arbitrary norm due to the norm equivalence property corresponding to the complex Euclidean space. By virtue of the  $T_\zeta$ -orthogonality property, we conclude that  $E_p(\theta) \in \mathfrak{M}_m^n$ . In accordance with the reasoning related to Formula (10), the mapping  $\arg\{\psi(X)\} : \mathfrak{M}_m^n \rightarrow \mathbb{J}$  is continuous. Thus, the mapping  $Y_p(\theta) : \mathbb{R}_0 \rightarrow \mathbb{J}$  is continuous and therefore its restriction to the set  $\mathbb{J}$  is continuous. In accordance with the Brouwer fixed-point theorem, which states that “Every continuous map of the closed unit ball in the Euclidean space into itself has a fixed point,” we conclude that there exists a fixed point  $\theta_p \in \mathbb{J}$ . Consider the points  $\mathbb{D} \cap \mathbb{J} = \{\zeta_1, \zeta_2, \dots, \zeta_z\}$ ,  $z = \text{card}(\mathbb{D} \cap \mathbb{J})$ . For simplicity, and without loss of generality, consider a case  $\zeta_1 = a$ ,  $\zeta_z = b$ , where  $\mathbb{J} := [a, b]$ . Let us show that, on the interval  $(\zeta_l, \zeta_{l+1})$ , in each case defined by the index  $p$ , there exists no more than one fixed point  $\theta_p$ . Firstly, let us note that, in accordance with Lemma 1, the function

$$\rho_p(\theta) = \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) \Psi(\theta) \mathbf{e}_{p_j}(\theta),$$

is analytic on the interval  $(\zeta_l, \zeta_{l+1})$ . Assume that  $\theta_p \in (\zeta_l, \zeta_{l+1})$ . Let us show that  $\rho'_p(\theta_p) = 0$ . Using Lemma 2, we get

$$\begin{aligned} \rho'_p(\theta) &= \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) \Psi'(\theta) \mathbf{e}_{p_j}(\theta) = \sum_{j=1}^m \mathbf{e}_{p_j}^*(\theta) i \left( e^{i\theta} L^* - e^{-i\theta} L \right) \mathbf{e}_{p_j}(\theta) = \\ &= ie^{i\theta} \text{tr}\{E_p^*(\theta) L^* E_p(\theta)\} - ie^{-i\theta} \text{tr}\{E_p^*(\theta) L E_p(\theta)\}. \end{aligned}$$

Therefore

$$\begin{aligned} \rho'_p(\theta_p) &= ie^{i\theta_p} \bar{\psi}(E_p(\theta_p)) - ie^{-i\theta_p} \psi(E_p(\theta_p)) = -2\text{Re}\left\{ie^{-i\theta_p} \psi(E_p(\theta_p))\right\} = \\ &= 2\text{Im}\left\{e^{-i\theta_p} \psi(E_p(\theta_p))\right\} = 2\text{Im}\left\{e^{-i\theta_p} e^{i\theta_p} |\psi(E_p(\theta_p))|\right\} = 0. \end{aligned}$$

Now if we assume that there exists a fixed point  $\tilde{\theta}_p \neq \theta_p$ ,  $\tilde{\theta}_p \in (\zeta_l, \zeta_{l+1})$ , then using the same reasoning, we will come to the conclusion  $\rho'_p(\tilde{\theta}_p) = 0$ . However, the latter contradicts the statement of Lemma 3, which claims that  $\rho''_p(\theta) < 0$ ,  $\theta \in (\zeta_l, \zeta_{l+1})$ ; thus, we conclude that the fixed point  $\theta_p$  is unique if it belongs to the interval  $(\zeta_l, \zeta_{l+1})$ . In this case, we have  $0 < \text{card } \mathbb{S}_p \leq \text{card}(\mathbb{D} \cap \mathbb{J}) - 1$ . The other cases related to the location of the points of the set  $\mathbb{D} \cap \mathbb{J}$  with respect to the segment  $\mathbb{J}$  can be described absolutely analogously and therefore are left to the reader who can state easily the general upper estimate  $\text{card } \mathbb{S}_p \leq \text{card}(\mathbb{D} \cap \mathbb{J}) + 1$ . The proof is complete.  $\square$

**Theorem 3.** The solutions of the stationary system (7) are given in the form

$$X = E_p(\theta), \Lambda = \text{diag}\{\phi_{p_1}, \phi_{p_2}, \dots, \phi_{p_m}\}, \theta \in \mathbb{S}_p, p = 1, 2, \dots, C_n^m.$$

Moreover, the following relation holds

$$\left| \text{tr}\{E_p^*(\theta) L E_p(\theta)\} \right| = \frac{1}{2} \rho_p(\theta), \theta \in \mathbb{S}_p.$$

**Proof.** Note that, in accordance with Lemma 4, there exists a fixed point  $\theta_p \in \mathbb{J}$  of the Equation (11). It is clear that, at the fixed point relation (9) can be rewritten in the form

$$H\mathbf{e}_{p_j} = |\psi(E_p)| \Psi(\theta_p) \mathbf{e}_{p_j} = \phi_{p_j} T_\zeta \mathbf{e}_{p_j}, j = 1, 2, \dots, m.$$

Therefore, the pair of matrices  $X = E_p(\theta_p)$ ,  $\Lambda = \text{diag}\{\phi_{p_1}, \phi_{p_2}, \dots, \phi_{p_m}\}$  represents the solution of the eigenvalue problem (8). Let us establish the representation for the objective function; we have

$$2|\psi(X)|^2 = \overline{\psi(X)}\text{tr}(X^*LX) + \psi(X)\text{tr}(X^*L^*X) = \text{tr}(X^*[\bar{\psi}L + \psi L^*]X) = \text{tr}(X^*HX).$$

Note that, at the point  $X$  satisfying the stationary condition, we have

$$2|\psi(X)|^2 = \text{tr}(X^*HX) = \sum_{j=1}^m (H\mathbf{x}_j, \mathbf{x}_j)_{\mathbb{C}^n} = \sum_{j=1}^m \lambda_j.$$

Taking into account the notation  $\mu_j(\theta) = \phi_j|\psi(X)|^{-1}$ ,  $j = 1, 2, \dots, n$ , substituting  $X = E_p(\theta_p)$ ,  $\Lambda = \text{diag}\{\phi_{p_1}, \phi_{p_2}, \dots, \phi_{p_m}\}$ , we get

$$2|\psi(E_p(\theta_p))| = \sum_{j=1}^m \mu_{p_j}(\theta_p) = \rho_p(\theta_p).$$

□

**Remark 1.** It is critical to observe that, instead of specifying the components of the phase vector  $\zeta$  arbitrarily, a highly natural and geometrically motivated choice is to set  $\zeta_j = -\arg(D_{jj})$ . Under this specific phase-compensation condition, the metric weight matrix  $T_\zeta$  collapses into a purely real diagonal matrix of absolute values, i.e.,  $(T_\zeta)_{jj} = |D_{jj}|$ , representing the absolute value of the complex graph vertex degree or the total graph nodal energy across both datasets. This adaptive choice principally simplifies the generalized eigenvalue problem in Step 5, Section 3.3. It completely eliminates local phase distortions, making the weight matrix invariant to local trigonometric shifts given by  $\arg D_{jj}$ . This stabilization fundamentally balances the trajectories of the eigenvectors, which depend continuously on the parameter  $\theta$ , on the Stiefel manifold. This geometric regularity directly simplifies the self-consistent algebraic equation in Step 6, Section 3.3.

The next step is to describe and classify the obtained stationary points.

### 3.2. Classification of the Stationary Points via the Hessian

The following reasoning is devoted to the classification of the stationary points. For this purpose, we will consider the Hessian. Assume that  $X = E_p(\theta)$ ,  $p = 1, 2, \dots, C_n^m$  and consider a differential  $dX$  in the direction along the tangent subspace. Using the orthogonal decomposition theorem, we have  $dX = XdY + dV$ , where  $dY$  is a matrix of the coefficients of the element decomposition in the basis formed by the columns of  $E_p(\theta)$ ; the second term is given by

$$dV \in E_p^\perp(\theta) = \mathbb{R}^m(L) \ominus_{T_\zeta} E_p(\theta),$$

where the orthogonal difference is understood in the  $T_\zeta$  sense, that is,  $X^*T_\zeta dV = 0$ ,  $X = E_p(\theta)$ . Denote  $\mathcal{B}(A, B) := \text{tr}\{A^*HB\} - \text{tr}\{\Lambda A^*T_\zeta B\}$ ,  $A, B \in \mathbb{C}^{n \times m}$ .

**Lemma 5.** The following representation holds

$$d^2\mathcal{L}(X, \Lambda) = 2|d\psi|^2 + 2\mathcal{B}(dV, dV).$$

**Proof.** In accordance with the above, we get

$$\mathcal{L}(X, \Lambda) = \psi(X)\overline{\psi(X)} - \text{tr}\{\Lambda(X^*T_\zeta X - I_m)\}.$$

Let us rewrite the first differential in the form

$$d\mathcal{L}(X, \Lambda) = \psi d\bar{\psi} + \bar{\psi} d\psi - \text{tr}\{\Lambda d(X^* T_{\zeta} X)\},$$

here, we have taken into account the fact that  $X \in \mathfrak{M}_m^n$  and therefore  $X^* T_{\zeta} X = I_m$ . However, regarding the first differential, we should assume generally that  $d(X^* T_{\zeta} X) \neq 0$  since we consider arbitrary directions  $dX$ . Thus, the second differential can be represented in the form

$$d^2\mathcal{L}(X, \Lambda) = 2|d\psi|^2 + \psi d^2\bar{\psi} + \bar{\psi} d^2\psi - \text{tr}\{d\Lambda d(X^* T_{\zeta} X)\} - 2\text{tr}\{\Lambda dX^* T_{\zeta} dX\}.$$

Consider

$$d^2\bar{\psi} = d\text{tr}\{d(X^* L^* X)\} = 2\text{tr}\{dX^* L^* dX\}, \quad d^2\psi = 2\text{tr}\{dX^* L dX\},$$

substituting, we get

$$\frac{1}{2} d^2\mathcal{L}(X, \Lambda) = |d\psi|^2 + \text{tr}\{dX^* H dX\} - \text{tr}\{\Lambda dX^* T_{\zeta} dX\}, \quad (12)$$

where we put  $d(X^* T_{\zeta} X) = 0$  since we are interested in the directions belonging to the tangent subspace. Further, we will focus on the form

$$\mathcal{B}(dX, dX) := \text{tr}\{dX^* H dX\} - \text{tr}\{\Lambda dX^* T_{\zeta} dX\}, \quad (13)$$

where  $X = E_p(\theta)$ ,  $p = 1, 2, \dots, C_n^m$ ,  $dX = X dY + dV$ . Let us show that the matrix  $dY$  is skew-Hermitian, i.e.,  $dY = -dY^*$ . For this purpose, using the connection condition, i.e., the fact of the given direction along the tangent subspace, we get  $X^* T_{\zeta} dX + dX^* T_{\zeta} X = 0$ . Substituting, we get

$$X^* T_{\zeta} (XdY + dV) + \{X^* T_{\zeta} (XdY + dV)\}^* = 0; \quad X^* T_{\zeta} X dY + \{X^* T_{\zeta} X dY\}^* = 0;$$

$$(X^* T_{\zeta} X)(dY + dY^*) = 0; \quad dY + dY^* = 0,$$

here we have used the connection condition  $X^* T_{\zeta} X = I_m$ . Now, let us show that the following additive property holds

$$\mathcal{B}(XdY + dV, XdY + dV) = \mathcal{B}(XdY, XdY) + \mathcal{B}(dV, dV).$$

Applying the cyclic property of the trace, we get  $\mathcal{B}(A, B) = \overline{\mathcal{B}(B, A)}$ . Therefore, to obtain the desired result, it is sufficient to prove that  $\mathcal{B}(dV, XdY) = 0$ . Substituting the stationary condition  $HX = T_{\zeta} X \Lambda$  corresponding to the argument  $\theta_p$ , taking into account that  $X^* T_{\zeta} dV = 0$ , we get

$$\mathcal{B}(dV, XdY) = \text{tr}\{dV^* H X dY\} - \text{tr}\{\Lambda dV^* T_{\zeta} X dY\} = \text{tr}\{dV^* T_{\zeta} X [\Lambda dY - dY \Lambda]\} = 0.$$

Let us show that  $\mathcal{B}(XdY, XdY) = 0$ . It is clear that

$$\mathcal{B}(XdY, XdY) = \text{tr}\{dY^* X^* H X dY - dY^* X^* T_{\zeta} X dY \Lambda\} = \text{tr}\{dY^* \Lambda dY - dY^* dY \Lambda\}.$$

Taking into account the cyclic property of the trace, we get  $\mathcal{B}(XdY, XdY) = \text{tr}\{\Lambda [dY, dY^*]\}$ . Since we have proved above that the matrix  $dY$  is skew-Hermitian,  $[dY, dY^*] = dY dY^* - dY^* dY = 0$ ; therefore,  $\mathcal{B}(XdY, XdY) = 0$ . Substituting into Equations (13) and (12), we obtain the desired result.  $\square$

**Theorem 4.** Assume that the segment  $\mathbb{J}$  does not contain the exceptional points; then there exist solutions  $E_1(\theta_1)$ ,  $E_2(\theta_2)$  of the problems PI, PII respectively. The number of solutions represented by the matrices formed from the eigenvectors is given by the unified formula

$$\text{card}\{\mu_{p_j} = \mu_k, j = 1, 2, \dots, m, k \notin \mathfrak{P}_p\}, p = 1, 2.$$

**Proof.** Assume that  $X = E_p(\theta)$ ,  $p = 1, 2, \dots, C_n^m$  and consider a differential  $dX$  in the direction along the tangent subspace. Using the orthogonal decomposition theorem, we have

$$dX = XdY + dV,$$

where  $dY$  is a matrix of the coefficients of the element decomposition in the basis formed by the columns of the matrix  $E_p(\theta)$ ; the second term has the following description

$$dV \in E_p^\perp(\theta) = \mathbb{R}^m(L) \ominus_{T_\zeta} E_p(\theta),$$

where the orthogonal difference is understood in the  $T_\zeta$  sense. In accordance with Lemma 5, we have

$$d^2\mathcal{L}(X, \Lambda) = 2|d\psi|^2 + 2\mathcal{B}(dV, dV).$$

Recall that, under the assumptions made, we have  $X^*T_\zeta dV = 0$ . In accordance with the orthogonal decomposition theorem, since the columns of the matrix  $dV := (d\mathbf{v}_1, d\mathbf{v}_2, \dots, d\mathbf{v}_m)$  belong to the orthogonal decomposition of the subspace generated by the eigenvectors  $\{\mathbf{e}_{p_j}\}_1^m$ , we get

$$d\mathbf{v}_s = \sum_{j \notin \mathfrak{P}_p} \alpha_{js} \mathbf{e}_j, \alpha_{js} \in \mathbb{C}. \quad (14)$$

Thus, we obtain the following representation

$$d\mathbf{v}_s^* H d\mathbf{v}_s = \sum_{j \notin \mathfrak{P}_p} \bar{\alpha}_{js} \mathbf{e}_j^* \sum_{j \notin \mathfrak{P}_p} \alpha_{js} H \mathbf{e}_j = \sum_{j \notin \mathfrak{P}_p} \bar{\alpha}_{js} \mathbf{e}_j^* \sum_{j \notin \mathfrak{P}_p} \alpha_{js} \phi_j T_\zeta \mathbf{e}_j = \sum_{j \notin \mathfrak{P}_p} |\alpha_{js}(\theta)|^2 \phi_j.$$

Analogously, we obtain

$$d\mathbf{v}_s^* T_\zeta d\mathbf{v}_s = \sum_{j \notin \mathfrak{P}_p} |\alpha_{js}(\theta)|^2.$$

On the other hand, using the accepted terms, we have

$$\mathcal{B}(dV, dV) = \sum_{s=1}^m (d\mathbf{v}_s^* H d\mathbf{v}_s - \lambda_s d\mathbf{v}_s^* T_\zeta d\mathbf{v}_s).$$

In accordance with Lemma 4, Theorem 3 there exists a unique fixed point  $\theta_p$ , i.e.,  $\text{card } \mathbb{S}_p = 1$ , corresponding to the stationary point  $\lambda_s = \phi_{p_s}$ ,  $s = 1, 2, \dots, m$ ; therefore,

$$\mathcal{B}(dV, dV) = \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} |\alpha_{js}|^2 (\phi_j - \phi_{p_s}).$$

In accordance with the given notation, in the cases  $p = 1$ ,  $p = 2$ , we have  $p_s = s$ ,  $p_s = n - m + s$ . Implementing the direct substitution, we obtain

$$\mathcal{B}(dV, dV) = \sum_{s=1}^m \sum_{j=m+1}^n |\alpha_{js}|^2 (\phi_j - \phi_s) > 0, \quad \mathcal{B}(dV, dV) = \sum_{s=1}^m \sum_{j=1}^{n-m} |\alpha_{js}|^2 (\phi_j - \phi_{n-m+s}) < 0.$$

Thus, we conclude that, at the point corresponding to  $\theta_1$ , we have a stable minimum, i.e.,

$$d^2\mathcal{L}(X, \Lambda) > 0.$$

Let us show that the stationary points satisfying the condition  $\exists l \notin \mathfrak{P}_p : \phi_{p_1} < \phi_l < \phi_{p_m}$  are the saddle points. The idea is to consider various differentials of the matrix-variable and establish in this way different signs of the second differential of the Lagrangian. Below, we present a general construction allowing us to obtain the desired result in various cases. Assume that  $X = E_p(\theta)$ ,  $dX = dV$ , using decomposition (14), we get

$$\begin{aligned}\mathrm{tr}(dV^* LX) &= \sum_{s=1}^m d\mathbf{v}_s^* L \mathbf{e}_{p_s} = \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} \bar{\alpha}_{js} \mathbf{e}_j^* L \mathbf{e}_{p_s}, \\ \mathrm{tr}(dV^* L^* X) &= \sum_{s=1}^m d\mathbf{v}_s^* L^* \mathbf{e}_{p_s} = \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} \bar{\alpha}_{js} \mathbf{e}_j^* L^* \mathbf{e}_{p_s} = \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} \bar{\alpha}_{js} \overline{\mathbf{e}_{p_s}^* L \mathbf{e}_j}.\end{aligned}$$

Substituting into the relation  $d\psi = \mathrm{tr}(dV^* LX) + \mathrm{tr}(X L dV^*)$ , we get

$$d\psi = \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} \{\bar{\alpha}_{js} a_{js} + \alpha_{js} b_{js}\}, \quad a_{js} := \mathbf{e}_j^* L \mathbf{e}_{p_s}, \quad b_{js} := \mathbf{e}_{p_s}^* L \mathbf{e}_j.$$

Thus, the second differential can be rewritten in the form

$$d^2\mathcal{L}(X, \Lambda) = 2 \left| \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} \{\bar{\alpha}_{js} a_{js} + \alpha_{js} b_{js}\} \right|^2 + 2 \sum_{s=1}^m \sum_{j \notin \mathfrak{P}_p} |\alpha_{js}|^2 (\phi_j - \phi_{p_s}).$$

The idea is to produce directions corresponding to the different signs of the Hessian. For this purpose, consider a concrete differential  $dV = (0, 0, \dots, d\mathbf{v}_m)$ ,  $d\mathbf{v}_m = \alpha_{lm} \mathbf{e}_l$ . In this case, we have

$$d^2\mathcal{L}(X, \Lambda) = 2|\bar{\alpha}_{lm} a_{lm} + \alpha_{lm} b_{lm}|^2 + 2|\alpha_{lm}|^2 (\phi_l - \phi_{p_m}).$$

Since, in accordance with the assumptions made, we have  $\phi_l - \phi_{p_m} < 0$ , it is sufficient to show that we can choose  $\alpha_{lm} \neq 0$  so that  $\bar{\alpha}_{lm} a_{lm} + \alpha_{lm} b_{lm} = 0$ . This leads to the homogeneous system

$$\begin{cases} \mathrm{Re}(a_{lm} + b_{lm}) \mathrm{Re} \alpha_{lm} + \mathrm{Im}(a_{lm} - b_{lm}) \mathrm{Im} \alpha_{lm} = 0 \\ \mathrm{Im}(a_{lm} + b_{lm}) \mathrm{Re} \alpha_{lm} - \mathrm{Re}(a_{lm} - b_{lm}) \mathrm{Im} \alpha_{lm} = 0 \end{cases}. \quad (15)$$

Since we are interested in the case when the determinant of the system equals to zero, we obtain the desired sufficient condition  $-\mathrm{Re}^2 a_{lm} - \mathrm{Re}^2 b_{lm} = \mathrm{Im}^2 a_{lm} - \mathrm{Im}^2 b_{lm}$ , that can be rewritten in the form  $|(L \mathbf{e}_{p_m}, \mathbf{e}_l)_{\mathbb{C}^n}| = |(L \mathbf{e}_l, \mathbf{e}_{p_m})_{\mathbb{C}^n}|$ . Using the symmetry property  $L^* = \bar{L}$ , separating the imaginary and real parts, we can prove easily that the latter relation holds. Thus, we have proved the existence of the non-trivial solution of the homogeneous system (15) corresponding to the eigenvectors having arbitrary phase factors, i.e., we obtain  $d\psi = 0$ ,  $\mathcal{B}(dV, dV) < 0$ . Having chosen the index  $p_1$  instead of the index  $p_m$ , implementing the same reasoning, we obtain  $d\psi = 0$ ,  $\mathcal{B}(dV, dV) > 0$ . Therefore, the points corresponding to the condition  $\phi_{p_1} < \phi_l < \phi_{p_m}$  are the saddle points. Eventually, we have in the remainder the description of the cases  $\phi_{p_m} \leq \phi_l$  and  $\phi_l \leq \phi_{p_1}$ , where in both cases,  $l \notin \mathfrak{P}_p$ . However,

the first case covers  $p = 1$ ; in accordance with the above, it corresponds to the minimum. Note that, in accordance with Theorem 3, we have

$$|\psi(E_p(\theta_p))| = \sqrt{\frac{1}{2} \sum_{j=1}^m \phi_{p_j}(\theta_p)} = \frac{1}{2} \rho_p(\theta_p). \quad (16)$$

Let us show that the minimum problem PI has a number of solutions equal to

$$\text{card}\{\mu_{p_j} = \mu_k, j = 1, 2, \dots, m, k \notin \mathfrak{P}_p\}, \quad (17)$$

where we put  $p = 1$ . Without loss of generality, assume that  $\mu_k = \mu_{1_m}$ ,  $k \notin \mathfrak{P}_1$ , having replaced the eigenvectors corresponding to the equal eigenvalues (multiple eigenvalues), we obtain a matrix  $E_q(\theta)$ ,  $q \in \{3, \dots, C_n^m\}$ . In accordance with the definition, we have  $\rho_p(\theta) = \rho_q(\theta)$ ,  $\theta \in \mathbb{R}_0$ . Applying the reasoning of Lemma 4, we get  $\rho'_p(\theta_p) = \rho'_q(\theta_q) = 0$ . On the other hand, in accordance with Lemma 3, we have  $\rho''_p(\theta) = \rho''_q(\theta) < 0$ , and therefore  $\theta_p = \theta_q$ . Using Formula (16), we obtain  $|\psi(E_1(\theta_1))| = |\psi(E_q(\theta_q))|$ . Absolutely analogously, having considered other cases corresponding to the condition given in (17), we obtain the desired result.

Applying the Weierstrass theorem and the method of elimination, we come to the conclusion that the case  $\phi_l \leq \phi_{p_1}$ ,  $l \notin \mathfrak{P}_p$  covers the maximum point. Following a line of reasoning absolutely analogous to the case corresponding to the minimum point, we conclude that the maximum problem PII has a number of solutions represented by Formula (17), where we put  $p = 2$ . The proof is complete.  $\square$

**Remark 2.** Note that the general case, i.e.,  $\text{card}(\mathbb{D} \cap \mathbb{J}) > 0$ ,  $\text{card } \mathbb{S}_p > 1$ , can be considered analogously. We should use Lemma 4 and consider an interval containing a point belonging to  $\mathbb{S}_p$ . Applying the same line of reasoning, we obtain the classification of the stationary points.

Eventually, the remaining problem is the location of exceptional points  $\mathbb{D}$  with respect to the fixed points  $\mathbb{S}_p$ . In accordance with Lemma 4, we have  $\text{card } \mathbb{S}_p < \infty$ , whereas according to [29] (p. 67), we have  $\text{card}(\mathbb{D} \cap \mathbb{J}) < \infty$ . Using a probabilistic approach, we conclude that the geometric probability of the random event of coincidence of the exceptional points and the fixed points equals zero in the case when the initial matrix  $W$  is formed from the elements of experimental origin. This clarification creates a complete theoretical foundation for prospective applications. This can be formulated in the form of a hypothesis.

**Hypothesis 1.** The intersection of the sets of exceptional and fixed points is empty.

### 3.3. Algorithmic Summary of the Coupled Manifold Alignment

To illustrate the practical application of the developed theoretical concept of the coupled unsupervised manifold alignment, we provide a concise step-by-step description of the proposed mathematical procedure. This summary establishes a rigorous connection between the extremal problems involving a non-selfadjoint operator and the corresponding computational algorithms under the constraints of the compact manifold homeomorphic to the Stiefel manifold, reducing complex mathematical notation for greater clarity.

1. **STEP 1. GRAPH CONSTRUCTION:** Given heterogeneous omics datasets measured across biological samples, construct their respective symmetric adjacency matrices  $A^{(1)}$  and  $A^{(2)}$  using either the geometrically motivated neighborhood method or the simple weight approach.

2. STEP 2. COMPLEX COUPLING MATRIX FORMULATION: Construct the complex matrix  $W$  of experimental origin, where the elements of the adjacency matrices  $A^{(1)}$  and  $A^{(2)}$  serve directly as its real and imaginary parts, respectively.
3. STEP 3. COUPLED LAPLACIAN CONSTRUCTION: Compute the diagonal degree matrix  $D$  based on the row sums of  $W$ , and form the non-selfadjoint coupled graph Laplacian operator  $L = D - W$ . To avoid trivial solutions, restrict further computational operations to the invariant range subspace of  $L$ .
4. STEP 4. METRIC WEIGHT CONSTRUCTION: Construct the positive definite metric weight matrix  $T_\zeta$  by taking the real part of the product of  $D$  and a diagonal phase-shifting matrix defined according to the phase vector  $\zeta = (\zeta_1, \zeta_2, \dots, \zeta_n)^T$ , where its components are arbitrarily specified such that  $\zeta_j \in (0, \pi/2)$ .
5. STEP 5. PARAMETRIC SPECTRAL DECOMPOSITION: Construct the parametric operator  $\Psi(\theta) = e^{-i\theta}L + e^{i\theta}L^*$  depending on the parameter  $\theta$ , and solve the corresponding generalized eigenvalue problem to obtain a complete system of  $T_\zeta$ -orthonormal eigenvectors.
6. STEP 6. FIXED-POINT SELECTION: Form the matrix  $E_p(\theta)$  from a selected subset of  $m$  eigenvectors corresponding to the target reduced dimensionality. Locate the stable fixed points  $\theta_p$  satisfying the self-consistent algebraic equation  $\arg \psi\{E_p(\theta)\} = \theta$ . Although the geometric probability of coincidence between the exceptional and fixed points is zero, this condition is verified experimentally to ensure that  $\theta_p \notin \mathbb{D}$ .
7. STEP 7. LATENT SPACE PROJECTION: Form the optimal matrix  $X = E_p(\theta_p)$  belonging to the manifold  $\mathfrak{M}_m^n$  whose columns form the  $T_\zeta$ -orthonormal basis, choosing the index  $p = 1$  for the minimum trace problem PI and  $p = 2$  for the maximum trace problem PII. The constructed correspondence

$$\mathfrak{A}_m^T : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{m \times n}, \quad \mathfrak{B}_m^T : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{m \times n}$$

produces the low-dimensional representations of the initial datasets in the target feature space whose internal structure is determined by the natural coupling inherent to the algebraic structure—the field of complex numbers.

## 4. Conclusions

This paper is a continuation of a series of papers by our research group devoted to the development of new mathematical methods for integrating multi-omics data. In our previous work [22], we laid the theoretical foundations for the topological alignment of heterogeneous data using the methods of the reproducing kernel Hilbert space theory. It has been shown that these mathematical objects admit the unification of an arbitrary number of datasets of different natures, and their further development towards quaternionic and hypercomplex numbers opens the way to the creation of a theoretically grounded general concept of integration.

In this paper, we expand this strategy, taking into account the biological limitations identified during the analysis of existing methods. Our research group has a unique set of multi-omics data, including genomic, transcriptomic, proteomic, lipidomic, and metabolomic profiles. In accordance with the adopted strategy, at the first stage, we conduct a detailed analysis of each omics dataset individually, which makes it possible to verify the reproducibility of the detected biological signals and eliminate the loss of significant information during subsequent integration. At the second stage, we apply existing tools for pairwise and multiple dataset integration, using the results obtained as a reference for evaluating reproducibility. At the third stage, we implement the mathematical approaches we are developing in the program code and apply them to integrate the entire dataset, comparing the results with those obtained in previous stages.

The central idea of the developed methods is not the mathematical alignment of datasets, but biologically meaningful integration, in which the structure of molecular interactions, the logic of enzymatic regulation and the dynamics of metabolic flows serve as biological constraints for the mathematical model. This approach aims to make the results of multi-omics analysis not only statistically reliable, but also directly interpretable in terms of cellular physiology, regulation of gene expression, and molecular pathology.

On the other hand, the constructed mathematical theory involving topological methods, operator theory methods, optimization theory, a probability theory approach, and biological data analysis deserves to be considered in itself. The idea to study a principally novel non-selfadjoint operator in the framework of the optimization theory, namely, the so-called coupled graph Laplacian, is very promising and at the same time harmonious from the operator theory point of view. The coupling of heterogeneous datasets in a natural manner is undoubtedly advantageous in comparison with the previously considered methods that partially deal with the artificial mathematical constructions based on the convenient relationships. The involved most general coupling structure such as an algebraic structure, in particular the field of the complex numbers, creates a principally new level of mathematical description of the problem. The further direct generalization appeals to the body of quaternions. The prospective most general representatives of the coupling algebraic structure are finite dimensional algebras over a field and Clifford algebras. Apparently, the generalization of the selfadjoint graph Laplacian operator to a non-selfadjoint operator implementing the coupling of the heterogeneous datasets satisfies the best traditions of functional analysis, which is invaluable from the point of view of a pure mathematician.

**Author Contributions:** Conceptualization, M.V.K., M.S.A., D.E.B. and A.V.C.; methodology, M.V.K. and A.V.C.; formal analysis, M.V.K.; investigation, M.V.K. and M.S.A.; resources, M.S.A.; data curation, M.S.A., D.E.B. and A.V.C.; writing—original draft, M.V.K.; supervision, A.V.C.; project administration, M.S.A. All authors have read and agreed to the published version of the manuscript.

**Funding:** State Assignment of Russian National Research Medical University No. 125022602916-4.

**Data Availability Statement:** No new data were created or analyzed in this study.

**Conflicts of Interest:** The authors declare no conflicts of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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