



On Geometric Properties of the Textile Set and Strict Textile Set

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Abstract. The textile plot is a tool for data visualisation proposed by Kumasaka and Shibata (2008). The textile set is a geometric object constructed to understand the textile plot outputs. In this study, we find additional facts on a proper subset called the strict textile set. Furthermore, we investigate differential and analytical geometric properties of the textile set.

Keywords: Textile plot · Textile set · Strict textile set · Submanifold · Canonical form

1 Introduction

The textile plot is a useful tool for data visualisation proposed by Kumasaka and Shibata [3]. The method transforms a given dataset consisting of continuous and/or categorical variables into a real matrix and draws a parallel coordinate plot based on it. The order of variables is determined using some variance criteria or clustering methods. We refer readers to [2] for a comprehensive study on parallel coordinate plots and [6] for geometric observation of parallel coordinate plots.

We first briefly review the textile plot (see [3] for details). We only consider continuous variables and fix the order of variables for simplicity. Suppose that a real matrix $\mathbf{X} = (x_{ti}) = (\mathbf{x}_1, \dots, \mathbf{x}_p) \in \mathbb{R}^{n \times p}$ is given. Let $y_{ti} = a_i + b_i x_{ti}$ for each t and i , where each a_i and b_i are determined as follows. Let $\bar{y}_t = p^{-1} \sum_{i=1}^p y_{ti}$ be the ‘horizontal’ mean. Then each a_i and b_i are determined in such a way that the deviation

$$\sum_{t=1}^n \sum_{i=1}^p (y_{ti} - \bar{y}_t)^2$$

is minimised under the restrictions of $y_{ti} = a_i + b_i x_{ti}$ and $\sum_t \sum_i y_{ti}^2 = 1$. The textile plot draws a line graph of $(y_{ti})_{i=1}^p$ for each t . Figure 1 explains the construction of the textile plot when $p = 5$.

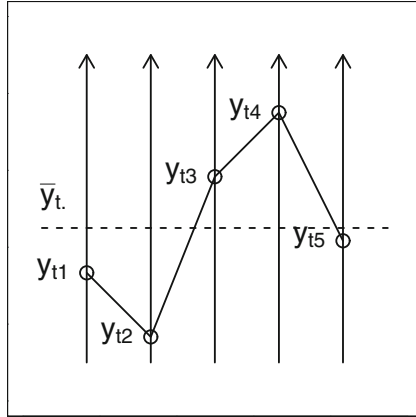


Fig. 1. Construction of the textile plot. The sum of deviations of y_{ti} against the horizontal average \bar{y}_t is minimised under the restrictions $y_{ti} = a_i + b_i x_{ti}$ and $\sum_{t,i} y_{ti}^2 = 1$.

The obtained matrix $\mathbf{Y} = (y_{ti})$ satisfies a set of conditions. A set of such matrices is called the textile set (see also [5]). In [5], we have shown that a canonical part of the textile set can be written as a union of submanifolds.

A visualisation method of linkage disequilibrium in genetic studies, where multiple-single nucleotide polymorphism (SNP) genotype data are considered, has been developed as an application of the textile plot [4]. Since the data considered in [4] are categorical, they are first quantified by dummy variables and then the textile plot is applied. See [3] and [4] for details.

In this study, we derive some geometric properties of the textile set that have not been explored in [5]. Furthermore, we define a proper subset called the strict textile set in order to fill the gap between the textile set and the textile plot.

The rest of this paper is organised as follows. In Sect. 2, we provide the definition of the textile set and represent it as an inverse image of a differentiable map. In Sect. 3, we define the strict textile set and investigate its representations. In Sect. 4, we investigate the textile set from the viewpoint of differential and analytic geometry. Section 5 concludes the paper.

2 The Textile Set

The matrix $\mathbf{Y} \in \mathbb{R}^{n \times p}$ constructed for the textile plot as described in Sect. 1 satisfies the following two conditions:

$$\exists \lambda \in \mathbb{R}, \quad \forall i \in \{1, \dots, p\}, \quad \sum_{j=1}^p \mathbf{y}_i^\top \mathbf{y}_j = \lambda \|\mathbf{y}_i\|^2 \quad (1)$$

and

$$\sum_{j=1}^p \|\mathbf{y}_j\|^2 = 1. \tag{2}$$

The two conditions are necessary for \mathbf{Y} to be an output of the textile plot but not sufficient. Indeed, two data matrices $\mathbf{Y} = (\mathbf{v}, \mathbf{v})$ and $\tilde{\mathbf{Y}} = (\mathbf{v}, -\mathbf{v})$ for any vector $\mathbf{v} \in \mathbb{R}^n$ with $\|\mathbf{v}\|^2 = 1/2$ satisfy the conditions (1) and (2) for $\lambda = 2$ and $\lambda = 0$, respectively, but only the former is the output of the textile plot.

The textile set is defined as follows (see also [5]).

Definition 1. A set of all matrices $\mathbf{Y} \in \mathbb{R}^{n \times p}$ satisfying Eqs.(1) and (2) is called the textile set and denoted by $T_{n,p}$.

We point out that the textile set is an inverse image of a differentiable map. Let $\mathcal{S}_+(p)$ be a set of all positive semi-definite matrices. For a data matrix $\mathbf{Y} \in \mathbb{R}^{n \times p}$, we denote the Gram matrix as $g(\mathbf{Y}) = \mathbf{Y}^\top \mathbf{Y} \in \mathcal{S}_+(p)$. Then, g is a function from $\mathbb{R}^{n \times p}$ to $\mathcal{S}_+(p)$. Let $T_+(p)$ be the image of $T_{n,p}$ by g . Explicitly, $T_+(p)$ consists of positive semi-definite matrices \mathbf{S} satisfying the following two conditions:

$$\exists \lambda \in \mathbb{R}, \quad \forall i \in \{1, \dots, p\}, \quad \sum_j S_{ij} = \lambda S_{ii},$$

$$\text{and} \quad \sum_j S_{jj} = 1.$$

The following theorem is important for understanding the structure of $T_{n,p}$.

Theorem 1. The textile set is given by $T_{n,p} = g^{-1}(T_+(p))$.

Proof. The proof is straightforward.

Figure 2 shows the relation of these objects. Note that $T_+(p)$ does not depend on n .

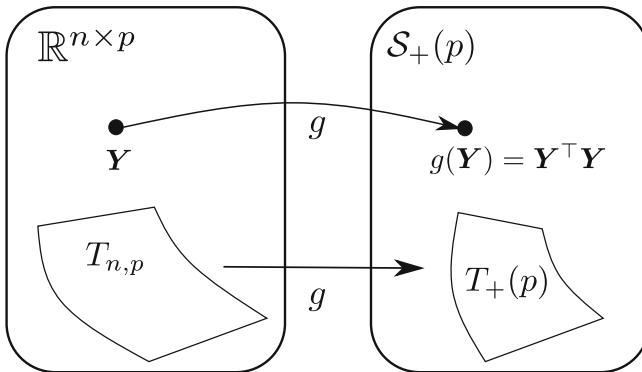


Fig. 2. The textile set $T_{n,p}$ as an inverse image.

3 The Strict Textile Set

In this section, we define the strict textile set as a proper subset of the textile set and characterise it.

The quantity λ in Eq. (1) is one of the eigenvalues of the correlation matrix $r_{ij} = \mathbf{y}_i^\top \mathbf{y}_j / (\|\mathbf{y}_i\| \|\mathbf{y}_j\|)$, where $\|\mathbf{y}_i\| \neq 0$ is assumed for simplicity. However, in the original definition of the textile plot (see [3]), λ is the maximum eigenvalue of the correlation matrix. The following lemma characterises the condition of maximality.

Lemma 1. *Let $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_p)$ be an element of $T_{n,p}$ and assume that $\|\mathbf{y}_i\| \neq 0$ for all i . Then λ in Eq. (1) is the maximal eigenvalue of $r_{ij} = \mathbf{y}_i^\top \mathbf{y}_j / \|\mathbf{y}_i\| \|\mathbf{y}_j\|$ if and only if a matrix*

$$Q_{ij} = \mathbf{y}_i^\top \left(\sum_{k=1}^p \mathbf{y}_k \right) \delta_{ij} - \mathbf{y}_i^\top \mathbf{y}_j \quad (3)$$

is positive semi-definite.

Proof. The maximality condition is equivalent to

$$\sum_i \sum_j a_i \frac{\mathbf{y}_i^\top \mathbf{y}_j}{\|\mathbf{y}_i\| \|\mathbf{y}_j\|} a_j - \lambda \sum_i a_i^2 \leq 0$$

for all $\mathbf{a} \in \mathbb{R}^p$. Let $b_i = a_i / \|\mathbf{y}_i\|$. Then we have

$$\sum_i \sum_j b_i (\mathbf{y}_i^\top \mathbf{y}_j) b_j - \lambda \sum_i b_i^2 \|\mathbf{y}_i\|^2 \leq 0.$$

Since Eq. (1) holds, this is further equivalent to

$$\sum_i \sum_j b_i \left(\mathbf{y}_i^\top \mathbf{y}_j - \mathbf{y}_i^\top \left(\sum_k \mathbf{y}_k \right) \delta_{ij} \right) b_j \leq 0,$$

and the proof is completed.

Now we define the strict textile set.

Definition 2. *The strict textile set $T_{n,p}^1$ consists of matrices $\mathbf{Y} \in T_{n,p}$ such that the matrix $\mathbf{Q} = (Q_{ij})$ defined by Eq. (3) is positive semi-definite.*

The matrix \mathbf{Q} is a function of the Gram matrix $\mathbf{S} = g(\mathbf{Y}) = \mathbf{Y}^\top \mathbf{Y}$. For the dependence, we can write

$$Q_{ij}(\mathbf{S}) = \sum_k S_{ik} \delta_{ij} - S_{ij}$$

or

$$\mathbf{Q}(\mathbf{S}) = \text{diag}(\mathbf{S}\mathbf{1}_p) - \mathbf{S},$$

where $\mathbf{1}_p$ is the all-ones vector and $\text{diag}(\mathbf{v})$ is the diagonal matrix with the diagonal part \mathbf{v} . We also define

$$T_+^1(p) := T_+(p) \cap \{\mathbf{S} \in \mathcal{S}_+(p) \mid \mathbf{Q}(\mathbf{S}) \in \mathcal{S}_+(p)\}. \quad (4)$$

Recall that $\mathcal{S}_+(p)$ is the set of positive semi-definite matrices. From the definition, we obtain the following lemma.

Lemma 2. *The strict textile set is given by $T_{n,p}^1 = g^{-1}(T_+^1(p))$.*

In what follows, we study the set $T_+^1(p)$ instead of $T_{n,p}^1$.

For example, if $p = 2$, then

$$\mathbf{Q}(\mathbf{S}) = \begin{pmatrix} S_{12} & -S_{12} \\ -S_{12} & S_{12} \end{pmatrix} = S_{12} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

The condition $\mathbf{Q} \succeq \mathbf{0}$ is obviously equivalent to $S_{12} \geq 0$.

If $p = 3$, then

$$\begin{aligned} \mathbf{Q}(\mathbf{S}) &= \begin{pmatrix} S_{12} + S_{13} & -S_{12} & -S_{13} \\ -S_{12} & S_{12} + S_{23} & -S_{23} \\ -S_{13} & -S_{23} & S_{13} + S_{23} \end{pmatrix} \\ &= S_{12} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + S_{13} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} + S_{23} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}. \end{aligned}$$

A sufficient condition for positive semi-definiteness of \mathbf{Q} is

$$S_{12} \geq 0, \quad S_{13} \geq 0, \quad S_{23} \geq 0.$$

This is not necessary: a counter-example is

$$\mathbf{S} = \begin{pmatrix} 100 & -1 & 10 \\ -1 & 100 & 10 \\ 10 & 10 & 100 \end{pmatrix}.$$

It is directly shown that \mathbf{Q} is positive semi-definite if and only if $S_{12} + S_{13} + S_{23} \geq 0$ and $S_{12}S_{13} + S_{12}S_{23} + S_{13}S_{23} \geq 0$.

Now let us consider general p . We denote the set appearing in the definition (4) as

$$\mathcal{A} := \{\mathbf{S} \in \mathcal{S}_+(p) \mid \mathbf{Q}(\mathbf{S}) \in \mathcal{S}_+(p)\}.$$

Theorem 2. *The set \mathcal{A} is a convex cone, which has an interior point.*

Proof. First, we show that \mathcal{A} is a convex cone. Let $\mathbf{S}_1, \mathbf{S}_2 \in \mathcal{A}$ and $c_1, c_2 \geq 0$. Then $c_1\mathbf{S}_1 + c_2\mathbf{S}_2 \in \mathcal{S}_+(p)$ and

$$\mathbf{Q}(c_1\mathbf{S}_1 + c_2\mathbf{S}_2) = c_1\mathbf{Q}(\mathbf{S}_1) + c_2\mathbf{Q}(\mathbf{S}_2) \in \mathcal{S}_+(p).$$

Hence $c_1\mathbf{S}_1 + c_2\mathbf{S}_2 \in \mathcal{A}$. Next, we prove that \mathcal{A} has an interior point. Observe that if $S_{ij} > 0$ for all pairs $i \neq j$, then $\mathbf{Q}(\mathbf{S}) \in \mathcal{S}_+(p)$. Hence, we obtain

$$\mathcal{S}_{++}(p) \cap \{\mathbf{S} \mid S_{ij} > 0, i \neq j\} \subset \mathcal{A},$$

where $\mathcal{S}_{++}(p)$ denotes a set of all positive definite matrices. Since the two sets in the left-hand side are open, it is sufficient to show that their intersection is not empty. Indeed, a matrix

$$\mathbf{S} = \begin{pmatrix} 2 & 1 & \cdots & 1 \\ 1 & 2 & & \vdots \\ \vdots & & \ddots & 1 \\ 1 & \cdots & 1 & 2 \end{pmatrix}$$

belongs to the two sets. This completes the proof.

We return to the space of \mathbf{Y} . Define

$$\begin{aligned} \mathcal{B} &:= g^{-1}(\mathcal{A}) \\ &= \{\mathbf{Y} \in \mathbb{R}^{n \times p} \mid \mathbf{Q}(\mathbf{Y}^\top \mathbf{Y}) \in \mathcal{S}_+(p)\}. \end{aligned}$$

The strict textile set is given by $T_{n,p}^1 = T_{n,p} \cap \mathcal{B}$. Indeed, we have

$$\begin{aligned} T_{n,p}^1 &= g^{-1}(T_+^1) \\ &= g^{-1}(T_+ \cap \mathcal{A}) \\ &= g^{-1}(T_+) \cap g^{-1}(\mathcal{A}) \\ &= T_{n,p} \cap \mathcal{B}. \end{aligned}$$

Corollary 1. *If $n \geq p$, then \mathcal{B} has an interior point.*

Proof. Note that $g(\mathbf{Y}) = \mathbf{Y}^\top \mathbf{Y}$ is continuous. If $n \geq p$, then g is also surjective. Indeed, for a given $\mathbf{S} \in \mathcal{S}_+(p)$, a matrix

$$\mathbf{Y} = \begin{pmatrix} \mathbf{S}^{1/2} \\ \mathbf{0} \end{pmatrix}$$

with the matrix square root $\mathbf{S}^{1/2}$ satisfies $g(\mathbf{Y}) = \mathbf{S}$. Since \mathcal{A} has an interior point, \mathcal{B} also has an interior point.

Figure 3 summarises the relations we obtained. Here we denote a set of all $p \times p$ symmetric matrices as $\mathcal{S}(p)$.

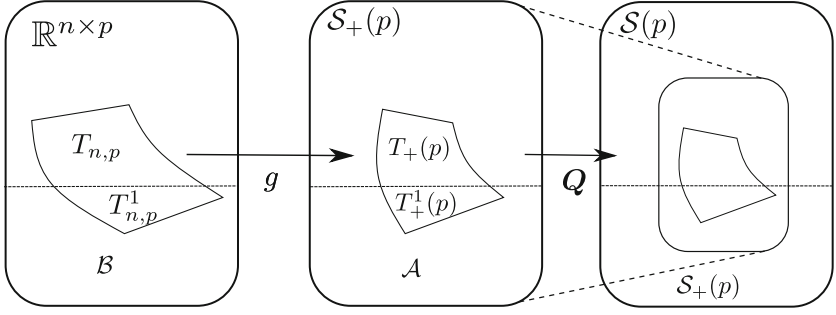


Fig. 3. The strict textile set $T_{n,p}^1$ and related objects.

4 Geometric Properties of the Textile Set from the Viewpoint of Differential and Analytic Geometry

In this section, we demonstrate that the textile set $T_{n,p}$ is a regular submanifold of $\mathbb{R}^{n \times p}$ with codimension $p + 1$. The result is independent from the preceding study presented in [5], where a canonical part of $T_{n,p}$ was studied. Furthermore, we obtain an envelope of the textile set and a canonical form of the envelope under the hypothesis that $n = p \geq 2$. Inselberg [1] has discussed the parallel coordinate from the analytical geometric point of view, which motivates our study.

Our observation starts with the quantity λ in Eq. (1).

Lemma 3. *Let $\mathbf{Y} \in T_{n,p}$. Then λ is bounded as follows:*

$$0 \leq \lambda \leq p.$$

Proof. For the lower bound, take the summation of Eq. (1) with respect to i and use Eq. (2) to obtain $\lambda = \|\sum_i \mathbf{y}_i\|^2 \geq 0$. For the upper bound, first consider the case $\|\mathbf{y}_i\| > 0$ for all i . Then Eq. (1) is equivalent to the condition that λ is an eigenvalue of the correlation matrix $r_{ij} = \mathbf{y}_i^\top \mathbf{y}_j / \|\mathbf{y}_i\| \|\mathbf{y}_j\|$ because $\sum_j r_{ij} \|\mathbf{y}_j\| = \lambda \|\mathbf{y}_i\|$. Since the trace of (r_{ij}) is p , we have $\lambda \leq p$. If $\|\mathbf{y}_i\|$ is zero for some i , consider a submatrix $(r_{ij})_{i,j \in I}$, where $I := \{i \mid \|\mathbf{y}_i\| > 0\}$. Note that I is not empty due to Eq. (2). It is shown that λ is an eigenvalue of the submatrix and therefore $\lambda \leq |I| \leq p$.

Remark 1. From the proof, we observe that $\lambda = 0$ if and only if $\sum_i \mathbf{y}_i = \mathbf{0}$, and that $\lambda = p$ if and only if $\mathbf{y}_1 = \dots = \mathbf{y}_p$.

For each $\lambda \in [0, p]$, define a map $f_\lambda: \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^{p+1}$ as

$$f_\lambda(\mathbf{y}_1, \dots, \mathbf{y}_p) := \left(\sum_{j=1}^p \mathbf{y}_1^\top \mathbf{y}_j - \lambda \|\mathbf{y}_1\|^2, \dots, \sum_{j=1}^p \mathbf{y}_p^\top \mathbf{y}_j - \lambda \|\mathbf{y}_p\|^2, \sum_{j=1}^p \|\mathbf{y}_j\|^2 - 1 \right).$$

Remark 2. $\{f_\lambda^{-1}(\mathbf{0}) \mid 0 \leq \lambda \leq p\}$ yields a classification of the textile set, i.e.,

$$T_{n,p} = \bigsqcup_{0 \leq \lambda \leq p} f_\lambda^{-1}(\mathbf{0}). \quad (5)$$

The following theorem is a result of the textile set from the viewpoint of differential geometry. This theorem shows that each $f_\lambda^{-1}(\mathbf{0})$ is an $np - (p + 1)$ -dimensional differentiable manifold.

Theorem 3. *Suppose that*

$$0 < \lambda (\leq p), \quad y_{11} \neq 0, \quad (6)$$

$$y_{11}y_{jj} - y_{1j}y_{j1} \neq 0, \quad j = 2, \dots, p, \quad (7)$$

$$\exists \ell \in \{2, \dots, p\}; \sum_{j=2}^p y_{ij} + y_{i\ell}(1 - 2\lambda) \neq 0, \quad i = 1, \dots, n. \quad (8)$$

We call the above equations the regularity condition, which implies that a natural inclusion map $\iota: f_\lambda^{-1}(\mathbf{0}) \hookrightarrow \mathbb{R}^{n \times p}$ is a homeomorphism onto its image. Then $f_\lambda^{-1}(\mathbf{0})$ is a regular submanifold of $\mathbb{R}^{n \times p}$ with codimension $p + 1$.

Proof. We outline the proof. We derive the sufficient condition for the Jacobi matrix of f_λ over $f_\lambda^{-1}(\mathbf{0})$ to be of full rank ($= p + 1$). Each of Eqs. (6)–(8) establishes the desired conclusion.

The following theorem shows an application of Theorem 3.

Theorem 4. *Assume that in Eq. (5), $T_{n,p}$ is given by the finitely disjoint union of $f_\lambda^{-1}(\mathbf{0})$ in addition to the regularity condition. Then, $T_{n,p}$ is an $np - (p + 1)$ -dimensional compact differentiable manifold, where its differential structure is induced from the disjoint union of open sets of the differential manifold $f_\lambda^{-1}(\mathbf{0})$.*

Proof. We outline the proof. We have observed that $T_{n,p}$ is compact (see [5] for details). Combining Theorem 3 with the assumption of the finiteness leads to the conclusion.

The remainder of this section is devoted to the study of the textile set from the viewpoint of analytic geometry. Let $n = p \geq 2$. The following lemma shows an envelope of $T_{n,n}$.

Lemma 4. *Fix $\lambda \in [0, n]$, $n \geq 2$. Let $F_\lambda: \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$ be a quadratic form defined as*

$$F_\lambda(\mathbf{y}_1, \dots, \mathbf{y}_n) := \sum_{i=1}^n \sum_{j=1}^n y_{ij} \left(\sum_{k \neq j} y_{ik} \right) - (\lambda - 1).$$

Then $T_{n,n} \subset F_\lambda^{-1}(0)$.

Proof. We deduce that Eqs. (1) and (2) yield the following quadric: for all $\mathbf{y}_1, \dots, \mathbf{y}_n \in T_{n,n}$,

$$F_\lambda(\mathbf{y}_1, \dots, \mathbf{y}_n) = 0, \quad 0 \leq \lambda \leq n. \tag{9}$$

This completes the proof.

We proceed with the study on the canonical form of the quadric given by (9). The following theorem is a result of the textile set from the viewpoint of analytic geometry.

Theorem 5. *Let F_λ be defined as in Lemma 4. Then, the canonical form of the quadric defined from F_λ is given as follows:*

$$\begin{aligned} & -\frac{1}{\lambda-1}z_1^2 - \dots - \frac{1}{\lambda-1}z_{n(n-1)}^2 \\ & + \frac{n-1}{\lambda-1}z_{n(n-1)+1}^2 + \dots + \frac{n-1}{\lambda-1}z_{n^2}^2 = 1, \quad \lambda \neq 1, \\ & -z_1^2 - \dots - z_{n(n-1)}^2 + (n-1)z_{n(n-1)+1}^2 + \dots + (n-1)z_{n^2}^2 = 0, \quad \lambda = 1, \end{aligned}$$

where each z_i , $i = 1, \dots, n^2$, denotes a transformed coordinate to obtain the stated canonical form.

Proof. We outline the proof. For each $i, j = 1, \dots, n$, identifying y_{ij} with $y_{(i-1)n+j}$ ($\in \mathbb{R}^{n^2}$), we can rewrite (9) as following:

$$F_\lambda(y_1, \dots, y_{n^2}) = (y_1, \dots, y_{n^2}) A (y_1, \dots, y_{n^2})^\top - (\lambda-1) = 0, \quad 0 \leq \lambda \leq n, \tag{10}$$

where

$$A := \begin{pmatrix} A_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & A_n \end{pmatrix}, \quad A_k := \begin{pmatrix} 0 & 1 & \dots & 1 \\ 1 & 0 & \dots & 1 \\ \vdots & \ddots & \ddots & \vdots \\ 1 & 1 & \dots & 0 \end{pmatrix}, \quad k = 1, \dots, n.$$

It can be noticed that the eigenvalues of A are given by -1 and $n-1$ with their multiplicities $n(n-1)$ and n , respectively. Hence, we have $\det A = ((-1)^{n-1}(n-1))^n \neq 0$ because $n \geq 2$, from which it can be derived that F_λ given by Eq. (10) is a central quadric. Consequently, a proper coordinate transformation gives us the desired conclusion.

5 Conclusions

In this study, we have obtained geometric properties of the textile and strict textile sets as follows: The textile set can be characterised as an inverse image of the map g (Theorem 1). We have also defined the strict textile set and demonstrated its relation to a convex cone (Theorem 2). Furthermore, we have investigated the textile set from the viewpoint of differential geometry (Theorems 3 and 4) and analytic geometry (Lemma 4 and Theorem 5).

In the future, we plan to practically apply the results reported here and describe the intrinsically differential and analytical geometric structure of employed datasets. In fact, R. Shibata, who proposed the textile plot in [3], has suggested this direction to us. We are also concerned with defining a proper metric for the textile set $T_{n,p}$ and its class $f_\lambda^{-1}(\mathbf{0})$ as a differentiable manifold (stated in Theorems 3 and 4), and a quadric of the textile set $T_{n,n}$ itself as well as its envelop.

We could not investigate probabilistic properties of \mathbf{Y} and $g(\mathbf{Y})$ defined in Sect. 2 when the data matrix \mathbf{X} is distributed according to some multivariate distributions. The distribution of \mathbf{Y} should be studied to understand the behaviour of the textile plot. For instance, the variable selection based on the norm $\|\mathbf{y}_i\|$ has to be justified in the framework of sampling distributions.

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