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OPTIMIZATION AND MATRIX CONSTRUCTIONS FOR CLASSIFICATION OF DATA

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Abstract. Max-plus algebras and more general semirings have many useful applications and have been actively investigated. On the other hand, structural matrix rings are also well known and have been considered by many authors. The main theorem of this article completely describes all optimal ideals in the more general structural matrix semirings. Originally, our investigation of these ideals was motivated by applications in data mining for the design of centroid-based classification systems, as well as for the design of multiple classification systems combining several individual classifiers.

1. Introduction

Semirings have been actively investigated, because they are important in mathematics and have many useful applications, see [10, 11]. As a special example of a semiring, let us only mention the max-plus algebra, which plays crucial roles in the study of discrete event systems, see [3, 10]. On the other hand, structural matrix rings have also been considered in the literature and many interesting results have been obtained (see, for example, [5, 8, 12, 22, 23]).

The present article is devoted to the investigation of the more general structural matrix semirings. Our main theorem gives a complete description of all ideals with largest weights in structural matrix semirings. Originally our investigation of these ideals was motivated by their applications to the design of classification systems, or classifiers, considered in data mining. We refer to the monograph [24] for more information on the design of classifiers and their roles in data mining. More detailed explanations are also given in Section 2 below. In particular, special sets satisfying certain optimal properties are required for the design of classifiers, as well as for the design of multiple classifiers combining several individual or initial classifiers, see [19, 20].

The paper is organised as follows. An overview of applications of matrix constructions for classification of data is given in Section 2 as motivation for this research. The main result of this paper is Theorem 1 in Section 3, which completely describes all ideals with largest weights in structural matrix semirings. A complete proof is given in Section 4.

Key words and phrases: matrix constructions, ideals, semirings, optimization.

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2. Motivation and Preliminaries

This section contains a concise review of the main definitions required for our new theorem. We use standard notions and terminology and refer the readers to [5, 6, 7, 9, 10, 11, 13, 14, 15, 16, 17, 18, 21, 24, 26] for more detailed discussions of these concepts and examples of recent results.

The design of efficient classifiers is very important in data mining, see [24]. Max-plus algebras, more general semirings, and matrix constructions over them can be used in order to generate convenient sets of centroids for centroid-based classifiers and to design combined multiple classifiers capable of correcting the errors of individual initial classifiers.

Classification deals with known classes of data. These classes are represented by given samples of data. The samples are used for supervised training of the classifier to enable it to recognize new elements of the same known classes. The classification process begins with feature extraction and representation of data in a standard vector space F^n , where F can be regarded as a semifield.

A semifield is a semiring, where the set of nonzero elements forms a group with respect to multiplication. Recall that a semiring is a set F with two binary operations, addition + and multiplication \cdot , such that the following conditions are satisfied:

- (S1) (F, +) is a commutative semigroup with zero 0,
- (S2) (F, \cdot) is a semigroup,
- (S3) multiplication distributes over addition,
- (S4) zero 0 annihilates F, i.e., $0 \cdot F = F \cdot 0 = 0$.

It is also often assumed that every semiring satisfies an additional property (S5) (F, \cdot) has an identity element 1.

Our results remain valid without assuming (S5), and so we consider more general semirings, which do not have to satisfy (S5). In analogy with a similar situation in ring theory, we then call every semiring satisfying (S5) a *semiring with identity element*. As usual, such more general terminology adds the convenience of allowing us to consider more general subsets as subsemirings without assuming that all subsemirings contain the identity element. Both terminologies are essentially equivalent, since it is always easy to adjoin an identity element in a standard fashion to every semiring that does not have one.

Every centroid-based classifier selects special elements c_1, \ldots, c_k in F^n , called *centroids* (see, for example, [4]). For $i = 1, \ldots, k$, each centroid c_i defines its class $N(c_i)$ consisting of all vectors v such that c_i is the nearest centroid of v. Every vector is assigned to the class of its nearest centroid.

On the other hand, multiple classifiers are often used in analysis of data to combine individual initial classifiers (see, for example, [27]). A well-known method for the design of multiple classifiers consists in designing several simpler initial or individual classifiers, and then combining them into one multiple classification scheme with several classes. This method is very effective, and is often recommended for various applications, see [24], Section 7.5 and [19]. The main advantage of using combined multiple classifiers is in their ability to correct errors of individual classifiers and produce correct classifications despite individual classification errors.

Denote the number of initial classifiers being combined by n. If o_1, \ldots, o_n are the outputs of the initial classifiers, then the sequence (o_1, \ldots, o_n) is called a *vector*

of outputs of the initial classifiers. In order to define the multiple classifier and enable correction of errors of the initial classifiers, a set of centroids c_1, \ldots, c_k is again selected in F^n . For $i = 1, \ldots, k$, the class $N(c_i)$ of the centroid c_i is again defined as the set of all observations with the vector outputs of the initial classifiers having c_i as its nearest centroid.

The design of multiple classifiers by combining individual classifiers is quite common in the literature. We refer to [19, 20] and [24] for a list of properties required of the sets of centroids. In particular, it is essential to find sets of centroids with large weights and small numbers of generators. The weight wt(v) of $v \in F^n$ is the number of nonzero components or coordinates in v. The weight of a set $C \subseteq F^n$ is the minimum weight of a nonzero element in C. For additional references and discussion of experimental research related to these properties we refer the readers to [19, 20].

The information rate of a class set C in F^m can be defined as $\log_{|F|}(|C|)/m$. It reflects the proportion of output of the individual initial classifiers used to produce the outcomes of the multiple classification, as opposed to additional efforts spent on increasing reliability and correcting classification errors.

All sequences of the centroid set C can be written down in a matrix M to discuss their properties. If M has two identical columns, this means that two initial classifiers produce identical outputs. This duplication is very inefficient, even though it could help to correct classification errors. Therefore, in a situation like this, one of these classifiers can be removed and a better scheme can be devised. Likewise, it is undesirable to have strong correlation or functional dependencies between very small sets of columns in M or between the initial classifiers.

According to [24], Section 7.5, for a classifier with a class set C to be efficient, the class C must satisfy the following most essential basic properties:

- (1) The set C must have a large weight.
- (2) The information rate of C must be large.
- (3) A small set of generators for the set C is essential in order to simplify computer storage and manipulation of the set.
- (4) If all vectors of C are recorded in a matrix M, then there should not be strong correlation or functional dependencies between small sets of columns of M. In particular, the matrix M should not have duplicate columns.

Thus, in particular, it is essential to find sets of centroids with large weights and small numbers of generators. For additional references and discussion of experimental research related to these properties we refer the readers to [19, 20, 26, 27].

The max-plus algebra is the set $\mathbb{R} \cup \{-\infty\}$ with two binary operations, max and +. It is very important in the investigation of discrete event systems, see [3]. The max-plus algebra is also sometimes called the *schedule algebra*, see [10]. Our main results remain valid in the more general case of all semifields, and so we record them in this setting.

Let F be a semiring. Consider the semiring $M_m(F)$ of all $m \times m$ matrices over F. Let ρ be a binary relation on the set $[1:m] = \{1, \ldots, m\}$. For $i, j \in [1:m]$ denote by $e_{i,j}$ the standard elementary matrix in $M_m(F)$ with 1 in the intersection of *i*-th row and *j*-th column and zeros in all other entries. It is well known and easy to verify that the set $M_{\rho}(F) = \bigoplus_{(i,j) \in \rho} Fe_{i,j}$ is a subsemiring of $M_m(F)$ if and only if the relation ρ is transitive. In this case $M_{\rho}(F)$ is called a *structural matrix*

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semiring. Many interesting results on structural matrix rings have been obtained in the literature (see, for example, [5, 8, 12, 22, 23]). Known facts and references concerning structural matrix rings can be also found in [14].

If $|\varrho| = n$, then the additive semigroup of $M_{\varrho}(F)$ is isomorphic to F^n and we can introduce multiplication in F^n by identifying it with $M_{\varrho}(F)$. Further we consider sets of centroids as subsets generated in $M_{\varrho}(F)$. Every set of elements $g_1, \ldots, g_k \in M_{\varrho}(F)$ generates the set $C(g_1, \ldots, g_k)$ of all sums of these elements and their multiples:

$$C(g_1, \dots, g_k) = \left\{ \sum_{j=1}^{m_1} \ell_{1,j} g_1 r_{1,j} + \dots + \sum_{j=1}^{m_k} \ell_{k,j} g_k r_{k,j} \middle| \ell_{i,j}, r_{i,j} \in M_{\varrho}(F) \cup \{1\} \right\}.$$
 (1)

The set $C(g_1, \ldots, g_k)$ is called an *ideal* generated by g_1, \ldots, g_k . The concept of an ideal is very important and has been actively investigated in several branches of modern mathematics. In particular, it is used in the investigation of modules over rings (see, for example, [1, 2]) and ring constructions (see, for example, [13, 14]).

3. Main Results

Let ρ be a binary relation on the set [1:m]. We introduce the following binary relations

$$\varrho_{\ell} = \{(i,j) \in \varrho \mid \exists k \in [1:m] : (k,i) \in \varrho\},$$

$$(2)$$

$$\varrho_r = \{(i,j) \in \varrho \mid \exists k \in [1:m] : (j,k) \in \varrho\}.$$
(3)

and put

$$M_Z = |\varrho \setminus (\varrho_r \cup \varrho_\ell)|. \tag{4}$$

For any $i \in [1:m]$, let us define the sets

$$\varrho(i) = \{j \mid (i,j) \in \varrho\},\tag{5}$$

$$\varrho^{-1}(i) = \{ j \mid (j,i) \in \varrho \},$$
(6)

$$R(i) = \{ j \mid (i,j) \in \varrho \setminus \varrho_r \}, \tag{7}$$

$$L(i) = \{ j \mid (j,i) \in \varrho \setminus \varrho_\ell \}.$$
(8)

We introduce the following nonnegative integers

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$$M_L = \max\{|L(i)| : i = 1, \dots, m\},$$
(9)

$$M_R = \max\{|R(i)| : i = 1, \dots, m\}.$$
(10)

Denote by \mathcal{G}_Z the set of all elements $g = \sum_{(i,j) \in \varrho \setminus (\varrho_r \cup \varrho_\ell)} f_{i,j} e_{i,j} \in M_\varrho(F)$, where $0 \neq f_{i,j} \in F$. Let \mathcal{G}_L be the set of all elements $g = \sum_{j \in L(i)} f_j e_{j,i} \in M_\varrho(F)$, where i runs over the set of all integers i such that $|L(i)| = M_L$, and where $0 \neq f_j \in F$. Denote by \mathcal{G}_R the set of all elements $g = \sum_{j \in R(i)} f_j e_{i,j} \in M_\varrho(F)$, where i runs over the set of all integers i such that $|R(i)| = M_R$, and where $0 \neq f_j \in F$. Our main theorem describes all sets $C(g_1, \ldots, g_k)$ with the largest weight in $M_\varrho(F)$.

Theorem 1. Let $M_{\varrho}(F)$ be a structural matrix semiring over a semifield F. Suppose that $C = C(g_1, \ldots, g_k)$ is an ideal with the largest weight in $M_{\varrho}(F)$. Then the following conditions are satisfied:

(i) wt(C) = max{1, M_Z, M_L, M_R };

(ii) if wt(C) > 1, then $C \cap (\mathcal{G}_Z \cup \mathcal{G}_L \cup \mathcal{G}_R)$ contains an element of weight wt(C);

(iii) $\operatorname{wt}(C(g)) = \operatorname{wt}(g) = M_Z$, for all $g \in \mathcal{G}_Z$;

- (iv) $\operatorname{wt}(C(g)) = \operatorname{wt}(g) = M_L$, for all $g \in \mathcal{G}_L$;
- (v) wt(C(g)) = wt(g) = M_R , for all $g \in \mathcal{G}_R$.

4. Proofs

For any semiring F, the *left annihilator* of F is the set

$$\operatorname{Ann}_{\ell}(F) = \{ x \in F \mid xF = 0 \}, \tag{11}$$

and the *right annihilator* of F is the set

$$\operatorname{Ann}_{r}(F) = \{ x \in F \mid Fx = 0 \}.$$
(12)

Lemma 2. For any structural matrix semiring $M_{\varrho}(F)$ over a semifield F, the following equalities are satisfied:

$$\operatorname{Ann}_{r}(M_{\rho}(F)) = M_{\rho \setminus \rho_{\ell}}(F), \tag{13}$$

$$\operatorname{Ann}_{\ell}(M_{\varrho}(F)) = M_{\varrho \setminus \varrho_r}(F).$$
(14)

Proof. Take any element r in $\operatorname{Ann}_r(M_\rho(F))$. It can be recorded as

$$r = \sum_{(i,j)\in\varrho} f_{i,j} e_{i,j},$$

where $f_{i,j} \in F$. Consider any pair (i, j) in ϱ_{ℓ} . There exists $k \in [1 : m]$ such that $(k, i), (k, j) \in \varrho$. Hence $e_{k,i} \in M_{\varrho}(F)$ and $f_{i,j}e_{k,i}e_{i,j}$ is a summand of the product $e_{k,i}r$ in $M_{\varrho}(F)$. Since $r \in \operatorname{Ann}_r(M_{\varrho}(F))$, we get $f_{i,j} = 0$. It follows that r belongs to $M_{\varrho \setminus \varrho_{\ell}}(F)$, and so $\operatorname{Ann}_r(M_{\varrho}(F)) \subseteq M_{\varrho \setminus \varrho_{\ell}}(F)$.

To prove the reversed inclusion, let us pick any element r in $M_{\varrho \setminus \varrho_{\ell}}(F)$. It can be written down as $r = \sum_{(i,j) \in \varrho \setminus \varrho_{\ell}} f_{i,j} e_{i,j}$, where $f_{i,j} \in F$. In order to verify that $M_{\varrho}(F)r = 0$, it suffices to show that $e_{a,b}r = 0$ for all $(a,b) \in \varrho$. Suppose to the contrary that $e_{a,b}r \neq 0$ for some $(a,b) \in \varrho$. Then it is clear that at least one of the summands $e_{a,b}f_{i,j}e_{i,j}$ is nonzero for some $(i,j) \in \varrho \setminus \varrho_{\ell}$. The definition of a structural matrix semiring implies that $f_{i,j} \neq 0$, b = i, $(a,i) = (a,b) \in \varrho$ and $(a,j) \in \varrho$. Hence $(i,j) \in \varrho_{\ell}$. This contradicts the choice of (i,j) in $\varrho \setminus \varrho_{\ell}$ and shows that $e_{a,b}r = 0$ for all $(a,b) \in \varrho$. Therefore $M_{\varrho}(F)r = 0$, which means that $r \in \operatorname{Ann}_r(M_{\varrho}(F))$. Thus $\operatorname{Ann}_r(M_{\varrho}(F)) \supseteq M_{\varrho \setminus \varrho_{\ell}}(F)$.

These two inclusions show that equality (13) always holds. The proof of equality (14) is dual and we omit it. $\hfill \Box$

Proof of Theorem 1. (iii): Consider any element $g \in \mathcal{G}_Z$. By definition, we know that

$$g = \sum_{(i,j)\in\varrho\setminus(\varrho_r\cup\varrho_\ell)} f_{i,j}e_{i,j}\in M_\varrho(F),$$

where $0 \neq f_{i,j} \in F$. Clearly, $\operatorname{wt}(g) = |\varrho \setminus (\varrho_r \cup \varrho_\ell)| = M_Z$. Since $\varrho \setminus (\varrho_r \cup \varrho_\ell) = (\varrho \setminus \varrho_r) \cap (\varrho \setminus \varrho_\ell)$, Lemma 2 and (1) show that C(g) coincides with the linear space Fg spanned by g. Since F is a semifield, it follows that all nonzero elements of C(g) have weights equal to the weight of g. Hence $\operatorname{wt}(C(g)) = \operatorname{wt}(g)$ in this case, and so condition (iii) holds.

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(iv): Choose any element $g \in \mathcal{G}_L$. It can be represented in the form

$$g = \sum_{j \in L(i)} f_j e_{j,i},$$

where $1 \leq i \leq m$, $|L(i)| = M_L$ and $0 \neq f_j \in F$. Hence we get $\operatorname{wt}(g) = |L(i)| = M_L$. It remains to verify that $\operatorname{wt}(C(g)) = \operatorname{wt}(g)$. To this end, we choose any nonzero element x in C(g) and are going to verify that $\operatorname{wt}(x) \geq \operatorname{wt}(g)$. It follows from (1) that

$$x = \sum_{j=1}^{k} \ell_j g r_j, \tag{15}$$

for some $\ell_j, r_j \in M_{\varrho}(F) \cup \{F\}$, where we may assume that only nonzero summands $\ell_j r \ell_j$ are included in the sum. Since $(j,i) \notin \varrho_\ell$ for all $j \in L(i)$, it follows from Lemma 2 that $\ell_j g = 0$ for every $\ell_j \in M_{\varrho}(F)$. Therefore we may assume that all the ℓ_j are equal to 1 in the expression (15) for x above.

Keeping in mind that $M_{\varrho}(F) = \bigoplus_{(a,b) \in \varrho} Fe_{a,b}$, the distributive law allows us to assume without loss of generality that every element $r_j \in M_{\varrho}(F)$ in the expression (15) for x belongs to the union $\cup_{a,b} Fe_{a,b}$. Since $gr_j \neq 0$, it follows that then all the r_j belong to $\cup_{(i,b) \in \varrho} Fe_{i,b}$. The transitivity of ϱ shows that $\varrho(i) \subseteq \varrho(j)$ for all j in L(i). Since $gr_j \neq 0$, we see that all the r_j belong to $\cup_{b \in \varrho(i)} Fe_{i,b}$. Since F is a semifield, it follows that $wt(gr_j) = wt(g)$ for all $j \in L(i)$. Therefore $wt(x) \ge wt(g)$, as required. Thus, condition (iv) holds.

(v): The proof of condition (v) is dual to that of (iv), and so we omit it.

(ii): Suppose that wt(C) > 1. Choose a nonzero element g of minimal weight in C and consider several cases.

Case 1. $g \notin \operatorname{Ann}_r(M_\rho(F)) \cup \operatorname{Ann}_\ell(M_\rho(F))$. By Lemma 2, we get

$$g \notin M_{\varrho \setminus \varrho_{\ell}}(F) \cup M_{\varrho \setminus \varrho_{r}}(F).$$

Therefore there exist $(a, b), (c, d) \in \varrho$ such that $e_{a,b}ge_{c,d} \neq 0$. However, $e_{a,b}ge_{c,d} \in C$ and wt $(e_{a,b}ge_{c,d}) = 1$. Hence wt(C) = 1. This contradicts the assumption that wt(C) > 1 and shows that Case 1 is impossible.

Case 2. $g \in \operatorname{Ann}_{\ell}(M_{\rho}(F)) \cap \operatorname{Ann}_{r}(M_{\rho}(F))$. Lemma 2 implies that

$$r \in M_{\varrho \setminus \varrho_\ell}(F) \cap M_{\varrho \setminus \varrho_\ell}(F).$$

It follows from the maximality of wt(C) and condition (iii), which we have already proved above, that wt(g) = M_Z . Therefore $g \in \mathcal{G}_Z$. Since wt(g) = wt(C), this means that condition (ii) holds in this case.

Case 3. $g \in \operatorname{Ann}_r(M_{\varrho}(F)) \setminus \operatorname{Ann}_{\ell}(M_{\varrho}(F))$. Then $ge_{i,t} \neq 0$ for some $(i,t) \in \varrho$. Obviously, wt $(ge_{i,t}) \leq wt(g)$. By the minimality of the weight wt(g) in C, we get wt $(ge_{i,t}) = wt(g)$, because $ge_{i,t} \in C$. Therefore there exists a subset $S \subseteq \varrho^{-1}(i)$ such that $g = \sum_{j \in S} f_j e_{j,i}$, where $0 \neq f_j \in F$. Clearly, |S| = wt(g). Since $g \in M_{\varrho}(F)$, we get $S \subseteq \varrho^{-1}(i)$. Lemma 2 and $g \in \operatorname{Ann}_r(M_{\varrho}(F))$ show that $(j,i) \in \varrho \setminus \varrho_{\ell}$ for all $j \in S$. Therefore $S \subseteq L(i)$.

The maximality of $\operatorname{wt}(C) = \operatorname{wt}(g) = |S|$ and condition (iv) proved above imply that $\operatorname{wt}(g) \geq M_L$. By the definition of M_L , we get $M_L \geq |S| = \operatorname{wt}(g)$. Therefore $|S| = M_L$ and S = L(i). It follows that $g \in \mathcal{G}_L$. This means that condition (ii) holds true in this case, too. **Case 4.** $g \in \operatorname{Ann}_{\ell}(M_{\varrho}(F)) \setminus \operatorname{Ann}_{r}(M_{\varrho}(F))$. In this case a dual proof to the proof of Case 3 demonstrates that $g \in \mathcal{G}_R$. Therefore condition (ii) always holds true.

(i): Clearly, condition (ii) implies that $wt(C) \leq max\{1, M_Z, M_L, M_R\}$. On the one hand, the maximality of wt(C) and conditions (iii), (iv), (v), (vi) show that

 $wt(C) \ge \max\{1, M_Z, M_L, M_R\}.$

Therefore condition (i) is satisfied. This completes our proof. \Box

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