Computing Connection Matrices via Persistence-like Reductions

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Abstract

Connection matrices are a generalization of Morse boundary operators from the classical Morse theory for gradient vector fields. Developing an efficient computational framework for connection matrices is particularly important in the context of a rapidly growing data science that requires new mathematical tools for discrete data. Toward this goal, the classical theory for connection matrices has been adapted to combinatorial frameworks that facilitate computation. We develop an efficient persistence-like algorithm to compute a connection matrix from a given combinatorial (multi) vector field on a simplicial complex. This algorithm requires a single-pass, improving upon a known algorithm that runs an implicit recursion executing two-passes at each level. Overall, the new algorithm is more simple, direct, and efficient than the state-of-the-art. Because of the algorithm's similarity to the persistence algorithm, one may take advantage of various software optimizations from topological data analysis.

1 Introduction

Connection matrix theory, originally developed by R. Franzosa [11, 12] as a tool for proving the existence of heteroclinic connections in dynamical systems, is a generalization of homological Morse theory in the setting of the Conley index theory [2]. Specifically, the connection matrix is the boundary operator in a chain complex constructed from Conley indices of Morse sets in a Morse decomposition of an isolated invariant set of a flow acting on a metrizable topological space. The topological space replaces the smooth manifold in the classical Morse theory, the flow replaces the gradient vector field, the Morse decomposition replaces the Morse function, and the individual Morse sets replace the critical points. The theory has found many applications, in particular in the study of ODEs and PDEs. For some early and very recent applications, see [22] and [14, 21] respectively and references therein.

Similar to the early Conley theory, the development of applications of connection matrices has been delayed by the limitation of manual, analytic calculations. The applicability of Conley theory rapidly changed about twenty years ago due to the development of modern, efficient homology algorithms. However, computation of connection matrices required more specialized algorithms. The first such algorithm, henceforth referred to as HMS algorithm, was presented in a recent paper by S. Harker, K. Mischaikow and K. Spendlove [13]. In this paper, connection matrices are studied from a computational point of view via a partially algebraic and partially geometric formulation based on a simplification of the theory for field coefficients presented by J. Robin and D. Salamon in [25].

As pointed out by Harker, Mischaikow and Spendlove in [13], developing an efficient computational framework for the connection matrix theory is particularly important in the context of the rapidly growing field of data science. Classical mathematical models, based on differential equations, are not adequate to deal with data for which the equations cannot be built from some first principles, like in physics, and more direct approaches are needed to address problems in dynamically changing data.

Among such approaches is the theory developed by R. Forman, which concerns dynamical systems that are generated by combinatorial vector fields [9, 10]. Recently, various authors have shown that

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the Conley theory holds in the more general setting of dynamical systems generated via combinatorial multivector fields [5, 6, 17, 20, 24, 23].

Harker, Mischaikow, and Spendlove first observed links between connection matrices and persistent homology [13]. A connection matrix may be viewed as a reduced matrix of a reduced filtered complex. In [13], the authors observed that that a certain construction of a gradient Forman vector field \mathcal{V} consistent with the given Morse decomposition reduces the problem of constructing connection matrix for a smaller complex unless \mathcal{V} consists only of critical cells. In the latter case the connection matrix is just the matrix of the boundary operator in the reduced complex. Hence, to compute the connection matrix they iteratively execute two-passes, one reducing the complex (called MATCHING in [13]) and another computing a boundary operator of this reduced complex (called GAMMA in [13]) until no more reductions are possible. In a sense, they operate *recursively* starting all over again on the reduced complexes.

The partial geometric flavor of HMS algorithm is due to the fact that the Forman vector field used to reduce the problem is constructed on the original basis acting as the phase space for the combinatorial dynamics. This helps guiding the intuition but results in the need of an implicit recursion executing two passes. In our algorithm we adopt this overall reduction approach while making it more efficient. In particular:

- 1. Analogous to the matrix based persistence algorithm [8], our algorithm requires no recursive behavior as in [13]. It makes a single pass over the filtered input matrix and performs column additions that implicitly execute the reductions simultaneously at both the complex and homology level. Then, the algorithm obtains the connection matrix by simply removing certain rows and columns. A key observation that facilitates this single pass execution is that reductions within Morse sets and across Morse sets, unlike in HMS algorithm, can be combined with suitable basis changes.
- 2. Like the persistence algorithm, for a multivector field on a simplicial complex comprising n simplices, our single pass matrix based algorithm runs in $O(n^3)$ time whereas the recursive HMS algorithm runs in $O(n^4)$ time as far as we can analyze (no time complexity analysis is given in [13]). Again, the advantage ensues from embedding the homology computation into the reduction phase.
- 3. The need of implicit recursion in HMS algorithm is closely related to the problem of the existence of a perfect Morse function that is a Morse function whose number of *n*-dimensional critical cells equals the *n*th Betti number of the complex. In general, a perfect Morse function may not exist. For instance, a Morse set or multivector in [23, Figure 5] has all Betti numbers zero but requires at least two critical cells in a gradient Forman vector field. Also, finding a constant-factor approximation of Morse function which minimizes the number of critical cells is NP-hard [19]. We avoid this problem entirely by not forcing the algorithm to run on a fixed basis. In that sense, analogous to the persistence algorithm, our algorithm is purely algebraic.
- 4. Our single pass persistence-like algorithm can take advantage of different optimizations that have been proposed to accelerate the persistence algorithm in TDA, e.g. [1, 3, 7, 18, 26].

2 Background and overview

2.1 Connection matrix

Connection matrices are a generalization of Morse boundary operators in classical Morse theory for gradient vector fields. They represent the connections between Morse sets in the dynamics using homological algebra.

The Conley index of a Morse set M encapsulates the behavior of the local dynamics in terms of the homology group of M relative to its exit set. In particular, it differentiates between repellers, attractors and saddles. Connection matrices, on the other hand, capture the dynamics at the global level by indicating the existence of connecting trajectories between Morse sets. In this sense, it is a useful invariant of the complete dynamics given by the input combinatorial vector field. Loosely speaking, if $H(M_p, E_p)$ denotes the Conley index for a Morse set M_p , that is, the homology group of M_p relative to the exit set E_p , then a connection matrix represents a boundary operator

$$\Delta: \bigoplus_{p \in P} H(M_p, E_p) \to \bigoplus_{p \in P} H(M_p, E_p).$$



Figure 1: (left) A continuous vector field, (middle) its discretization with Forman vectors, (right) and its Conley complex represented with 5 cells and their incidence structure.

Alternatively, a connection matrix can be viewed as a simplification of the vector field producing what is called a Conley complex which is a generalization of the Morse complex studied in Morse theory. It embodies the essential dynamics by coalescing the trivial Morse sets into larger invariant sets with a homotopy. See e.g. Figure 1 where a vector field with two repellers, one saddle, and one attracting orbit is simplified with five cells, two 2-cells representing two 2-dimensional repellers, one 1-cell representing the saddle, and another 1-cell together with a 0-cell representing the attracting orbit. The continuous vector field shown in left may be discretized with a combinatorial vector field on a simplicial complex. Conley complex essentially simplifies this input complex to a cell complex while preserving the Morse sets. Depending on how the input boundary operator at the chain level of the simplicial complex is provided for the Morse decomposition, the homotopy-induced simplification can be different resulting in different Conley complexes. In Figure 1, these different Conley complexes indicate the fact that the system, while preserving the Morse sets, may be deformed by breaking the attracting periodic orbit into an attracting stationary point and a saddle. This extra saddle may be reached from only one of the two repellers. Depending on whether this is the right or the left repeller, we get two different Conley complexes. See, for example, two Conley complexes in Figure 2 (right). Corresponding to these two Conley complexes, we have two different connection matrices shown in Figure 3.

2.2 Combinatorial multivector field and Morse decomposition

In this subsection, we introduce some of the basic definitions from combinatorial (multi)vector field theory that are necessary for this work; see [4, 5, 20, 23] for more details. Throughout this paper, we restrict our attention to simplicial complexes of arbitrary but finite dimension. For a simplicial complex K, we use \leq to denote the face relation, that is, $\sigma \leq \tau$ if σ is a face of τ . We define the *closure* $cl(\sigma)$ of σ as $cl(\sigma) := \{\tau \mid \tau \leq \sigma\}$ and we extend the notion to a set of simplices $A \subseteq K$ as $cl(A) := \bigcup_{\sigma \in A} cl(\sigma)$. The set A is *closed* if A = cl(A).

Definition 2.1 (Multivector and multivector field). Given a finite simplicial complex K, a multivector $V \subset K$ is a subset that is convex under face-poset relation, that is, if $\sigma, \tau \in V$ with $\sigma \leq \tau$ then every simplex μ with $\sigma \leq \mu \leq \tau$ is in V. A multivector field \mathcal{V} on K is a partition of K into multivectors.

Following [20], a notion of dynamics on a combinatorial multivector field can be introduced. These dynamics take the form of a multivalued map $F_{\mathcal{V}}$: $K \multimap K$, with $F_{\mathcal{V}}(\sigma) = [\sigma]_{\mathcal{V}} \cup cl(\sigma)$ where $[\sigma]_{\mathcal{V}} \subset K$ is the unique element of the partition \mathcal{V} containing σ . A finite sequence of simplices $\sigma_1, \sigma_2, \ldots, \sigma_n$ is a *path* if for $i = 2, \ldots, n$, we have $\sigma_i \in F_{\mathcal{V}}(\sigma_{i-1})$.

Definition 2.2 (Morse sets and decomposition). Given a multivector field \mathcal{V} on a finite simplicial complex K, a subset $M \subseteq K$ is called a *Morse set* if for every path $\sigma_1, \sigma_2, \ldots, \sigma_n$ in K with $\sigma_1, \sigma_n \in M$, each $\sigma_i, i \in \{1, \ldots, n\}$ is necessarily in M. A collection of Morse sets $\mathcal{M} = \{M_p \mid p \in P\}$ indexed by a poset (P, \leq) is called a *Morse decomposition* of \mathcal{V} if we have the disjoint union $K = \sqcup_{p \in P} M_p$ and $p \leq q$ if and only if there is a path $\sigma_1, \ldots, \sigma_n$ with $\sigma_1 \in M_p$ and $\sigma_n \in M_q$.

An astute reader will recognize that the Morse decomposition defined here differs slightly from the earlier definitions introduced in [4, 6, 20]. Definition 2.2 liberates us from a need of introducing additional concepts such as the invariant part Inv M of a Morse set M, thereby simplifying the presentation of the algorithm. Nevertheless, the Morse decomposition in the sense of previous works can be easily retrieved by taking $\mathcal{M}' := \{ \operatorname{Inv} M_p \mid p \in P \}$ (see e.g. [20] for the precise definition of the combinatorial invariance). In particular, Definition 2.2 lets us incorporate trivial Morse sets into the structure, i.e. sets $M \in \mathcal{M}$ such that $\operatorname{Inv} M = \emptyset$.



Figure 2: (left) Vector field $\mathcal{V} = \{\{A, AB\}, \{B, BC\}, \{C, CD\}, \{D, DA\}, \{CA\}, \{ABC\}, \{CDA\}\},$ (middle) A Morse decomposition consisting of 4 Morse sets, triangles CDA, ABC, edge CA, and the orbit $\{\{A, AB\}, \{B, BC\}, \{C, CD\}, \{D, DA\}\}$, (right) Two Conley complexes; the left one corresponds to a connection matrix shown in Figure 3 (top) and the right one corresponds to a connection matrix shown in Figure 3 (bottom).

2.3 Overview of the algorithm

Let \mathcal{V} be a multivector field defined on a simplicial complex K. The algorithm takes the boundary operator $\partial_K : C_*(K) \to C_*(K)$ in matrix form, where the matrix is filtered according to a Morse decomposition of \mathcal{V} . This means that if M_i and M_j are two Morse sets with i < j, then simplices in the Morse set M_i necessarily come before those in the Morse set M_j in the columns ordered from left to right. A Morse decomposition can be obtained from \mathcal{V} by computing strongly connected components in a directed graph constructed as follows. Each simplex $\sigma \in K$ is represented as a node in the graph and a directed edge goes from a node σ to a node τ if and only if $\tau \in F_{\mathcal{V}}(\sigma)$. It is known that the strongly connected components in this graph constitute what are called the *minimal Morse* sets [Theorem 4.1,[4]]. We do not elaborate on this aspect any further as this is not the focus of this paper, and we assume that the matrix ∂_K is given.

We perform column additions (source column added to a target column) respecting the filtration to arrive at a reduced matrix which is analogous to the persistence algorithm; see Algorithm CONNECTMAT in Section 4. However, there are crucial differences in reducing the matrix and in outputting the result. For reductions the differences are: (i) column additions are performed not only to resolve conflicts at the lowest non-zero entries, but also if the target column has a conflict for other entries with the lowest entry of the source column, (ii) source columns are always to the left of the target column across Morse sets, but there is no such restrictions within a Morse set, (iii) a source column triggers a conflict only if it is *homogeneous*, that is, its lowest entry comes from a simplex that is in the same Morse set.

In Figure 3, we show the boundary operator filtered according to the Morse decomposition in Figure2(left). It is represented by two matrices which differ only in the order of cells within the Morse sets. We describe the working of our algorithm on the matrix shown in top row. The column AB is added to column BC because of the conflict in the row B even though it does not contain the lowest 1 in column BC. Similarly, column BC is added to column CD because of a conflict in row C and the column CD is added to DA because of a conflict in row D. All these additions happen within the same Morse set. Next addition happens between columns BC and CA which belong to different Morse sets, but the addition is allowed because the lowest entry for BC represents the simplex C which belongs to the same Morse set as BC. The column ABC does not trigger any conflict. The final column CAD has a conflict with the lowest entry in column ABC. However, ABC is not added to CAD because it is not homogeneous since its lowest entry representing the simplex CA in ABC does not come from the same Morse set.

The other main departure from the classical persistence algorithm is in the way we output the result which is not the entire reduced matrix but only a submatrix. A column in the reduced matrix is called *targetable* if its simplex appears as a lowest entry in a homogeneous column. For example, the columns B, C, D are targetable as they appear as the lowest entry in the homogeneous columns AB, BC, and CD respectively. All homogeneous and targetable columns and their corresponding



Figure 3: Working of the algorithm on two different boundary matrices for the example in Figure 2, computed connection matrices are shown on right.

rows are eliminated from the output. The resulting 5×5 connection matrix is shown which represents the dynamics depicted in the Conley complex shown in Figure 2 (right). The column for CDA in the connection matrix has two 1's in rows CA and DA signifying that the dynamics flow from the repeller triangle CDA to the existing saddle edge CA and the new saddle edge DA rising from breaking the attracting periodic orbit. Similarly, the column ABC has a single 1 in row CA but no 1 in row DAindicating that dynamics can flow from the triangle ABC only to the repeller edge CA.

Applying the same algorithm on the boundary matrix shown in the bottom row, we arrive at a different connection matrix. Observe the difference in the entries for columns ABC and CDA which corresponds to the difference in the Conley complexes shown in Figure 2.

3 Algebraic formulation

Although connection matrices were constructed by R. Franzosa in [11, 12] as a tool facilitating the detection of heteroclinic connections between invariant sets of dynamical systems, they may be decoupled from dynamics, defined purely algebraically and studied as a part of homological algebra. A formal setting is that the input multivector field \mathcal{V} as a partition of a simplicial complex K is presented with a Morse decomposition. This decomposition is viewed as a *chain complex* with a *boundary map* that is *filtered* with a poset $\mathbb{P} = (P, \leq)$ over which the Morse decomposition is supported. This input chain complex is successively converted to other chain complexes, the last one being the source of a Conley complex. Successive chain complexes are always kept connected with isomorphic *chain maps* presented as matrices w.r.t. some appropriate bases. The Conley complex is extracted from the last chain complex by an implicit chain homotopy that is implemented by a simple removal of a coefficient for each individual simplicial complex in the *filtered chain complexes*, we obtain *graded vector spaces* connected by *filtered linear maps* induced by chain maps. Our algebraic framework builds on these concepts/objects, which have been used in earlier works in the context of connection matrix [14, 24].

Before presenting this formal, purely algebraic definition of connection matrix, we present some general assumptions, notations, and some basic facts from homological algebra.

3.1 Algebraic preliminaries

Throughout the paper we consider only finite dimensional vector spaces over the field \mathbb{Z}_2 and matrices with \mathbb{Z}_2 entries. Let V be an n-dimensional vector space over \mathbb{Z}_2 . Set $\mathbb{I}_n := \{1, 2, ..., n\}$. Since in the paper the order of vectors in a basis $B = \{b_1, b_2, \ldots, b_n\}$ of V matters, we consider the basis as a map $b : \mathbb{I}_n \ni i \mapsto b_i \in V$. Given a basis B, we denote the associated scalar product by $\langle \cdot, \cdot \rangle$. More precisely, $\langle \cdot, \cdot \rangle$ is the bilinear form $C_q \times C_q \to \mathbb{Z}_2$ defined on generators $b, b' \in B$ by $\langle b, b' \rangle = 1$ if b = b'and 0 otherwise. An example of an *n*-dimensional vector space over \mathbb{Z}_2 is the coordinate space \mathbb{Z}_2^n . The *canonical basis* $\mathbf{E}_n = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$ consists of vectors \mathbf{e}_i in which all coordinates except the *i*th are zero.

Given a matrix A, we denote its *i*th row by $A[i, \cdot]$, its *j*th column by $A[\cdot, j]$ and its entry in *i*th row and *j*th column by A[i, j]. By $low_A(j)$ we denote the row index of the lowest 1 in $A[\cdot, j]$ if the column is nonzero and we set $low_A(j) = 0$ otherwise. If $i := low_A(j)$ is defined, we say that column $A[\cdot, i]$ is the *target* of column $A[\cdot, j]$.

Let V' be an n'-dimensional vector space over \mathbb{Z}_2 with basis $B' = \{b'_1, b'_2, \ldots, b'_{n'}\}$. Given a linear map $h: V \to V'$, its matrix in bases B and B' is the matrix (h_{ij}) where

$$h_{ij} := \langle hb_j, b'_i \rangle \text{ for } i \in \mathbb{I}_{n'} \text{ and } j \in \mathbb{I}_n.$$

$$\tag{1}$$

Conversely, given a \mathbb{Z}_2 -matrix $A = (a_{ij})$ with n' rows and n columns we have a linear map $h_{B,A,B'}$: $V \to V'$ defined on basis $B = \{b_1, b_2, \ldots, b_n\}$ by $h_{B,A,B'}(b_j) := \sum_{i=1}^{n'} a_{ij}b'_i$. Then, clearly, A is the matrix of $h_{B,A,B'}$. If bases B and B' are clear from context, we adopt the simplified notation h_A .

Given a fixed basis B of V, we identify V with the coordinate space \mathbb{Z}_2^n via isomorphism h_{B,I_n,\mathbf{E}_n} where I_n denotes an $n \times n$ identity matrix. Under this identification, composition of linear maps corresponds to multiplication of matrices.

We recall (see, for instance, [15, Section 3.1]) that for $1 \le i < j \le n$ the operation of adding *i*th column to *j*th column followed by adding *j*th row to *i*th row in an $n \times n \mathbb{Z}_2$ -matrix A results in a new matrix A' such that

$$E_{i,j}A' = AE_{i,j} \tag{2}$$

where $E_{i,j}$ (illustrated below) is the sum of the identity matrix and the matrix whose all entries are zero except a one in *i*th row and *j*th column. We call it the *column/row addition* matrix.



We recall that a *chain complex* with \mathbb{Z}_2 coefficients is a pair (C, d) where $C = \bigoplus_{q \in \mathbb{Z}} C_q$ is a \mathbb{Z}_2 vector space with gradation $C = (C_q)_{q \in \mathbb{Z}}$ and $d : C \to C$ is a linear map satisfying $d(C_q) \subset C_{q-1}$ and $d^2 = 0$. Given another such chain complex (C', d'), a *chain map* $\varphi : (C, d) \to (C', d')$ is a linear map such that $\varphi(C_q) \subset C'_q$ and $d'\varphi = \varphi d$. A chain map is a *chain isomorphism* if it is an isomorphism as a linear map. Two chain maps $\varphi, \psi : (C, d) \to (C', d')$ are *chain homotopic* if there exists a linear map $S : C \to C'$ satisfying $S(C_q) \subset C'_{q+1}$ and $\psi - \varphi = d'S + Sd$. Such an S is called a *chain homotopy*. Two chain complexes (C, d), (C', d') are *chain homotopic* if there exist chain maps $\varphi : (C, d) \to (C', d')$ and $\psi : (C', d') \to (C, d)$ such that $\psi \varphi$ is chain homotopic to id_C and $\varphi \psi$ is chain homotopic to $\mathrm{id}_{C'}$. In what follows, we consider only finite dimensional chain complexes that allow us to work with finite bases.

3.2 Algebraic connection matrices

Let P be a finite set. By a P-gradation of a finite dimensional \mathbb{Z}_2 -vector space V we mean the collection $\{V_p \mid p \in P\}$ of subspaces of V such that $V = \bigoplus_{p \in P} V_p$. We call such a vector space with a given P-gradation a P-graded vector space. We say that basis $B = \{b_1, b_2, \ldots, b_n\}$ is P-graded if $B \subset \bigcup_{p \in P} V_p$. Note that for each basis vector $b_i \in B$ there is exactly one $p \in P$ such that $b_i \in V_p$. We denote this p by $gr_P(b_i)$. Clearly, every P-graded vector space admits a P-graded basis.

Given a *P*-graded vector space $V = \bigoplus_{p \in P} V_p$ we denote by $\iota_q^V : V_q \to V$ and $\pi_p^V : V \to V_p$ respectively the inclusion and projection homomorphisms. Given another *P*-graded vector space

 $V' = \bigoplus_{p \in P} V'_p$ we identify linear map $h: V \to V'$ with the matrix $[h_{pq}]_{p,q \in P}$ of partial linear maps $h_{pq}: V_q \to V'_p$ where $h_{pq}:=\pi_p^{V'} \circ h \circ \iota_q^V$. Consider now a fixed finite poset $\mathbb{P}:=(P,\leq)$ and a linear map $h: V \to V'$. We say that h is

 \mathbb{P} -filtered or briefly filtered when \mathbb{P} is clear from the context if

$$h_{pq} \neq 0 \Rightarrow p \le q. \tag{3}$$

The following proposition is straightforward.

Proposition 3.1. If h is \mathbb{P} -filtered then it is \mathbb{P}' -filtered for any poset $\mathbb{P}' = (P, \leq')$ with partial order <' extending <.

Given a fixed P-graded basis B of V and B' of V', we say that an $n' \times n$ matrix A is P-filtered w.r.t. B, B' or briefly *filtered* when \mathbb{P} , B and B' are clear from the context and if the linear map $h_A: V \to V'$ is P-filtered. One can easily verify the following proposition.

Proposition 3.2. The product of \mathbb{P} -filtered matrices is \mathbb{P} -filtered and the inverse of an invertible \mathbb{P} -filtered matrix is \mathbb{P} -filtered.

By a \mathbb{P} -filtered chain complex we mean a chain complex (C, d) with field coefficients and a given gradation $C = \bigoplus_{p \in P} C_p$ such that the boundary homomorphism d is \mathbb{P} -filtered. Given another \mathbb{P} filtered chain complex (C', d') we define a \mathbb{P} -filtered chain map $\varphi : (C, d) \to (C', d')$ as a chain map which is also P-filtered as a homomorphism. One can easily check that a composition of filtered chain maps is a filtered chain map. We say that φ is a filtered chain isomorphism if it is a filtered chain map which is also an isomorphism. Note that trivially the identity homomorphism on (C, d), denoted id_C , is a filtered chain isomorphism. Two filtered chain complexes (C, d) and (C', d') are filtered chain isomorphic if there exist filtered chain maps $\varphi: (C,d) \to (C',d')$ and $\varphi': (C',d') \to (C,d)$ such that $\varphi' \circ \varphi = \mathrm{id}_C$ and $\varphi \circ \varphi' = \mathrm{id}_{C'}$.

Two filtered chain maps $\varphi, \varphi' : (C, d) \to (C', d')$ are said to be *filtered chain homotopic* if there exists a chain homotopy joining φ with φ' which is also filtered as a homomorphism. Two filtered chain complexes (C, d) and (C', d') are filtered chain homotopic if there exist filtered chain maps $\varphi: (C,d) \to (C',d')$ and $\varphi': (C',d') \to (C,d)$ such that $\varphi' \circ \varphi$ is filtered chain homotopic to id_C and $\varphi \circ \varphi'$ is filtered chain homotopic to $\mathrm{id}_{C'}$.

Following [13, 24] we define Conley complex of a filtered chain complex (C, d) as any filtered chain complex $(\overline{C}, \overline{d})$ which is filtered chain homotopic to (C, d) and satisfies $\overline{d}_{pp} = 0$ for all $p \in \mathbb{P}$. The following theorem may be easily obtained as a consequence of results in [25, Theorem 8.1, Corollary 8.2] and [13, Proposition 4.27].

Theorem 3.1. For every finitely generated chain complex (C, d) there exists a Conley complex and any two Conley complexes of (C, d) are filtered chain isomorphic.

Theorem 3.1 lets us define a *connection matrix* of (C, d) as the matrix of homomorphisms $[d_{pq}]_{p,q \in \mathbb{P}}$ for any Conley complex (\bar{C}, \bar{d}) of (C, d). We note that each homomorphism in the connection matrix is represented itself as a matrix. Moreover, this matrix is often 1×1 matrix, consisting of just one number, which is the case in our setting.

Algorithm 4

In this section we present algorithm CONNECTMAT which computes a connection matrix of a filtered chain complex (C, d). The algorithm has a reduction phase followed by a simple extraction step whose correctnesses are argued in subsections 4.1 and 4.2 respectively.

4.1Reductions

We need to choose a special basis of C, given by the following definition.

Definition 4.1. We say that a \mathbb{P} -graded basis B of chain complex (C, d) is d-admissible if there exists an extension of the partial order $\leq in \mathbb{P}$ to a linear order \leq_{lin} such that

$$i \leq j \Rightarrow \operatorname{gr}_{\mathsf{P}}(\mathsf{b}_{\mathsf{i}}) \leq_{lin} \operatorname{gr}_{\mathsf{P}}(\mathsf{b}_{\mathsf{i}}) \text{ for } i, j \in \mathbb{I}_{n}.$$
 (4)

and the matrix A of the boundary operator d in this basis is strictly upper triangular, i.e.,

$$A[i,j] \neq 0 \implies i < j. \tag{5}$$

As an immediate consequence of (4) we get that for every d-admissible basis B

$$\operatorname{gr}_{\mathsf{P}}(\mathsf{b}_{\mathsf{i}}) < \operatorname{gr}_{\mathsf{P}}(\mathsf{b}_{\mathsf{j}}) \Rightarrow \mathsf{i} < \mathsf{j}.$$
 (6)

Proposition 4.1. Filtered Chain complex (C, d) admits a d-admissible basis.

Proof: A linear extension of \leq always exists. Arbitrarily fix one and set $\mathbb{P}_{\text{lin}} := (P, \leq_{\text{lin}})$. Let *B* be a \mathbb{P} -graded basis of *C*. By reordering its elements we can assure that (4) is satisfied. Then (5) follows from (6) if $\text{gr}_{\mathsf{P}}(\mathsf{b}_i) \neq \text{gr}_{\mathsf{P}}(\mathsf{b}_j)$ and when $\text{gr}_{\mathsf{P}}(\mathsf{b}_i) = \text{gr}_{\mathsf{P}}(\mathsf{b}_j)$, (5) may be achieved by a suitable rearrengement of basis elements with the same grade.

In the sequel we assume that B is a fixed d-admissible basis of chain complex (C, d) and $\mathbb{P}_{\text{lin}} := (P, \leq_{\text{lin}})$ stand for the associated linear extension of poset \mathbb{P} . It follows from (5) that

$$low_A(j) < j \text{ for all } j \in \mathbb{I}_n.$$

$$\tag{7}$$

Algorithm 1: CONNECTMAT
Data: An $n \times n$ matrix A of a filtered boundary homomorphism d
Result: A connection matrix
1 for $j := 1$ to n do
2 for $i := low_A(j)$ down to 1 do
3 $s := 0;$
4 if $A[i, j] = 1$ then
5 S := { $s \in \mathbb{I}_n \mid \mathbf{s} \neq \mathbf{j} \& \log_{\mathbf{A}}(s) = i \& \mathbf{A}[\cdot, \mathbf{s}] \text{ is homogeneous } ;$
$6 \mathbf{if} \ S \neq \varnothing \ \mathbf{then}$
$7 \mathbf{s} := \min S;$
8 add column $A[\cdot, \mathbf{s}]$ to column $A[\cdot, \mathbf{j}];$
9 add row $A[j, \cdot]$ to row $A[s, \cdot] /*$ needed only to prove correctness $*/$;
10 $J := \mathbb{I}_n \setminus J_h(\mathbb{A}) \setminus J_t(\mathbb{A});$
11 return A restricted to columns and rows with indices in J

The algorithm CONNECTMAT computing a connection matrix of \mathbb{P} -filtered chain complex (C, d) is presented in Algorithm 1. In order to explain the algorithm and discuss its features we first make some assumptions and introduce some notation. We assume that CONNECTMAT takes on input a filtered matrix A of the boundary homomorphism d in a fixed d-admissible basis $B = \{b_1, b_2, \ldots b_n\}$. We denote the associated linear extension of the partial order in \mathbb{P} by \leq_{lin} . As we already mentioned in Section 3, fixing basis B lets us identify (C, d) with (\mathbb{Z}_2^n, A) where n is the dimension of C and A is the matrix of the boundary homomorphism d in basis B. For $i \in \mathbb{I}_n$ we set $\nu(i) := \operatorname{gr}_{\mathsf{P}}(\mathsf{b}_i)$. By (4) we have

$$i \le j \Rightarrow \nu(i) \le_{\text{lin}} \nu(j) \text{ for } i, j \in \mathbb{I}_n.$$
 (8)

We call a column j of matrix A homogeneous if it is nonzero and $\nu(j) = \nu(\log_A(j))$. We call a column j targetable if it is a target of a homogeneous column. We denote the set of homogeneous and targetable columns of A respectively by $J_h(A)$ and $J_t(A)$.

Let K be the number of times the inner **for** loop is executed by the algorithm. Clearly, K is finite. Let $\mathbf{A} = A_0$ be the initial matrix before entering the **for** loop and $\mathbf{A} = A_k$ be the matrix after the kth execution of the inner **for** loop for k = 1, 2, ..., K. Let i_k , j_k and s_k denote the corresponding values of the variables \mathbf{i} , \mathbf{j} and \mathbf{s} respectively. Let $d_k := h_{A_k}$ and set $E_k := E_{s_k, j_k}$ if $s_k \neq 0$ and the identity matrix otherwise. We get from (2) that for k = 1, 2, ..., K

$$A_k = E_k^{-1} A_{k-1} E_k. (9)$$

Proposition 4.2. For every $k \in \mathbb{I}_N$ matrices A_k and E_k are filtered. Moreover, (C, d_k) is a filtered chain complex which is filtered chain isomorphic to (C, d).

Proof: Clearly, $A_0^2 = 0$, because A_0 equals the matrix on input which is the matrix of a boundary operator. Therefore, by induction argument we get $A_k^2 = E_k^{-1}A_{k-1}^2E_k = 0$ which shows that $d_k = h_{A_k}$ is a boundary operator. Moreover, we get from (9) that $e_k := h_{E_k}$ is a chain map and by definition it is an isomorphism from (C, d_{k-1}) to (C, d_k) . Therefore, it is a chain isomorphism.

We will prove by induction on k that A_k is filtered. Again, A_0 as the matrix on input is filtered. Assume A_{k-1} is filtered for some k satisfying $1 \le k \le K$. We first show that E_k is filtered. To this end assume that $(h_{E_k})_{pq} \ne 0$ for some $p, q \in \mathbb{P}$. In view of the structure of matrix E_k either $(h_{E_k})_{pq}$ contains a diagonal entry which immediately implies p = q, or it contains the unique off-diagonal nonzero entry in s_k th row and j_k th column. Consider the latter case. Then $p = \nu(s_k)$ and $\nu(j_k) = q$. Since variable **A** is modified, the condition in the **if** statement is satisfied and the properties of the set **S** hold. Hence, we have $A_{k-1}[i_k, j_k] = 1$ and $\log_{A_{k-1}}(s_k) = i$. We also know that column s_k is homogeneous. Since A_{k-1} is filtered by induction assumption, we get $\nu(i_k) \le \nu(j_k)$. Combining all these properties we get

$$p = \nu(s_k) = \nu(\log_{A_{k-1}}(s_k)) = \nu(i_k) \le \nu(j_k) = q.$$

Hence, in both bases we get $p \leq q$, which proves that E_k is filtered and in view of Proposition 3.2 we get from (9) that A_k is filtered. Thus, we have filtered chain complexes (C, d_k) for $k = 0, 1, \ldots, K$ and all these chain complexes are filtered chain isomorphic.

Proposition 4.3. For every $j \in \mathbb{I}_n$ the *j*th column of matrix **A** does not change after completing the *j*th pass of the outer **for** loop.

Proof: Fix a $j \in \mathbb{I}_n$. Note that the only modifications of matrix **A** happen in the addition of columns and rows inside the inner **for** loop. Consider column and row additions on *k*th pass of the outer **for** loop with k > j. Clearly, column additions modify *k*th column but not *j*th column. A row addition on *k*th pass of the outer **for** loop adds *k*th row to another row. Note that by (7) we have $\log_A(j) < j < k$. Therefore, A[k, j] = 0, which means that such an addition of rows cannot modify *j*th column as well.

Proposition 4.4. The value of A[i, j] settled after completing the inner for loop with the index variables i = i and j = j remains unchanged till the end of the algorithm.

Proof: Assume by contrary that such a change happens on the pass of the inner **for** loop when j = j' and i = i'. By Proposition 4.3 we must have j' = j and since the inner **for** loop which is a downwards loop, we have i' < i. The change of A[i, j] may happen only via addition of columns or rows inside **if** statement. Therefore, for some s', we have $low_A(s') = i' < i$, which implies A[i, s'] = 0. In consequence, addition of column $A[\cdot, s']$ to $A[\cdot, j]$ cannot change A[i, j]. Addition of row $A[j, \cdot]$ to $A[s', \cdot]$ can change A[i, j] only if s' = i and A[j, j] = 1 which clearly is not the case. This contradiction proves our claim.

Proposition 4.5. For every $j \in \mathbb{I}_n$ after completing *j*th pass of the outer **for** loop if A[i, j] = 1 for some $i \leq low_A(j)$, then there is no homogeneous column $A[\cdot, s]$ with $s \neq j$ and $low_A(s) = i$.

Proof: Assume on the contrary that for some $j \in \mathbb{I}_n$ after completing *j*th pass of the outer for loop there is an $i \leq \log_A(j)$ such that A[i, j] = 1 and a homogeneous column $A[\cdot, s]$ with $s \neq j$ and $\log_A(s) = i$. Consider the value of A[i, j] immediately before entering the inner for loop with index variables $\mathbf{i} = i$ and $\mathbf{j} = j$ for the inner and outer for loops respectively. We claim that regardless of the value of A[i, j], we have A[i, j] = 0 after completing this pass of the inner for loop. Indeed, if the initial value is zero, then the condition of **if** statement is not satisfied. Consequently, A[i, j] is not modified and remains zero after completing the inner for loop with $\mathbf{i} = i$. If the value is one, then **if** statement is executed and addition of columns modifies A[i, j] to zero. This proves our claim. Now, by Proposition 4.4 the value of A[i, j] is also zero when the *j*th pass of the outer for loop is completed, a contradiction.

We say that a filtered matrix A is *reduced* if it satisfies the following three conditions:

- (R1) the map $\alpha: J_h(A) \ni j \mapsto low_A(j) \in J_t(A)$ is a well defined bijection,
- (R2) $J_h(A) \cap J_t(A) = \emptyset$, and
- (R3) if A[i, j] = 1 for some $i \leq low_A(j)$, then there is no $s \in J_h(A)$ with $s \neq j$ and $low_A(s) = i$.

Proposition 4.6. Matrix A_K , that is the final state of the variable A, is reduced.

Proof: To simplify the notation, denote by $A := A_K$ the final state of variable A. By definition of $J_t(A)$, the map α is well defined and is a surjection. The fact that it is an injection follows immediately from Proposition 4.5. This proves property (R1).

To prove (R2) assume on the contrary that there is an $i \in J_h(A) \cap J_t(A)$. Then, there is a $j \in J_h(A)$ such that $low_A(j) = i$. Since column j is homogeneous, we have $\nu(i) = \nu(low_A(j)) = \nu(j)$. Let $t := low_A(i)$. Since $i \in J_h(A)$, we have t > 0. Proof of Proposition 4.2 implies that $A^2 = 0$. Thus, we have

$$0 = A^{2}[t, j] = \sum_{s=1}^{n} A[t, s]A[s, j] = \sum_{s=t+1}^{i} A[t, s]A[s, j] = \sum_{s=t+1}^{i-1} A[t, s]A[s, j] + 1,$$

because A[t,s] = 0 for $s \le t$, A[s,j] = 0 for s > i and A[t,i] = 1 = A[i,j]. Hence, there is an s_0 such that $t < s_0 < i$ and $A[t,s_0] = 1 = A[s_0,j]$. In particular, since $A[t,s_0] = 1$, we get from Proposition 4.5 that there is no reducible column $A[\cdot,u]$ such that $low_A(u) = t$. However, $A[\cdot,i]$ is exactly such a column, a contradiction. Finally, property (R3) follows immediately from Proposition 4.5.

We say that a filtered matrix A is cropped if $J_h(A) = \emptyset$. Then, necessarily also $J_t(A) = \emptyset$.

Proposition 4.7. Consider matrix A of the boundary operator d in a fixed d-admissible basis B of filtered chain complex (C,d). If A is cropped, then (C,d) is its own Conley complex and A is a connection matrix of (C,d).

Proof: Clearly (C, d) is filtered chain homotopic to itself. Hence, we only need to check that $d_{pp} = 0$ for $p \in \mathbb{P}$. Assume by contrary that there is a $p \in \mathbb{P}$ such that $d_{pp} \neq 0$. We have $d = h_A$, therefore there are $i, j \in \mathbb{I}_n$ such that $\nu(i) = \nu(j) = p$ and A[i, j] = 1. It follows that the *j*th column of A is nonzero. Since $J_h(A) = \emptyset$, we have $\nu(\operatorname{low}_A(j)) \neq \nu(j)$. We also have $A[\operatorname{low}_A(j), j] = 1$ which gives $\nu(\operatorname{low}_A(j)) \leq \nu(j)$. Therefore, $\nu(\operatorname{low}_A(j)) < \nu(j) = \nu(i)$. We get from (6) that $\operatorname{low}_A(j) < i$. But, from the definition of low_A we have $i \leq \operatorname{low}_A(j)$, a contradiction proving that $d_{pp} = 0$ for $p \in \mathbb{P}$.

4.2 Extracting the connection matrix

Observe that the algorithm outputs the cropped matrix A, which by Proposition 4.7 is a connection matrix of the chain complex (\bar{C}, \bar{d}) where A represents the boundary operator \bar{d} . Now we show that the (\bar{C}, \bar{d}) is filtered chain homotopic to the input chain complex (C, d). This establishes that the output matrix A is the connection matrix of (C, d).

We say that a basis B of a chain complex (C,d) is \mathbb{Z} -graded if $B \subset \bigcup_{q \in \mathbb{Z}} C_q$. Let $B = \{b_1, b_2, \ldots, b_n\}$ be a fixed \mathbb{Z} -graded basis of C. We say that a pair (i_0, j_0) of indexes in \mathbb{I}_n is a reduction pair if $b_{i_0}, b_{j_0} \in B$ are such that $\langle db_{j_0}, b_{i_0} \rangle = 1$. Given a fixed reduction pair (i_0, j_0) denote by \overline{C} the subspace of C spanned by $\overline{B} := B \setminus \{b_{i_0}, b_{j_0}\}$ and consider maps

$$\bar{d}: \bar{C} \ni c \mapsto dc + \langle dc, b_{i_0} \rangle db_{j_0} + \langle dc, b_{j_0} \rangle b_{j_0} \in \bar{C}$$

$$\tag{10}$$

$$\pi: \bar{C} \ni c \mapsto c + \langle c, b_{i_0} \rangle db_{j_0} + \langle c, b_{j_0} \rangle b_{j_0} \in C$$

$$\tag{11}$$

$$\iota: C \ni c \mapsto c + \langle dc, b_{i_0} \rangle b_{j_0} \in \bar{C}$$

$$\tag{12}$$

$$\gamma: C \ni c \mapsto \langle c, b_{i_0} \rangle b_{j_0} \in C.$$
(13)

The following theorem is based on results in [16].

Theorem 4.1. (see [16]) The pair (C, \overline{d}) is a finite dimensional chain complex with coefficients in \mathbb{Z}_2 . Moreover, ι and π are chain maps and γ is a chain homotopy such that

$$\pi\iota = \mathrm{id}_C + d\gamma + \gamma d$$
 and $\iota \pi = \mathrm{id}_{\bar{C}}$.

In particular, chain complexes (C, d) and $(\overline{C}, \overline{d})$ are chain homotopic. We refer to complex $(\overline{C}, \overline{d})$ as the (i_0, j_0) -reduction of complex (C, d).

Proof: The first part of the theorem is a special case of [16, Theorem 1]. The second part is implicitely contained in the proof of [16, Theorem 2]. \Box

Proposition 4.8. Consider a filtered chain complex (C, d) so that the matrix (d_{ij}) of d in a d-admissible basis $B = \{b_1, b_2, \ldots, b_n\}$ is reduced. Let $j_0 \in J_h(A)$ and let $i_0 := \mathsf{low}(j_0)$. Then (i_0, j_0) is a reduction pair. Moreover, if (\bar{C}, \bar{d}) is the (i_0, j_0) -reduction of complex (C, d) as in Theorem 4.1, then the matrices of maps given by formulas (10-13) may be characterized as follows. The matrix (\bar{d}_{ij}) of \bar{d} in base \bar{B} satisfies for $i, j \in \bar{B}$

$$\bar{d}_{ij} = d_{ij}.\tag{14}$$

The matrix (π_{ij}) of π in bases B and \overline{B} satisfies for $i \in \overline{B}$ and $j \in B$

$$\pi_{ij} = \begin{cases} \delta_{ij} & \text{if } j \neq i_0, \\ d_{ij_0} & \text{otherwise,} \end{cases}$$
(15)

where δ_{ij} is zero unless i = j when it is one. The matrix (ι_{ij}) of ι in bases \overline{B} and B satisfies for $i \in B$ and $j \in \overline{B}$

$$\iota_{ij} = \begin{cases} \delta_{ij} & \text{if } i \neq j_0, \\ d_{i_0j} & \text{otherwise.} \end{cases}$$
(16)

The matrix (γ_{ij}) of γ in base B satisfies for $i, j \in B$

$$\gamma_{ij} = \begin{cases} 1 & \text{if } i = j_0 \text{ and } j = i_0, \\ 0 & \text{otherwise.} \end{cases}$$
(17)

Proof: Since $i_0 := low(j_0)$, clearly (i_0, j_0) is a reduction pair. To prove (14) observe that by (1) and (10) we have

$$\bar{d}_{ij} = \langle db_j, b_i \rangle + \langle db_j, b_{i_0} \rangle \langle db_{j_0}, b_i \rangle + \langle db_j, b_{j_0} \rangle \langle b_{j_0}, b_i \rangle = d_{ij} + \langle db_j, b_{i_0} \rangle \langle db_{j_0}, b_i \rangle,$$

because $i \in B$ implies $\langle b_{j_0}, b_i \rangle = 0$. Since $j_0 \in J_h(A)$, we cannot have $d_{i_0j} = \langle db_j, b_{i_0} \rangle \neq 0$, because the matrix d_{ij} of d is reduced. Hence $\langle db_j, b_{i_0} \rangle \neq 0$ and (14) follows.

To prove (15) observe that

$$\pi_{ij} = \langle b_j, b_i \rangle + \langle b_j, b_{i_0} \rangle \langle db_{j_0}, b_i \rangle + \langle b_j, b_{j_0} \rangle \langle b_{j_0}, b_i \rangle = \delta_{ij} + \langle b_j, b_{i_0} \rangle \langle db_{j_0}, b_i \rangle,$$

because $i \in \overline{B}$ implies $\langle b_{j_0}, b_i \rangle = 0$. Hence, if $j \neq i_0$, we get $\langle b_j, b_{i_0} \rangle = 0$ and $\pi_{ij} = \delta_{ij}$. Since $i \neq i_0$, in the case $j = i_0$ we get $\delta_{ij} = 0$ and $\pi_{ij} = \langle db_{j_0}, b_i \rangle = d_{ij_0}$. This proves (15).

To prove (16) observe that

$$\iota_{ij} = \langle b_j, b_i \rangle + \langle db_j, b_{i_0} \rangle \langle b_{j_0}, b_i \rangle$$

Hence, if $i \neq j_0$, we get $\langle b_{j_0}, b_i \rangle = 0$ and $\iota_{ij} = \langle b_j, b_i \rangle = \delta_{ij}$. Since $j \neq i_0$, in the case $i = j_0$ we get $\delta_{ij} = 0$ and $\iota_{ij} = \langle db_j, b_i_0 \rangle = d_{i_0j}$. This proves (16).

Finally, to prove (17) observe that

$$\gamma_{ij} = \langle b_j, b_{i_0} \rangle \langle b_{j_0}, b_i \rangle.$$

Therefore, $\gamma_{ij} = 0$ unless $i = j_0$ and $j = i_0$ when $\gamma_{ij} = 1$. This proves (17).

Proposition 4.9. Under assumptions of Proposition 4.8, the associated (i_0, j_0) -reduction of (C, d), denoted (\bar{C}, \bar{d}) , is a filtered chain complex, filtered chain homotopic to (C, d). Moreover, the matrix of \bar{d} in basis $B \setminus \{b_i, b_j\}$ is precisely the matrix of d with i_0 th and j_0 th columns and rows removed. In particular, it is also reduced.

Proof: We get from Theorem 4.1 that (\bar{C}, \bar{d}) is a chain complex which is chain homotopic to (C, d). To see that (\bar{C}, \bar{d}) is a filtered chain complex, we need to prove that \bar{d} is filtered. For this end assume that $\bar{d}_{pq} \neq 0$ for some $p, q \in P$. Then, there are $i, j \in \mathbb{I}_n$ such that $b_i, b_j \in \bar{B}, \nu(i) = p, \nu(j) = q$, and $\bar{d}_{ij} \neq 0$. Then, by (14), we have $d_{ij} = \bar{d}_{ij} \neq 0$ and, since d is filtered, we get $p = \nu(i) \leq \nu(j) = q$, which proves that \bar{d} is filtered.

To prove that (\bar{C}, \bar{d}) is filtered chain homotopic to (C, d) we only needs to verify that also π , ι and γ are filtered. This follows immediately from formulas (15), (16), (17) and the fact that d is filtered. Finally, formula (14) implies that the matrix of \bar{d} coincides with that of d with i_0 th and j_0 th columns and rows removed. This immediately implies that the matrix of \bar{d} is reduced.

Theorem 4.2. Given an $n \times n$ matrix of a filtered chain complex (C, d) in a fixed d-admissible basis on input, CONNECTMAT outputs a connection matrix of (C, d) in $O(n^3)$ time; the output does not change if row additions in the inner **for** loop are dropped.

Proof: Let A be the final contents of variable A, that is matrix $A := A_K$ and let A be the matrix on output of algorithm CONNECTMAT. First observe that by Proposition 4.2 chain complex (C, h_A) is filtered chain isomorphic to (C, d). By Proposition 4.6 matrix A is reduced. We proceed by induction in the cardinality of $J_h(A)$. If $J_h(A) = \emptyset$, the conclusion follows from Proposition 4.7. If the cardinality of $J_h(A)$ is positive, we first observe that by the definition of reduced matrix and Proposition 4.5 the pair $(low_A(j), j)$ for $j \in J_h(A)$ is an elementary reduction pair. Therefore, by the inductive assumption of Proposition 4.9, CONNECTMAT outputs a connection matrix. The inner for loop runs in $O(n^2)$ time (similar to the persistence algorithm) for all column additions incurring an $O(n^3)$ total time complexity.

Finally, observe that dropping the addition of rows inside the inner for loop modifies only the rows corresponding to homogeneous columns and such rows and columns are removed from the matrix on output. \Box

5 Conclusions

We have presented a simple, direct, single-pass, persistence-like algorithm for computing connection matrices from a given boundary matrix filtered according to a Morse decomposition of a multivector field. Since connection matrices need not be unique in general, it would be interesting to know whether the presented algorithm can be made to produce all possible connection matrices. There is a choice in extending the partial order in \mathbb{P} to the linear order of columns in the filtered matrix, which actually may lead to different connection matrices. It is proven in [24] that, for a Forman gradient field, there is a unique connection matrix. This seems to be related to the fact that each critical Morse set in such a field consists of a single simplex (single column) thus leaving no choice for reductions.

Now that we have a persistence-like algorithm for connection matrices, can we extend it for persistence of connection matrices across fields? We plan to address these questions in future work.

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