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► **To cite this version:**

Sammy Khalife, Yann Ponty, Laurent Bulteau. Sequence graphs realizations and ambiguity in language models. COCOON 2021 - 27th International Computing and Combinatorics Conference, Oct 2021, Tainan, Taiwan. hal-02495333v3

**HAL Id: hal-02495333**

**<https://hal.science/hal-02495333v3>**

Submitted on 13 Jan 2021 (v3), last revised 18 May 2023 (v4)

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# Sequence graphs realizations and ambiguity in language models

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## Abstract

Several language models rely on an assumption modeling each local context as a (potentially oriented) bag of words, and have proven to be very efficient baselines. Sequence graphs are the natural structures encoding their information. However, a sequence graph may have several realizations as a sequence, leading to a degree of ambiguity. In this paper, we study such degree of ambiguity from a combinatorial and computational point of view. In particular, we present theoretical results concerning the family of sequence graphs. Several combinatorial problems are presented, depending on three levels of generalisation (window size, graph orientation, and weights), and whether some of these are NP-complete is left opened. We establish different algorithms, including an integer program and a dynamic programming formulation to respectively recognize a sequence graph and to count the number of its distinct realizations. This allows us to show that this model assumption can induce an important number of sentences to have the same representations. We empirically compare the representations obtained with a recurrent neural networks for different realizations of sequence graphs.

**2012 ACM Subject Classification** Mathematics of computing → Combinatoric problems; Mathematics of computing → Combinatorics on words; Mathematics of computing → Graph algorithms; Theory of computation → Complexity classes; Theory of computation → Problems, reductions and completeness

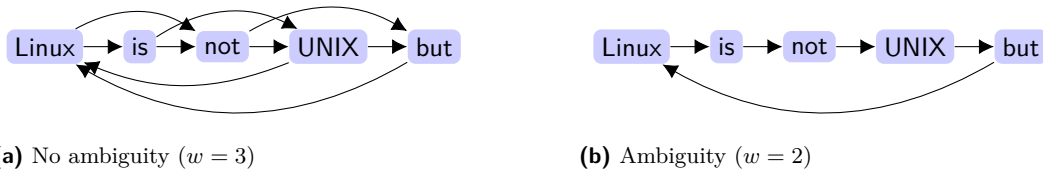
**Keywords and phrases** Graphs, Sequences, Combinatorics, Inverse problem, Complexity class

## 1 Introduction

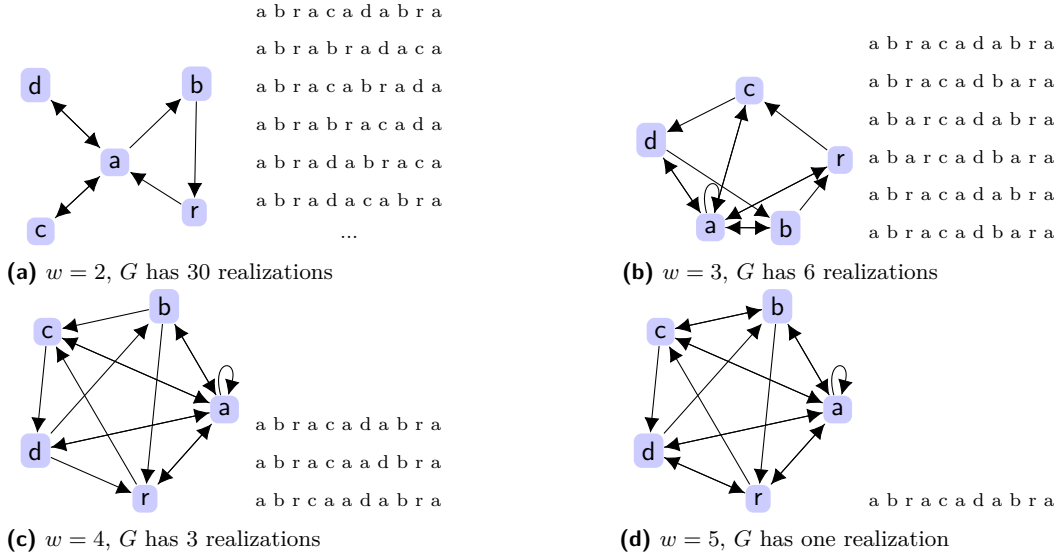
The automated treatment of familiar objects, either natural or artifacts, always relies on a translation into entities manageable by computer programs. However, the correspondence between the object to be treated and "its" representation is not necessarily one-to-one. The representations used for learning algorithms are no exception to this rule. In particular, natural language words and textual documents representations are essential for several tasks, including document classification [23], role labelling [19], and named entity recognition [16]. The traditional models based on pointwise mutual information, or graph-of-words (GOW), [9, 17, 20], supplement the content of bag-of-words (TF, TFIDF) with statistics of co-occurrences within a **window** of fixed size  $w$ , introduced to mitigate the degree of ambiguity. Several models [2, 14, 18, 21] also use the same type of information and constitute strong baselines for natural language processing.

While these representations are more precise than the traditional bag-of-words (e.g Parikh vectors), they still induce some level of ambiguity, *i.e.* a given graph can represent several sequences. Our study is thus motivated by a quantification of the level of ambiguity, seen

## Sequence graphs realizations and ambiguity in language models



■ **Figure 1** Sequence graphs (or *graphs-of-words*) built for the sentence “Linux is not UNIX but Linux” using window sizes 3 (a) and 2 respectively (b). In the second case, the sequence graph is ambiguous, since any circular permutation of the words admits the same representation.



■ **Figure 2** Sequence graphs (or *graphs-of-words*) built for the sentence “a b r a c a d a b r a” using window sizes 2 (a), 3 (b), 4 (c) and 5 (d).

46 as an algorithmic problem, coupled with an empirical assessment of the consequences of  
 47 ambiguity for the representations.

48 After introducing in Section 2 the formal definition of a sequence graph and the descriptions  
 49 of our main problems, we establish in Section 3.1 complexity aspects of deciding the existence  
 50 and counting sequences in GOWs associated with a window size  $w = 2$ . Then we consider  
 51 in Section 3.2 the general case  $w \geq 3$ , and propose a integer program and a dynamic  
 52 programming algorithm to respectively recognize a sequence graph and count admissible  
 53 sequences. Finally, we assess the prevalence of ambiguity within a synthetic dataset, and  
 54 observe that sequences invariant with respect to the GOW representation do not lead to  
 55 invariance with respect to recurrent neural networks such as Long Short Term Memory  
 56 networks (LSTMs).

### 57 Related work

58 Sequence graphs encode the information of several co-occurrences based models [2, 15, 18]. To  
 59 the best of our knowledge, the ambiguity and realizability questions addressed in this work  
 60 were never systematically addressed by prior work in computational linguistics. Furthermore,  
 61 we believe the problems studied in this paper are interesting from an algorithmic point of  
 62 view, and appear to be devoid of reduction to other well-known problems.

63 However, some similarities exist between our problem and others studied in the Distance  
 64 Geometry (DG) literature. In distance geometry, the input consists of a set of pairwise  
 65 distances between points, having unknown positions in a  $d$ -dimensional space. The problem  
 66 then consists in determining (the existence of) a set of positions for the points, satisfying the  
 67 distance constraints. Since a position is fully characterized from  $d + 1$  constraining neighbors,  
 68 the problem can be solved by finding a sequential order for processing points, such that the  
 69 assignment of a point is always by at least  $d + 1$  among its neighbors [13]. This statement  
 70 shares some level of similarity with our problem since an admissible sequence for a window  
 71  $w = d + 2$  also represents a linear ordering of its nodes, in which  $w - 1 = d + 1$  of the  
 72 neighbors have lower value with respect to the order.

73 The reasons for the insufficiency of linear ordering in DG to solve our realizability problem  
 74 are threefold. First, each element of the sequence  $x$  associated to the protein backbone is  
 75 associated a unique vertex. This is not the case we investigate here, since a symbol can be  
 76 repeated several times, but only one vertex is created in the graph. This implies that the  
 77 vertex associated to the  $i^{\text{th}}$  element ( $i \geq w$ ) of  $x$  can have strictly less than  $w - 1$  distinct  
 78 neighbors in its predecessors in  $x$ . Second, the absence of loops in distance geometry, because  
 79 an element is at distance 0 from itself. Finally, the graphs are always undirected in distance  
 80 geometry.

## 81 2 Definitions and problem statement

82 Let  $x = x_1, x_2, \dots, x_p$  be a finite sequence of discrete elements among a finite vocabulary  
 83  $X$ . Without loss of generality, we can suppose that  $X = \{1, \dots, n\}$ . In the following, let  
 84  $I_p = \{1, \dots, p\}$ . This motivates the following definition:

85 ► **Definition 1.**  $G = (V, E)$  is the graph of the sequence  $x$  with window size  $w \in \mathbb{N}^*$  if and  
 86 only if  $V = \{x_i \mid i \in I_p\}$ , and

$$87 \quad (i, j) \in E \iff \exists(k, k') \in I_p^2, |k - k'| \leq w - 1, x_k = i \text{ and } x_{k'} = j \quad (1)$$

88 For digraphs, Eq. (1) is replaced with

$$89 \quad (i, j) \in E \iff \exists(k, k') \in I_p^2, k \leq k' \leq k + w - 1, x_k = i \text{ and } x_{k'} = j. \quad (2)$$

90 Finally, a weighted sequence graph  $G$  is endowed with a matrix  $\Pi(G) = (\pi_{ij})$  such that

$$91 \quad \pi_{ij} = \text{Card} \{(k, k') \in I_p^2 \mid k \leq k' \leq k + w - 1, x_k = i \text{ and } x_{k'} = j\} \quad (3)$$

92 We say that  $x$  is a  $w$ -admissible sequence for  $G$  (or a realization of  $G$ ), if  $G$  is the graph of  
 93 sequence  $x$  with window size  $w$ .

94 The natural integers  $\pi_{ij}$  represent the number of co-occurrences of  $i$  and  $j$  in a window  
 95 of size  $w$ . Hence, the graph of sequence is unique. An linear time algorithm to construct a  
 96 weighted sequence digraph is presented in Sec. A of the appendix. Other cases are obtained  
 97 similarly. The procedure in algorithm 1 defines a correspondence between the sequence set  
 98  $X^*$  into the graph set  $\mathcal{G} : \phi_w : X^* \rightarrow \mathcal{G}, x \mapsto G_w(x)$ . Based on these definitions, we consider  
 99 the following problems:

100 ► **Problem 1** (Weighted-REALIZABLE (W-REALIZABLE) ).

101 **Input:** Possibly directed graph  $G$ , matrix weights  $\Pi$ , window size  $w$

102 **Output:** True if  $(G, \Pi)$  is the  $w$ -sequence graph of some sequence  $x$ , False otherwise.

103 ► **Problem 2** (Unweighted-REALIZABLE (U-REALIZABLE) ).

104 *Input:* Possibly directed graph  $G$ , window size  $w$

105 *Output:* True if  $G$  is the  $w$ -sequence graph of some sequence  $x$ , False otherwise.

106 We denote  $D$ -REALIZABLE (resp.  $G$ -) the restricted version of REALIZABLE where the  
 107 input graph  $G$  is directed (resp. undirected), and  $W$ -REALIZABLE (resp.  $U$ -) the restricted  
 108 version of REALIZABLE where the input graph  $G$  is weighted (resp. unweighted), possibly  
 109 in combination with the  $D$ - or  $G$ - variants. We write  $\text{REALIZABLE}_w$  for the case where  $w$   
 110 is a fixed (given) constant. We also consider the variants of  $W$ -REALIZABLE, denoted  $WG$ -  
 111 REALIZABLE and  $WD$ -REALIZABLE where the input graph is restricted to be respectively  
 112 undirected and directed. We define  $UG$ -REALIZABLE and  $UD$ -REALIZABLE similarly. Finally,  
 113 we write  $(WG\text{-}, WD\text{-}, \dots)\text{REALIZABLE}_w$  for the case where  $w$  is a fixed strictly positive integer.

114 ► **Problem 3** (Unweighted-NUMREALIZATIONS (U-NUMREALIZATIONS) ).

115 *Input:* Possibly directed graph  $G$ , window size  $w$

116 *Output:* The number of **realizations** of  $G$ , i.e. preimages of  $G$  through  $\phi_w$  such that  
 117  $|\{x \in X^* \mid \phi_w(x) = G\}|$  if finite, or  $+\infty$  otherwise.

118 ► **Problem 4** (Weighted-NUMREALIZATIONS (W-NUMREALIZATIONS)).

119 *Input:* Possibly directed graph  $G$ , matrix weights  $\Pi$ , window size  $w$

120 *Output:* The number of **realizations** of  $G$  in the weighted sense.

121 Similarly, we use the same prefix for the directed or undirected versions of ( $D$ -,  $G$ -, i.e.  
 122  $DU$ - for directed and unweighted). We also denote  $\text{NUMREALIZATIONS}_w$  for the case where  
 123  $w$  is a fixed strictly positive integer. Note that  $\text{NUMREALIZATIONS}$  strictly generalizes the  
 124 previous one, as  $\text{REALIZABLE}$  can be solved by testing the nullity of the number of suitable  
 125 realization computed by  $\text{NUMREALIZATIONS}$ .

126 

<b>DW</b> Directed weighted	<b>DU</b> Directed unweighted
<b>GW</b> Undirected weighted	<b>GU</b> Undirected unweighted

### 127 **3 Theoretical results**

128 In this section, we present our main theoretical results. Due to length limitations, some of  
 129 the proofs are left in the appendix.

#### 130 **3.1 A complete characterization of 2-sequence graphs**

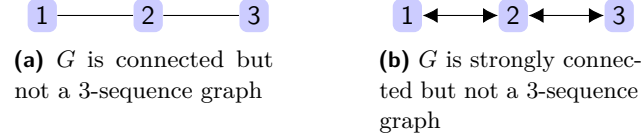
131 A graph has a sequential realization with  $w = 2$  when there exists a path visiting every vertex  
 132 and covering all of its edges (at least once for the unweighted case and exactly  $\pi_e$  for the  
 133 edge  $e$  in the weighted case). This characterization enables relatively simple characterization  
 134 and algorithmic treatment, leading to the results summarized in Table 2.

■ **Table 1** Complexity for various instances of our problems ( $w = 2$ )

Data Instance	NUMREALIZATIONS <sub>2</sub>		REALIZABLE <sub>2</sub>	
	Complexity	#Sequences	Complexity	Characterization
Unweighted graph	P	$\{0, +\infty\}$	P	$G$ connected
Weighted graph	#P-hard	$\{0, 1\} \cup 2\mathbb{N}^*$	P	$\psi(G)$ (semi) Eulerian
Unweighted digraph	P	$\{0, 1, +\infty\}$	P	Theorem 14
Weighted digraph	P	$\mathbb{N}$ (BEST Theorem)	P	$\psi(G)$ (semi) Eulerian

### 135 3.2 General sequence graphs and $\text{REALIZABLE}_{w \geq 3}$

136 The characterization of more general sequence graphs, such as 3-graphs is not the same for  
 137 2-graphs, as shows the counter-example in Fig 3a: the depicted graph has no self-edge so  
 138 there must at least one clique of size 3. Similarly, Fig. 3b depicts a counter example for  
 139 directed graphs:  $G$  does not have loops, so if it had a 3-admissible sequence, such sequence  
 140 must be of the form  $\{1231\dots, 1321\dots, 2312\dots, 3213\dots, 2132\dots\}$  but then  $(2, 1)$  would form  
 141 an edge.



■ Figure 3 Counter examples for  $w = 3$

### 142 3.3 A polynomial time algorithm for $\text{GU-REALIZABLE}_w$

143 Similarly to the procedure in Sec. B, we will use an auxiliary graph built on  $G$ . Let  
 144  $H(G) = (E, H_E)$  be the new graph obtained with the following procedure. Two edges  
 145  $e = (v_1, v_2)$ ,  $f = (v_3, v_4)$  of  $E$  are connected in  $H(G)$  if and only if:

$$146 \quad v_2 = v_3 \text{ and } (v_1, v_4) \in E \quad (4)$$

147 This defines an injective function  $\tilde{h} : E_H \rightarrow V^3$ : an edge of  $H(G)$  can be seen as an  
 148 unique triplet  $v_1, v_2, v_3$  where  $(v_1, v_2), (v_1, v_3)$  and  $(v_2, v_3) \in E$ . Therefore, by definition, a  
 149 walk  $P$  in  $H(G)$  is always of the form:

$$150 \quad P = (t_1, t_2), \dots, (t_{p-1}, t_p) \text{ s.t } \forall i \in \{1, \dots, p-1\}, (t_i, t_{i+1}) \in E \quad (5)$$

151 It is clear that if  $H(G)$  is a 2-graph, then  $G$  is a 3-graph since there is a walk going  
 152 through all edges of  $H(G)$  (so visiting every non isolated node and creating all edges of  $G$ ).  
 153 However, the converse is not true as depicted in Fig. 4. In order to determine if  $G = (V, E)$   
 154 has an admissible sequence in the general case, a procedure is to recursively merge pairs of  
 155 vertices, maintaining constraints depending on  $E$ . These constraints are similar to Eq. 4. We  
 156 adopt the following notations,  $u_{i,j} = (u_i, u_j)$  and  $u_{1:k} = (u_1, \dots, u_k)$ . The iterative procedure  
 157 for  $w \geq 3$  is summed up in the following equation. Namely,  $\forall k \in \{2, \dots, w-2\}$ , one has

$$158 \quad E^{(k)} = \{u_{1:k+1} \in V^{k+1} \mid u_{1:k} \in E^{(k-1)}, u_{2:k+1} \in E^{(k-1)} \wedge (u_1, u_{k+1}) \in E\} \quad (6)$$

159 Let  $H^{(k)} = (E^{(k)}, E^{(k+1)})$ , it can be defined recursively through:

$$160 \quad H^{(0)} = G \quad \forall k \in \mathbb{N}^*, H^{(k)} = f(H^{(k-1)}) \quad (7)$$

162 where  $f$  transforms edges into vertices and creates edges between new vertices that verify  
 163 Eq. 6.

164 ► **Definition 2.** Let  $u$  be a vertex of  $H^{(k)}$  for  $k \in \mathbb{N}$ ,  $u = (u_1, \dots, u_k, u_{k+1})$ . The sequence  
 165  $u_1, \dots, u_{k+1}$  is the **authentic** sequence of  $u$ . We also call an authentic sequence of a walk on  
 166  $H^{(k)}$ :  $P = (x_1, \dots, x_{k+1}), (x_2, \dots, x_{k+2}), \dots, (x_v, \dots, x_{v+k})$  the sequence  $x_1, x_2, \dots, x_{v+k}$ .

167 In order to obtain admissible sequences of length  $p$ , the computation of  $H^{(p)}$  requires  $p$   
 168 iterations, and the number of vertices and edges of  $H^{(k)}$  can increase during iterations (the  
 169 complete graph is an example for which these numbers increase exponentially).

170 ► **Proposition 3.** *Let  $x = x_1, \dots, x_p$  be a  $w$ -admissible sequence of a graph (or digraph)  
 171  $G = (V, E)$ . If  $w \leq p$ ,  $x$ , then  $x$  is an authentic sequence of a walk of length  $p - w + 1$  on  
 172  $H^{(w-2)}$ .*

**Proof.** Due to length limitation, we provide a proof sketch, full proof is left in the appendix.  
 The following property by induction on  $k$ :

$$\forall k \in \{w, \dots, p\}, \exists \text{ walk } P \text{ on } H^{(w-2)} \text{ such that :}$$

$$x_{1:k} = P[1]_1, P[2]_1, \dots, P[k-w]_1, P[k-(w-1)]_{1:(w-1)}$$

173 • Initialisation:  $k = 1$ . By construction of  $H^{(w-2)}$ ,  $x_1$  is the first element of the “static  
 174 walk”:  $x_{1:w-1} \in H^{(w-2)}$ .

175 • Induction: Verification that if  $x_{1:k}$  is a walk of length  $k - w + 1$ , one can find a walk of  
 176 length  $(k + 1) - w + 1$  to generate  $x_{1:(k+1)}$ . ◀

177 ► **Theorem 4.** *Let  $w \in \mathbb{N}^*$ .  $\text{GU-REALIZABLE}_w$  is in  $P$ .*

178 **Proof.** The case for  $w = 1$  is trivial, and  $w = 2$  has been treated. For  $w \geq 3$ , an algorithm  
 179 is obtained by going through all the connected components of  $H^{(w-2)}$ . Let  $C_1, \dots, C_m$  the  
 180 connected components of  $H^{(w-2)}$ . On the one hand, it is possible to compute them in  
 181 polynomial time. On the other hand, it is possible to construct walks covering all of their  
 182 respective edges in polynomial time (for instance iteratively using shortest paths). Let  
 183  $W_1, \dots, W_m$  such walks and  $X_1, \dots, X_m$  their respective admissible sequences.

184 Using Prop. 3,  $G$  is a  $w$ -sequence graph if and only if there exists a walk  $\tilde{W}_{i_0}$  on some  
 185  $C_{i_0}$  creating exactly the edges of  $G$ . However,  $W_{i_0}$  creates more edges than any walk on  $C_{i_0}$   
 186 by construction.

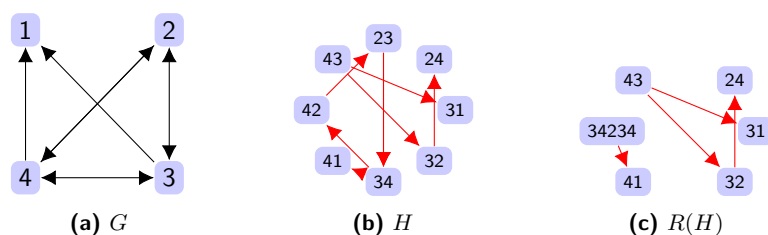
In conclusion, the assertion:

$$\exists i \in \{1, \dots, m\}, \phi_w(X_i) = G$$

187 is a characterization that  $G$  is a  $w$ -sequence. This assertion is decidable in polynomial time  
 188 since for all  $i$ ,  $\phi_w(X_i)$  is computable in polynomial time (cf. Algorithm 1). ◀

189 For digraphs, the analogue of the aforementioned procedure would consist in enumerating  
 190 all paths in the DAG  $R(H^{(w-2)})$ . However, the number of paths can be exponential, even for  
 191 a sequence graph. In the next subsection, we will prove that  $\text{DU-REALIZABLE}_w$  is actually  
 192 NP-hard. Finally, if  $x_1, \dots, x_c$  are vertices of a strongly component of  $H^{(w-2)}$ , which order  
 193 should be considered to form a new vertex attribute  $x_C$ ? The following lemma shows that  
 194 this order is not important, as long as it represents a walk in the component. Moreover, it  
 195 is possible to reconstruct all admissible sequences from walks on  $R(H^{(w-2)})$ . With the same  
 196 notations:

197 ► **Lemma 5.** *Let  $x$  a walk on  $H^{(w-2)}$  whose authentic sequence is  $w$ -admissible for  $G$ . If  $x$   
 198 goes through a strongly component  $C$  of  $H^{(w-2)}$ , adding any supplementary path included in  
 199  $C$  is stable for  $w$ -admissibility. Any graph generated by a walk on  $H^{(w-2)}$  can be generated  
 200 by a walk on  $R(H^{(w-2)})$ .*



■ **Figure 4** Procedure to find a 3-admissible sequence. 34234, 41: is 3-admissible, with authentic sequence 342341

201 **Proof.** We present a proof sketch. The first statement concerning stability requires a  
 202 straightforward verification using the definition of  $H^{(w-2)}$ . Second, a procedure to generate  
 203  $G$  from a walk on  $R(H^{(w-2)})$  using a walk  $x_{1:p}$  on  $H^{(w-2)}$  is to consider an iterative scheme,  
 204 and discuss three cases:

- 205 ■ (i)  $x_i$  and  $x_{i+1}$  are not in a strongly connected component (SCC)
- 206 ■ (ii)  $x_i$  is not in a SCC and  $x_{i+1}$  is in a SCC
- 207 ■ (iii)  $x_i$  and  $x_{i+1}$  are both in SCCs

208 For case (i), we just keep  $x_i$  and  $x_{i+1}$ . For cases (ii) and (iii), we use the first part result of  
 209 the Lemma and add covering walks over the strongly connected components. ◀

### 210 3.4 Main complexity results

211 In this subsection we present the remaining complexity results, which are summarized in  
 212 Table 2. In the previous subsection, we proved that  $\text{GU-REALIZABLE}_w \in P, \forall w \geq 3$ . Besides,  
 213 for GU, the number of realizations of a graph  $G$  is either 0 (not realizable),  $+\infty$  (realizable  
 214 and there exists a cycle in a component of  $H$  generating  $G$ ), or 1 (realizable but no cycle  
 215 in any component of  $H$  generating  $G$ ). These three cases can be tested in polynomial time  
 216 using our algorithm, showing that  $\text{GU-NUMREALIZATIONS}_w \in P, \forall w \geq 3$ . In the remaining  
 217 of this section, we present the reductions we used for the other instances.

■ **Table 2** Complexity for various instances of our problems ( $w \geq 3$ ). We remind that a para-NP-hard problem does not admit any XP algorithm unless  $P=NP$ .

Variation	Constant $w, w \geq 3$		Parameter $w$	
	$\text{NUMREALIZATIONS}_w$ Complexity	$\text{REALIZABLE}_w$ Complexity	$\text{NUMREALIZATIONS}$ Complexity	$\text{REALIZABLE}$ Complexity
GU	P	P	W[1]-hard; XP	W[1]-hard; XP
GW	NP-hard	NP-hard	para-NP-hard	para-NP-hard
DU	NP-hard	NP-hard	para-NP-hard	para-NP-hard
DW	NP-hard	NP-hard	para-NP-hard	para-NP-hard

218 ▶ **Proposition 6.** CLIQUE admits a polynomial time parameterized reduction into GU-  
 219 REALIZABLE.

220 **Proof.** Let  $G = (V, E)$  be a simple graph. Let  $G'$  be a graph constructed from  $G$  adding  
 221 two nodes  $a$  and  $b$  with loops, such that  $a$  and  $b$  are connected to each vertex of  $G$ . Let  $k$  be  
 222 a strictly positive integer and  $w = k + 1$ . We will show that  $G$  has a  $k$ -clique if and only if  
 223  $G'$  is  $w$ -realizable.



First, let us suppose that  $G$  has a  $k$ -clique. Let  $C$  be an arbitrary sequence of the vertices of one of its  $k$ -clique. Let  $v_1, \dots, v_{|V|}$  be the vertices of  $G$  and  $(u_1, u'_1), \dots, (u_{|E|}, u'_{|E|})$  be its edges. In the following  $x^w$  represents the  $w$ -repetition of  $x$ . Then, the following sequence is a  $w$ -realization of  $G'$ :

$$a^w u_1 u'_1 a^w u_2 u'_2 a^w \dots a^w u_{|E|} u'_{|E|} a^w C b^w v_1 b^w v_2 b^k \dots b^w v_{|V|}$$

224 Now let us suppose that  $G'$  is  $w$ -realizable and let  $x = x_1, \dots, x_p$  be a  $w$ -realization of  $G'$ .  
 225 Without loss of generality, let us suppose  $a$  appears before  $b$  in  $x$ . Let  $i_b$  be the index of  
 226 the first appearance of  $b$  and let  $i_a$  be the largest index of the appearance of  $a$  before  $i_b$ .  
 227 Then  $i_b - i_a \geq w$ , otherwise there would be an edge between  $a$  and  $b$ . Furthermore, since  
 228  $G$  is simple, there cannot be two repetitions of a vertex in the sequence  $x_{i_a+1}, \dots, x_{i_a+w-1}$ .  
 229 Due to the definition of a sequence graph, all vertices  $\{x_{i_a+1}, \dots, x_{i_a+w-1}\}$  are connected,  
 230 forming a clique in  $G$  of size  $w - 1 = k$ , which ends the proof. ◀

231 ▶ **Corollary 7.** GU-REALIZABLE is  $W[1]$ -hard for parameter  $w$ .

232 **DU-Realizable is NP-hard for  $w \geq 3$**

233 Consider the following intermediate problem:

234 **OptionalRealizable $_w$**  Given a directed unweighted graph  $D = (V, A)$ , a subset  $A' \subseteq A$  of  
 235 *compulsory arcs*, two distinguished vertices  $s, s' \in V$ . Is there a sequence  $S$  such that the  
 236 graph of  $S$  contains only arcs in  $A$  and (at least) all arcs in  $A'$ .

237 We first prove that this problem is NP-hard, then show how it reduces to DU-Realizable.

238 **OptionalRealizable $_w$ ,  $w \geq 3$  is NP-hard**

239 Given  $G = (V, A)$  and a start vertex  $s$ , build a directed weighted graph  $G' = (V', A')$  as  
 240 follows:

- 241 ■ Vertex set:  $V = \bigcup_{v \in V} \{v_0 \mid v_1\} \cup \{x_p^i, 1 \leq p \leq 2n + 1, 1 \leq i \leq w - 2\}$
- 242 ■ Arc set,
  - 243 ■ optional arcs  $(x_{2p-1}^i, v_0), (v_0, x_{2p}^i), (x_{2p}^i, v_1), (v_1, x_{2p+1}^i)$  for each  $v \in V, 1 \leq p \leq n,$   
 244  $1 \leq i \leq w - 2.$
  - 245 ■ optional arcs  $(u_1, v_0)$  for each  $(u, v)$  in  $A$
  - 246 ■ compulsory arcs  $(v_0, v_1)$  for each  $v \in V$
  - 247 ■ optional arcs  $(x_p^i, x_p^j)$  for  $i < j$  and  $(x_p^i, x_{p+1}^j)$  for  $j \leq i$

248 Start vertices are  $(x_0^1, \dots, x_0^{k-2}, s)$ .

249  $G'$  is a yes-instance  $\Leftrightarrow G$  admits a hamiltonian path

250  $\Leftarrow$  Let  $v^p$  be the  $p$ th vertex of  $V$  in the hamiltonian path. Let  $X^p$  be the sequence  
 251  $x_{2p-1}^0 \dots x_{2p-1}^{w-2} v_0^p x_{2p}^0 \dots x_{2p}^{w-2} v_1^p$ . Let  $X^{n+1} = x_{2n}^0 \dots x_{2n}^{w-2}$ , and  $S$  be the concatenation  
 252  $X^1 \dots X^{n+1}$ . It can be checked that  $S$  contains only arcs of  $A$  and all compulsory arcs.

253  $\Rightarrow$  Consider a sequence  $S$ , an occurrence of  $x_p^i$  in  $S$  for some  $1 \leq i \leq w - 2, 1 \leq p \leq n$   
 254 (note that  $p \neq n + 1$ ), and let  $S'$  be the subsequence of  $S$  containing the  $w - 1$  characters  
 255 following  $x_{2p+1}^i$ . Let  $T = x_p^{i+1} \dots x_p^{w-2}$  and  $U = x_{p+1}^1 \dots x_{p+1}^i$  (note that  $T$  is possibly  
 256 empty).  $T$  and  $U$  are seen both as strings and as sets of vertices. The out-neighborhood  
 257 of  $x_p^i$  contains all vertices of  $T \cup U$ , as well as all vertices  $v_q$  for  $v \in V$ , where  $q = 0$  if  $p$  is  
 258 odd and  $q = 1$  if  $p$  is even. Since there are  $k - 2$  vertices in  $T \cup U$ , and no vertex has a  
 259 self-loop, then by the pigeon-hole principle string  $S'$  must contain at least one vertex  $v^q$ ,  
 260  $v \in V$ . Since there are no arc  $(v^q, v'^q)$  for  $v, v' \in V$ ,  $S'$  contains exactly one vertex  $v^q$ , thus

261 it also contains all vertices of  $T \cup U$ . Based on the direction of the arcs in  $T \cup U \cup \{v^q\}$ , it  
 262 follows that  $S' = T \cdot v^q \cdot U$ .

Let  $X_p$  be the string  $x_p^1 \dots x_p^{w-2}$ . From the arguments above, and the fact that  $S$  starts with  $X_1$ , there exist indices  $i_1, j_1, \dots, i_n, j_n$  such that

$$S = X_1 v_{i_1}^0 X_2 v_{j_1}^1 X_3 v_{i_2}^0 X_4 v_{j_3}^1 X_5 \dots X_{2n+1}$$

263 From the window size  $w$ , there must exist an arc  $(v_{i_p}^0, v_{j_p}^1)$  for each  $p$ , so by construction  
 264  $i_p = j_p$ . Furthermore, these arcs are compulsory for each vertex  $v^0$ , so  $(i_1, \dots, i_n)$  is a  
 265 permutation of  $\{1, \dots, n\}$ . Finally, there also exist an arc  $(v_{j_p}^1, v_{i_{p+1}}^0)$  in  $G'$ , so there exists  
 266 an arc  $(v_{i_p}, v_{i_{p+1}})$  in  $G$ . Thus,  $(v_{i_1}, \dots, v_{i_n})$  is a hamiltonian path in  $G$ .

### 267 **DU-Realizable<sub>w</sub> is NP-hard**

268 By reduction from **OptionalRealizable<sub>w</sub>**. Given a directed unweighted graph  $G = (V, A)$ , a  
 269 subset  $A' \subseteq A$  of compulsory arcs (let  $A'' = A \setminus A'$  be the set of optional arcs), an integer  $w$ ,  
 270 and  $w - 1$  distinguished vertices  $s_1 \dots s_{w-1} \in V$ .

Let  $m = |A''|$ , write  $A'' = \{(u_1, v_1), \dots, (u_m, v_m)\}$ . Create  $G'$  by adding  $w(m + 1)$  separator vertices  $y_p^i$ ,  $1 \leq p \leq m + 1$  and  $1 \leq i \leq w$  and  $m$  vertices  $z_p$ . Build the strings

$$Z = \left( \prod_{p=1}^m (y_p^1 \dots y_p^w u_p z_p v_p) \right) y_{m+1}^1 \dots y_{m+1}^w$$

$$Z' = Z s_1 \dots s_{w-1}$$

271 . Add all arcs realized by  $Z'$  involving  $y_p^i$  and/or  $z_p$  to  $G'$ .

272  $G$  has a realization with optional arcs  $\Leftrightarrow G'$  has a realization

273  $\Rightarrow$  Build a realization for  $G'$  by concatenating  $Z$  with the realization for  $G$  starting with  
 274  $s_1 \dots s_{w-1}$ . All optional arcs of  $G'$  are realized in  $Z$ , all compulsory arcs of  $G'$  are realized  
 275 in the suffix (the realization of  $G'$ ), and all arcs involving a separator are realized in  $Z'$ . No  
 276 forbidden arc is realized.

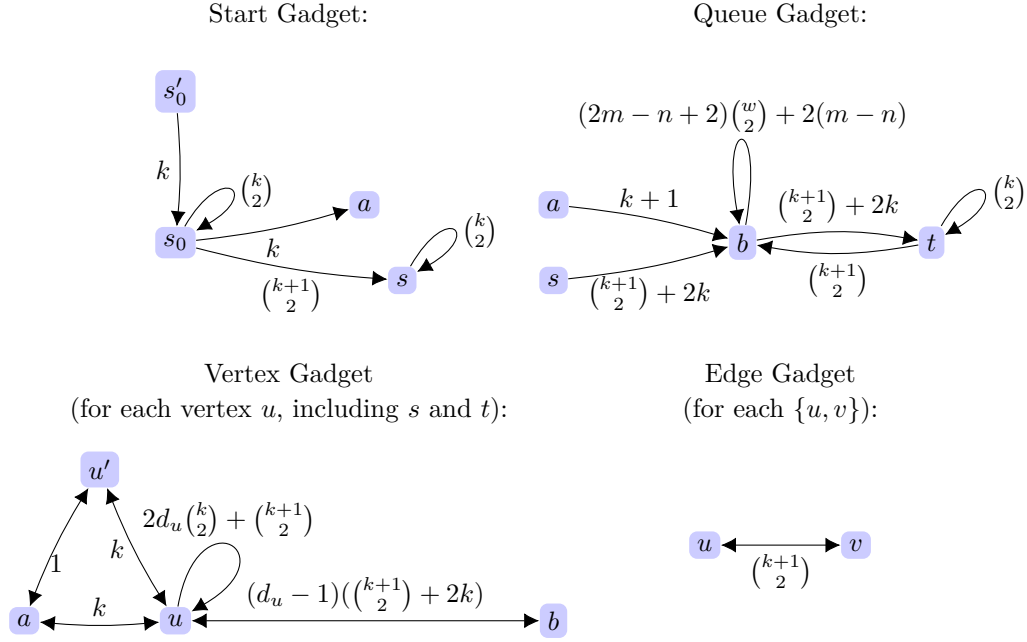
277  $\Leftarrow$  Let  $S$  be a realization of  $G'$ . The set of in-neighbors of any separator has size at most  
 278  $w - 1$  and induce a tournament in  $G'$  (this is clear for all arcs involving separators, it is also  
 279 true for a potential pair of vertices  $(u_i, v_i)$  of  $G$  since  $G$  has no length-2 cycle. So the  $w - 1$   
 280 characters before any separator are ordered as in  $Z$ . Furthermore each separator (except  
 281  $y_1^1$ ) contains at least one other separator in each in-neighborhood, so any occurrence of a  
 282 separator is actually the last character of a substring of  $S$  equal to a prefix of  $Z$ . Since  $y_1^1$   
 283 has in-degree 0, it may only appear as the first character of  $S$ , and any prefix of  $Z$  in  $S$   
 284 is also a prefix of  $S$ . Moreover since  $y_{m+1}^w$  must appear in  $S$ , we have  $S = ZS'$  with no  
 285 separator appearing in  $S'$ . Thus  $S'$  realizes only arcs from  $G$ . From the out-neighborhood of  
 286  $y_{m+1}^1, \dots, y_{m+1}^w$ , we have that  $S$  starts with  $s_1, \dots, s_{w-1}$ . Moreover no compulsory arc of  $G$  is  
 287 realized in  $Z$ , nor with one vertex in  $Z$  and one in  $S'$  (since such arcs start with a separator),  
 288 so all compulsory arcs are realized in  $S'$ . Overall,  $G$  is a yes-instance of **OptionalRealizable<sub>w</sub>**  
 289 with sequence  $S'$ .

### 290 **GW-Realizable<sub>w</sub>, DW-Realizable<sub>w</sub> are NP-hard for all $w \geq 3$**

291 By reduction from a variant of hamiltonian path:

292 **Input:** Undirected graph  $G$  with two degree-1 vertices.

293 **Question:** Does  $G$  have a hamiltonian path?



■ **Figure 5** Subgraphs used in the reduction from Hamiltonian Path to DW-Realizable<sub>3</sub>. Weights on double arcs apply to both directions. Note that some arcs appear in different gadgets, in which case the weights should be summed (in particular, so loops on  $s$  and  $t$  have total weight  $2d_u \binom{k}{2} + \binom{k+1}{2}$ )

294 Note that this variant of HP is easily shown to be NP-hard from Hamiltonian cycle via  
 295 the following reduction: given a graph  $G$  on which we need to find a hamiltonian cycle,  
 296 pick any vertex  $v$ , duplicate it into  $v_1, v_2$  (each edge  $\{u, v\}$  becomes two edges  $\{u, v_1\}$  and  
 297  $\{u, v_2\}$ ), and add pending vertices  $s$  and  $t$  connected to  $v_1$  and  $v_2$  respectively.

#### 298 **Reduction for DW-Realizable**

299 Given  $G = (V, E)$  with degree-1 vertices  $s$  and  $t$ , build a directed weighted graph  
 300  $G' = (V', A)$  as follows:

301 **Vertex set.** For each  $u \in V$ , create a vertex denoted  $u'$ . Create two additional dummy  
 302 vertices  $a$  and  $b$ . Let  $V' := \{a, b, s_0, s'_0\} \cup \bigcup_{u \in V} \{u, u'\}$ . The arcs are given in Figure 5, as  
 303 the union of the start gadget, the queue gadget, and the vertex and edge gadgets respectively  
 304 for each vertex and edge of  $G$ .

#### 305 **Reduction for GW-Realizable**

306 Build the directed graph  $G'$  as above, and let  $G'_u$  be the undirected version of  $G'$ : remove  
 307 arc orientations, for  $u \neq v$  the weight of  $\{u, v\}$  is the sum of the weight of  $(u, v)$  and  $(v, u)$  in  
 308  $G'$  (the weight of loops is unchanged).

#### 309 **Main claims**

310 We prove the following three claims:

- 311 (i)  $G$  hamiltonian  $\Rightarrow G'$  has a realization
- 312 (ii)  $G'$  has a realization  $\Rightarrow G'_u$  has a realization
- 313 (iii)  $G'_u$  has a realization  $\Rightarrow G$  hamiltonian

314 All together, they show the correctness of the reductions for both GW-Realizable and  
 315 DW-Realizable since they yield :

316  $G$  hamiltonian  $\Leftrightarrow G'$  has a realization

317  $G$  hamiltonian  $\Leftrightarrow G'_u$  has a realization

318

319 **Proof of Claim (i).**  $G$  has a hamiltonian path, let  $(u_1 = s, u_2, \dots, u_n = t)$  be its hamiltonian  
 320 path and  $(v_1, w_1), \dots, (v_{m'}, w_{m'})$  be the pairs of connected verices except pairs  $(u_i, u_{i+1})$  (i.e.  
 321 the set  $\bigcup_{\{u,v\} \in E} \{(u,v), (v,u)\} \setminus \{(u_i, u_{i+1}) \mid 1 \leq i < n\}$ . Note that  $m' = 2m - (n - 1)$ .  
 322 Define sequence  $S$  as follows.

$$S := \left| \begin{array}{l} s'_0 s_0^k a s^k s' s^k a u_2^k u_2^k u_2^k a \dots a u_{n-1}^k u_{n-1}^k u_{n-1}^k a t^k t' t^k a \\ b^w v_1^k b w_1^k b^w v_2^k b w_2^k \dots b^w v_{m-n}^k b w_{m-n}^k b^w \end{array} \right.$$

323 Note that a sequence of the form  $x^k a y^k$  yields  $\binom{k}{2}$  loops for  $x$ ,  $\binom{k}{2}$  loops for  $y$ , as well  
 324 as  $\binom{k+1}{2}$  arcs  $(x, y)$  (indeed, there are  $1 + 2 + \dots + w - 2 = \binom{k+1}{2}$  such arcs). A sequence  
 325 of the form  $b x^k b^w$  yields in particular an arc  $(b, x)$  of weight  $k$  and arc  $(x, b)$  of weight  
 326  $\binom{k+1}{2} + k$ . ◀

327 **Proof of Claim (ii).** Clear, any realization for  $G'$  is a realization for  $G'_u$ . ◀

328 **Proof of Claim (iii).** Pick a realization  $S$  of  $G'_u$ . Define the weight of a vertex in  $G_u$  as the  
 329 sum of the weights of its incident edges (counting loops twice). From the construction, we  
 330 obtain the following weights for a selection of vertices:

- 331 ■  $s'_0$  has weight  $w - 1$
- 332 ■  $u'$  has weight  $2(w - 1)$  for  $u \in V$
- 333 ■  $a$  has weight  $2(n + 1)(w - 1)$

334 From the weight of  $s'_0$ , it follows that this vertex must be an endpoint of  $S$  (wlog,  $S$   
 335 starts with  $s'_0$ ). It follows that for any other vertex  $v$  with weight  $2i(w - 1)$ ,  $v$  must have  
 336 exactly  $i$  occurrences in  $S$  (in general it can be either  $i$  or  $i + 1$ , but if  $v$  has  $i + 1$  occurrences  
 337 it must be both the first and last character of  $S$ , i.e.  $v = s'_0$ : a contradiction). Thus each  $u'$   
 338 occurs once and  $a$  occurs  $n + 1$  times in  $S$ .

339 Each  $u'$  occurs once, so order vertices of  $V$  according to their occurrence in  $S$  (i.e.  
 340  $V = \{u_1, \dots, u_n\}$  with  $u'_1$  appearing before  $u'_2$ , etc.). For each  $i$ , the neighborhood of  $u'_i$  in  
 341  $S$  contains  $a$  twice, one  $a$  on each side (since there is no  $(a, a)$  loop). Other neighbors of  
 342  $u'_i$  may only be occurrences of  $u_i$ , so each  $u'_i$  belongs to a factor, denoted  $X_i$ , of the form  
 343  $au_i^* u'_i u_i^* a$ . Two consecutive factors  $X_i, X_{i+1}$  may overlap by at most one character ( $a$ ), and  
 344 if they do, then there exists an edge  $\{u_i, u_{i+1}\}$  (since  $w \geq 3$ ) in  $G$ . There are  $n$  such factors  
 345  $X_{u_i}$ , and only  $n + 1$  occurrences of  $a$ , so all  $as$  except extreme ones belong to the overlap of  
 346 two consecutive  $X_j$ s, and there exists an edge  $\{u_i, u_{i+1}\}$  for each  $i$ . Thus  $(u_1, \dots, u_n)$  is a  
 347 hamiltonian path of  $G$ . ◀

## 348 4 Effective general algorithms

### 349 4.1 REALIZABLE<sub>w</sub> Linear integer programming formulation

350 Let  $G = (V, E)$  be a graph with integer weights  $\pi_{e \in E}$ . In this model, we represent a sequence  
 351  $x$  over the alphabet  $\{1, \dots, n\}$ , as a  $(0 - 1)$  matrix  $X \in \mathbb{M}_{n,p}(\{0, 1\})$  encoding the sequence  $x$ :

$$352 X_{i,j} = \begin{cases} 1 & \text{if } x_j = i \\ 0 & \text{otherwise} \end{cases}$$

It should be noted that the set sequence of sequences over the alphabet  $\{1, \dots, n\}$  is exactly represented by the  $(0 - 1)$  matrices such that

$$\forall j \in \{1, \dots, p\} \quad \sum_{i=1}^n X_{i,j} = 1$$

353 Given a window size  $w$ , a unit of  $\pi_{e=(v_1, v_2)}$  corresponds to the appearance of two elements  
 354  $v_1, v_2$  at a distance  $i \in \{1, \dots, w - 1\}$  in the sequence. Now, let us consider a fixed distance  $i$ ,  
 355 and a starting index  $j \in \{1, \dots, p - i\}$ , we use a intermediary slack variable  $y_j^e(i) \in \{0, 1\}$  to  
 356 model the presence of such appearance using the constraint:

$$357 \quad X_{v_1, j} X_{v_2, j+i} = y_j^e(i) \quad (8)$$

358 Then, the Boolean variable  $y_j^e(i)$  is equal to 1 when  $v_1$  is located at position  $j$  and  $v_2$  at  
 359 position  $j + i$ . We linearise Eq. 8 as:

$$360 \quad \begin{aligned} -X_{v_1, j} \quad \quad \quad + y_j^e(i) &\leq 0 \\ -X_{v_2, j+i} + y_j^e(i) &\leq 0 \\ X_{v_1, j} + X_{v_2, j+i} - y_j^e(i) &\leq 1 \end{aligned} \quad (9)$$

Each slack variable  $y_k^e(i)$  is attributed to an edge  $e$ , a relative distance  $i \in \{1, \dots, w - 1\}$  and a starting position  $k \in \{1, \dots, p - i\}$ . Given our constraint formulation, every slack variable is attributed 3 constraints. For a digraph, the number of possible pair positions for a unit of  $\pi_{e=(v_1, v_2)}$  is given by:

$$C = \sum_{i=1}^{w-1} (p - i) = p(w - 1) - \frac{w(w - 1)}{2} = (w - 1)(p - \frac{w}{2})$$

361 Therefore, in our model,  $C$  corresponds to the number of slack variables attributed to  
 362 constraints for an edge of the graph.

363 On the contrary, the absence of an edge  $e = (v_1, v_2)$ , corresponding to  $\pi_e = 0$ , can be  
 364 modeled for a distance  $i \in \{1, \dots, w - 1\}$  and a starting position  $j \in \{1, \dots, p - i\}$  as:

$$365 \quad X_{v_1, j} + X_{v_2, j+i} \leq 1$$

366 Then,  $\text{REALIZABLE}_w$  can be formulated as the following linear integer program:

$$367 \quad \min_{X \in \{0, 1\}^{p \times n}, y \in \{0, 1\}^{|E| \times C}} \sum_{e \in E} \sum_{i \in \{1, \dots, w-1\}} y_1^e(i) + \dots + y_{p-i}^e(i)$$

368 under the constraints

$$369 \quad \forall j \in \{1, \dots, p\} \quad \sum_{i=1}^n X_{i,j} = 1$$

$$370 \quad \forall e = (v_1, v_2) \in E \quad \begin{cases} -X_{v_1, 1} \quad \quad \quad + y_1^e(i) \leq 0 \\ \quad \quad \quad - X_{v_2, 1+i} + y_1^e(i) \leq 0 \\ X_{v_1, 1} + X_{v_2, 1+i} - y_1^e(i) \leq 1 & X_{v'_1, 1} + X_{v'_2, 1+i} \leq 1 \\ \quad \quad \quad \vdots & \quad \quad \quad \vdots \\ -X_{v_1, p-i} \quad \quad \quad + y_{p-i}^e(i) \leq 0 & X_{v'_1, p-i} + X_{v'_2, p} \leq 1 \\ \quad \quad \quad - X_{v_2, p} + y_{p-i}^e(i) \leq 0 \\ X_{v_1, p-i} + X_{v_2, p} - y_{p-i}^e(i) \leq 1 \end{cases}$$

$$\text{and } \forall e \in E \quad \sum_{i \in \{1, \dots, w-1\}} y_1^e(i) + \dots + y_{p-i}^e(i) \geq \pi_e$$

If the objective function reaches  $\sum_{e \in E} \pi_e$  at its minimum then the output of  $\text{REALIZABLE}_w(G, \Pi)$  is True, and False otherwise.

## 4.2 NUMREALIZATIONS<sub>w</sub> Dynamic programming formulation

We did not present a way to count admissible sequences in the general case. Although the tractability of our problems (NP-hardness of  $\text{REALIZABLE}_w$ , #P-hardness of  $\text{NUMREALIZATIONS}_w$ ) currently remains open for some cases, we present in this subsection a method based on dynamic programming valid for all cases.

The recursion proceeds by extending a partial sequence, initially set to be empty, keeping track of for represented edges along the way. Namely, consider  $N_w[\Pi, p, \mathbf{u}]$  to be the number of  $w$ -admissible sequences of length  $p$  for the graph  $G = (V, E)$ , respecting a weight matrix  $\Pi = (\pi_{ij})_{i,j \in V^2}$ , preceded by a sequence of nodes  $\mathbf{u} := (u_1, \dots, u_{|\mathbf{u}|}) \in V^*$ . It can be shown that, for all  $\forall p \geq 1$ ,  $\Pi \in \mathbb{N}^{|V|^2}$  and  $\mathbf{u} \in V^{\leq w}$ ,  $N_w[\Pi, p, \mathbf{u}]$  obeys the following formula, using the notations of Section 3.2:

$$N_w[\Pi, p, \mathbf{u}] = \sum_{v \in V} \begin{cases} N_w[\Pi'_{(\mathbf{u}, v)}, p-1, (u_1, \dots, u_{|\mathbf{u}|}, v)] & \text{if } |\mathbf{u}| < w-1 \\ N_w[\Pi'_{(\mathbf{u}, v)}, p-1, (u_2, \dots, u_{w-1}, v)] & \text{if } |\mathbf{u}| = w-1 \end{cases} \quad (10)$$

with  $\Pi'_{(\mathbf{u}, v)} := (\pi_{ij} - |\{k \in [1, |\mathbf{u}|] \mid (u_k, v) = (i, j)\}|)_{(i,j) \in V^2}$ . The base case of this recurrence corresponds to  $p = 0$ , and is defined as

$$\forall \Pi, N_w[\Pi, 0, \mathbf{u}] = \begin{cases} 1 & \text{if } \Pi = (0)_{(i,j) \in V^2} \\ 0 & \text{otherwise.} \end{cases} \quad (11)$$

The total number of admissible sequences is then found in  $N_w[\Pi, p, \varepsilon]$ , *i.e.* setting  $\mathbf{u}$  to the empty prefix  $\varepsilon$ , allowing the sequence to start from any node.

The recurrence can be computed in  $\mathcal{O}(|V|^w \times \prod_{i,j \in V^2} (\pi_{i,j} + 1))$  time using memoization, for  $p$  the sequence length. The complexity can be refined by noting that:

$$\sum_{i,j \in V^2} \pi_{i,j} \leq w \times p$$

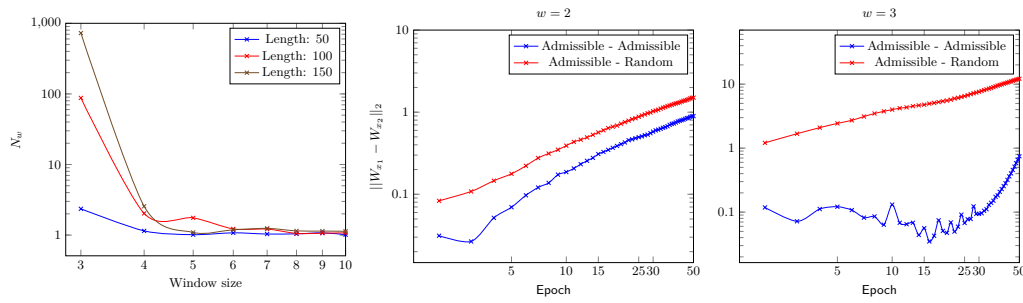
To investigate the worst case scenario, we can consider the optimisation problem:

$$\max_{\Pi} \prod_{i,j \in V^2} (\pi_{i,j} + 1) \text{ such that } \sum_{i,j} \pi_{i,j} = w p. \quad (12)$$

This problem is equivalent to maximise a product under a budget constraint. When  $n^2 \geq w \times p$ , which is the case in practice, the maximum is reached for a Boolean matrix  $\Pi = (\pi_{i,j}) \in \{0, 1\}^{|V|^2}$ , verifying the constraint. This property can be deduced from the inequality:

$$\begin{aligned} 1 \leq a < b-1 &\implies \log a + \log b < \log(a+1) + \log(b-1) \\ &\implies ab < (a+1)(b-1) \end{aligned}$$

It follows that, in the worst-case scenario,  $\prod_{i,j \in V^2} (\pi_{i,j} + 1) \in \mathcal{O}(2^{w p})$ . Thus, despite the, apparently extreme complexity of our algorithm, it is still possible to compute  $N_w[\Pi, p, u_{1:w}]$  for “reasonable” values of  $p$  and  $w$ .



■ **Figure 6** Left plot: Average lower bound ( $N_w$ ) on the average number of sequences. Two right plots:  $\|W_{x_1} - W_{x_2}\|_2 = f(\text{Epoch})$  - LSTM, log - log scale

## 5 Application to sequential models

### 5.1 Number of equivalent sequences for weighted sequence digraphs

Since the dynamic programming method in Sec. 4.2 is exponential in the worst case, we provide results for relatively short sequences generated from text data (a dump of English Wikipedia, 2016) of 500 documents, each of them having a length  $p \in \{50, 100, 150\}$ . Each document contained a minimum of  $\frac{3}{4}p$  distinct words. For each  $w \in 3 \rightarrow 10$ , we estimate the number of admissible sequences yielding the same representations for a set of documents and different window size using the procedure described in Sec. 4.2 to compute  $N_w$ . Due to memory limitations, it should be noted that  $N_w$  is a lower bound of the number of total admissible sequences, since a starting pattern (first  $w$  tokens) is fixed.

Results are reported in the left plot of Fig. 6. For  $w = 2$ , the number of sequences (obtained using Prop. 19) was significantly larger ( $> 10^5$ ), so not reported in the figure for clarity. As expected, the number of distinct admissible sequences tends to 1 when the window size increases. This suggests that window sizes used in skip gram models should be usually larger or equal to 5. In natural language processing, a frequent configuration is  $w = 10$  [18, 21]. However, some examples with different realizations exist, even for  $w = 10$  and  $p = 50$ .

### 5.2 Comparison with a recurrent neural network

The second experiment we consider is to evaluate the difference of the parameters between a sequential model trained on two admissible sequences of a given graph. The sequential model we are considering are a class of recurrent dynamical recurrent models, referred to as long short term memory (LSTM) networks [12]. These models have attracted new interest due to experimental progress for time series prediction [11] and natural language processing [3, 6, 25]. Given a window size  $w$ , the task we consider is to predict the next element of the sequence given the  $w - 1$  previous ones. If the sequences were equivalent for the sequential model, the weights should numerically converge after training.

To generate pairs of admissible sequences encoding for non trivial graphs (i.e not the complete graph), we used algorithm based on Lemma 5. We generate  $w$ -admissible sequence (thousand tokens long), for  $w \in \{2, 3\}$ , but could not provide other pairs for  $w > 3$  due to computational time. We compare the pairs of admissible sequences with a pair of one of the sequence, and a sequence generated randomly uniformly on the same vocabulary. We implemented the LSTM network using the Python library Keras [7], a high-level API

434 running over TensorFlow [1]. In order to remove randomness from the training algorithm,  
 435 we froze the seed generating initial weights (the optimization directions being fixed by the  
 436 data). We chose tanh as main activation function, sigmoid for the recurrent activations, with  
 437 2 units. The number of units is chosen relatively low in order to obtain a reasonable number  
 438 of weights (in this case 16).

439 Two right plots of Fig. 6 reports the results for  $w \in \{2, 3\}$ ,  $W_x$  represents all the weights  
 440 of the network for a sequence  $x$ . For  $w = 2$ , there the difference of the weights for 2 admissible  
 441 sequences is lower than with one of the sequence and a random one, but this proximity does  
 442 not appear to be significant compared with a random sequence. For  $w = 3$ , the recurrent  
 443 network has relatively close weights for two admissible sequences when compared with a  
 444 random one.

## 445 **6 Conclusion**

446 In this study, we revisited a series of problems related to the ambiguity of sequence graphs  
 447 representations, which are popular in the context of text mining and natural language  
 448 processing. We derived theoretical properties and practical algorithms for the family of  
 449 sequence graphs.

450 This study can be of use used for several sequential models, such as continuous bag of  
 451 words (CBOW), skip-grams ([10, 14, 24]), pointwise mutual information models [2, 18, 21].

## 452 **Acknowledgments**

453 The authors wish to express their gratitude to Guillaume Fertin and an anonymous reviewer  
 454 of an earlier version of this manuscript, for their valuable suggestions and constructive  
 455 criticisms.

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526 **A Additional figures**

■ **Algorithm 1** Construction of a sequence digraph

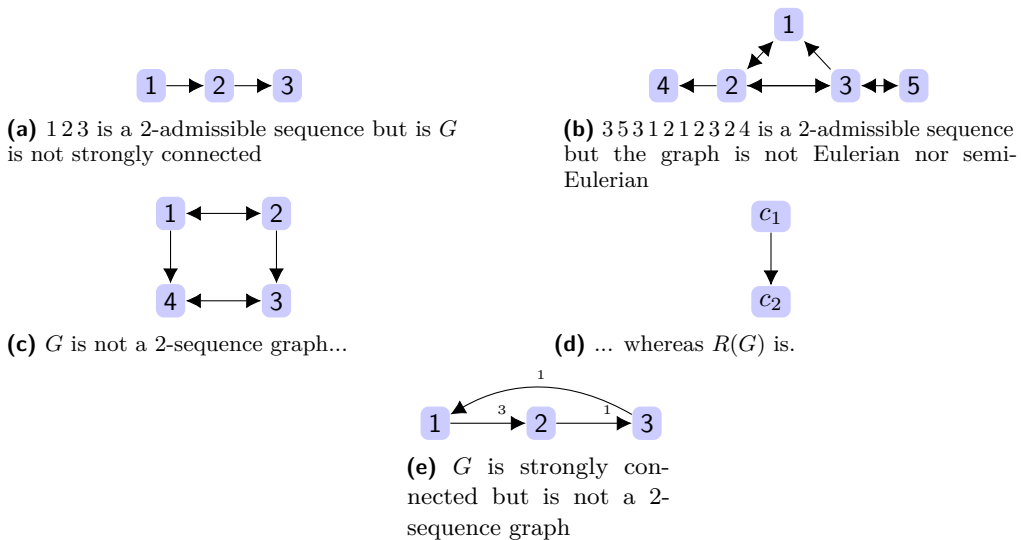
**Input:** Sequence  $x$  of length  $p$ , window size  $w$ ,  $p \geq w \geq 2$

**Parameter:** Optional list of parameters

**Output:**  $(G_w(x), \Pi)$

```

1:  $V \leftarrow \emptyset$ 
2: Initiate  $\Pi = (\pi_{i,j})$  to  $d \times d$  matrix of zeros
3: for  $i = 1 \rightarrow p - 1$  do
4:    $V \leftarrow V \cup \{x_i, x_{i+1}\}$ 
5:   for  $j = i + 1 \rightarrow \min(i + w - 1, p)$  do
6:      $\pi_{x_i, x_j} \leftarrow \pi_{x_i, x_j} + 1$ 
7:   end for
8: end for
9: return solution
    
```



■ **Figure 7** Counter examples for  $w = 2$

527 **B Results and proofs Sec. 3.1 ( $w = 2$ )**

528 In this section, we present the results for digraphs and  $w = 2$ . Obviously, the simplest case  
 529 concerns undirected graphs as stated in:

530 ► **Proposition 8.** *If  $G = (V, E)$  is unweighted and undirected, with  $|V| > 1$ , the following  
 531 are equivalent:*

- 532 (i)  $G$  is connected
- 533 (ii)  $G$  has a 2-admissible sequence
- 534 (iii)  $G$  admits an infinite number of 2-admissible sequences

535 *In these conditions, a 2-admissible sequence can start and end at any vertex.*

536 **Proof.** Let us suppose  $G$  has an admissible sequence  $u$ . Let  $a, b$  two distinct vertices of  $G$ .  
 537 Then using the definition,  $a$  and  $b$  must appear at least once in the sequence  $u$ , i.e  $u_{i_a} = a$   
 538 and  $u_{i_b} = b$ . If  $i_a < i_b$ , then the sequence  $s = (u_i \mid i_a \leq i \leq i_b)$  defines a path from  $a$  to  $b$   
 539 since  $\forall i, e_{s_i s_{i+1}} \in E$ . The case  $i_b > i_a$  is dealt similarly. ◀

540 The previous characterization is wrong for digraphs, even with strongly connectivity. A  
 541 counter example is depicted in Fig. 7a. However, strong connectivity remains a sufficient  
 542 condition:

543 ▶ **Proposition 9.** *Let  $G = (V, E)$  a unweighted digraph. If  $G$  is strongly connected then*  
 544  *$G \in \text{Im } \phi_2$ . A 2-admissible sequence can start or end at any given vertex of  $G$ .*

545 **Proof.** This can be proved similarly to (i)  $\implies$  (ii) for proposition 9 by replacing connectivity  
 546 with strong connectivity. ◀

547 ▶ **Proposition 10.** *Let  $G = (V, E)$  an unweighted digraph. If  $G$  is Eulerian or semi-Eulerian,*  
 548 *then  $G \in \text{Im } \phi_2$ .*

549 **Proof.** If  $G$  is Eulerian or semi-Eulerian, there exists a walk going through all edges, this  
 550 walk defines a 2-admissible sequence. ◀

551 Again the converse of Prop. 10 does not hold as depicted in Fig. 7b. The characterization  
 552 of sequence digraph is more subtle. As a start, it is natural to consider directed acyclic  
 553 graphs (DAGs):

554 ▶ **Proposition 11.** *Let  $G = (V, E)$  a DAG.  $G$  is a 2-sequence graph if and only if it is a*  
 555 *directed path, i.e  $G$  is a directed tree where each node has at most one child and at most one*  
 556 *parent. In this case,  $G$  has a unique 2-admissible sequence.*

557 **Proof.** If  $G$  is directed path, since  $G$  is finite, it admits a source node. Therefore a 2-  
 558 admissible sequence is obtained by simply going through all vertices from the source node.  
 559 This is obviously the only one.

560 Conversely, let us suppose  $G$  is a DAG and a 2-sequence graph. If  $G$  is not a directed  
 561 path, there are two cases: either there exists a vertex having two children, or two parents.  
 562 Let  $s$  be a vertex having 2 distinct children  $c_1$  and  $c_2$ . This is not possible since there cannot  
 563 be a walk going through  $(s, c_1)$  and  $(s, c_2)$ :  $G$  would have a cycle otherwise. Finally a vertex  
 564  $v$  cannot have two parents  $p_1$  and  $p_2$ : if a 2-admissible sequence existed, it would have to go  
 565 through  $(p_1, v)$  and  $(p_2, v)$ , creating a cycle, hence the contradiction. ◀

566 Every directed graph  $G$  is a DAG of its strongly connected components. In the following,  
 567 let  $R(G)$  be the DAG obtained by contracting the strongly connected components of  $G$ .

568 ▶ **Proposition 12.** *Let  $G = (V, E)$  a digraph. If  $G$  is a 2-sequence graph then  $R(G)$  is a*  
 569 *2-sequence graph.*

570 **Proof.** Let  $G$  be a 2-sequence graph, and let us suppose that  $R(G)$  is not a 2-sequence graph.  
 571 Since  $R(G)$  is a (weakly) connected DAG, then using Prop. 11, it cannot be a directed path,  
 572 so  $R(G)$  has either a node having two children or two parents. Let  $S$  be a node of  $R(G)$   
 573 having at least 2 distinct children  $C_1$  and  $C_2$ . This means that there exist three distinct  
 574 corresponding nodes in  $V$ ,  $s$ ,  $v_1$  and  $v_2$  such that  $(s, v_1) \in E$  and  $(s, v_2) \in E$ . Since  $G$  is a  
 575 2-sequence graph, there exists a walk covering  $(s, v_1)$  and  $(s, v_2)$ , such walk would make  $S$ ,  
 576  $C_1$  and  $C_2$  the same node in  $H(G)$ , hence the contradiction. The case for which a vertex has  
 577 two parents is dealt with similarly. ◀

578 The converse of Prop. 12 does not hold as depicted in Fig. 7c, 2. However, let us add a  
579 weight compatibility in  $R(G)$  as follows:

580 ► **Definition 13.** *Let  $G$  be a digraph, and  $R^+(G)$  be the weighted DAG obtained from  $R(G)$ ,  
581 such that the weight of an edge is attributed the number of distinct arcs from two strongly  
582 connected components in  $G$ .*

583 ► **Theorem 14.** *Let  $G = (V, E)$  be an unweighted digraph.*

584  *$G$  is a 2-sequence graph if and only if  $R^+(G)$  is a directed path and its weights are all  
585 equal to 1.*

586 **Proof.** If  $G$  is a 2-sequence graph,  $R(G)$  is a 2-sequence graph using Prop. 12. Also Prop. 11  
587 implies that  $R(G)$  and  $R^+(G)$  are directed paths. Moreover, if  $R^+(G)$  had a weight strictly  
588 greater than 1, then there would be strictly more than one edge between two connected  
589 components  $C_1$  and  $C_2$ . All these edges go in the same direction otherwise  $C_1 \cup C_2$  would  
590 form a strongly connected component. This is a contradiction since any 2-admissible sequence  
591 would have to go from  $C_1$  to  $C_2$  and then come back to  $C_1$  (or conversely) which would  
592 would make  $C_1 \cup C_2$  a strongly connected component.

593 Conversely, let us suppose  $R^+(G)$  is a directed path and its weights are equal to one.  
594 First, there exists a walk  $x_1, \dots, x_p$  covering all edges of  $R^+(G)$  verifying: (i)  $\forall i, x_i \in V$  or  $x_i$   
595 represents a strongly connected component of  $G$ , (ii) there is only one edge in  $G$  between  
596 from  $x_i$  to  $x_{i+1}$  and (iii)  $x$  has no repetition, i.e there is no common vertex in  $G$  between  $x_i$   
597 and  $x_{i+1}$ . We construct a 2-admissible sequence  $y$  for  $G$  by means of the following procedure.

598 **Initialisation:** If  $x_1 \in V$ , we simply set  $y \leftarrow x_1$ . Otherwise,  $x_1$  corresponds to a strongly  
599 connected component  $C_1$  of  $G$  and we add to  $y$  any 2-admissible sequence of  $C_1$ .

600 For  $i \in \{1, \dots, p-1\}$ :

- 601 • If  $(x_i, x_{i+1}) \in E$ : we add  $x_{i+1}$  to the sequence  $y$ .
- 602 • If  $x_i \in V$  and  $x_{i+1}$  is a strongly connected component  $C_i$  of  $G$ : By assumption, there  
603 exists only one edge of  $G$  from  $x_i$  to a vertex of  $C_i$ , say  $c_0^i$ . Since  $C_i$  is strongly connected,  
604 using Prop. 9,  $C_i$  has a walk going through all of its edges and starting in  $c_0^i$ , say  $c_0^i, \dots, c_p^i$ .  
605 We add  $c_0^i, \dots, c_p^i$  to  $y$ .
- 606 • If  $x_i$  corresponds to a strongly connected component  $C_i$  and  $x_{i+1} \in V$ : we perform  
607 similar operations by stopping on the single node of  $C_i$  that has an edge to  $x_{i+1}$  (this is  
608 possible thanks to Prop. 9).
- 609 •  $x_i$  and  $x_{i+1}$  both correspond to strongly connected components  $C_i$  and  $C_{i+1}$ , there  
610 exists only one edge between in  $E$  between  $C_i$  and  $C_{i+1}$ , say  $e_i = (v_i, v_{i+1})$ . We can complete  
611  $y$  by a walk from the last vertex visited which belong to  $C_i$  and  $v_i$ , and then by a 2-admissible  
612 sequence through  $C_{i+1}$  starting in  $v_i$  and ending in  $v_{i+1}$ .

613 End For

614 The process stops when  $i = p-1$ , and all edges are covered by the sequence  $y$ . ◀

615 Therefore, an algorithm to decide if a digraph is a 2-sequence is obtained by extract its  
616 connected components (there exist linear time algorithms e.g [22]), and to count the number  
617 of distinct edges between these.

618 ► **Corollary 15.** *Let  $G$  an unweighted digraph. The possible numbers of 2-admissible sequences  
619 for  $G$  is exactly  $\{0, 1, +\infty\}$ . Moreover,  $G$  admits a unique 2-admissible sequence if and only  
620 if  $G$  is a directed path.*

621 **Proof.** Let  $G$  a 2-sequence graph and let us show that  $G$  has either a unique or an infinite  
622 number of 2-admissible sequence.  $G$  verifies characterization of Theorem 14. If  $R(G)$  has

623 a vertex representing a strongly connected component of  $G$  (or a vertex with a self loop),  
 624 then by adding an arbitrary number of cycles to  $y$ , the obtained walk is still admissible.  
 625 Otherwise, if every vertex of  $R(G)$  is in  $V$  without self-loops in  $E$ , then  $G$  is a DAG. Using  
 626 Prop. 11,  $y$  is the unique 2-admissible sequence. ◀

## 627 Weighted 2-sequence graphs

628 The weighted case cannot be treated similarly due to the weight constraints implying that a  
 629 weighted graph has a finite number of admissible sequences. A counter example is depicted  
 630 in Fig. 7e.

631 ▶ **Definition 16.** Let  $\psi(G)$  be the multigraph with the same vertices as  $G = (V, E)$  and with  
 632  $\pi_{ij}$  edges between  $(i, j) \in V^2$ .

633 Due to the previous study, the characterization of weighted 2-sequence graphs using  $\psi(G)$  is  
 634 immediate.

635 ▶ **Theorem 17.** If  $G$  is a weighted graph (directed or not), with  $\Pi(G) \in \mathcal{M}_d(\mathbb{N})$ , then:  
 636  $G \in \text{Im } \phi_2 \iff \psi(G)$  is connected and semi-Eulerian.

637 **Proof.**  $G \in \text{Im } \phi_2$  means that there is a trail going through each edge  $(i, j) \in E$  exactly  $\pi_{i,j}$   
 638 times. This trail corresponds to a semi-Eulerian path in  $\psi(G)$ . ◀

639 ▶ **Lemma 18.** Let  $G = (V, E)$  a weighted 2-sequence graph (possibly oriented). Let  $\mathcal{E}$  be the  
 640 set of Eulerian paths of  $\psi(G)$  and  $\mathcal{S}$  be the set of 2-realizations of  $G$ . Then

$$641 \quad \mathcal{E} = (\#\mathcal{S}) \prod_{e \in E} \pi_e! \quad (13)$$

642 **Proof.** We will first prove it for digraphs. If  $e = (v_1, v_2)$  is an edge of a digraph, we will  
 643 represent the source and target vertex of  $e$  as  $e(s)$  and  $e(t)$ . Let  $(e_1, e_2, \dots, e_h)$  be a Eulerian  
 644 path of  $\psi(G)$  defined as a sequence of its edges. Then  $\forall (i, j) \in \{1, \dots, h\}^2$ ,  $e_i \neq e_j$  and  
 645  $\forall i \in \{1, \dots, h-1\}$ ,  $e_i(t) = e_{i+1}(s)$ . Let us consider the transformation:

$$646 \quad \begin{aligned} \mathcal{E} &\longrightarrow \mathcal{S} \\ (e_1, e_2, \dots, e_h) &\mapsto (e_1(s), e_2(s), \dots, e_{p-1}(s), e_h(t)) \end{aligned} \quad (14)$$

647 We have already shown this transformation is surjective: any 2-sequence of  $G$  can be  
 648 obtained with a Eulerian path of  $\psi(G)$ . We will now consider the action of  $\mathfrak{S}_h$  on  $\mathcal{E}$ .  
 649 For a Eulerian path, let us suppose that two edges of  $\psi(G)$  have been permuted, say  
 650  $e_1$  and  $e_{i_0}$  without loss of generality. If the two corresponding sequences are the same:  
 651  $(e_{i_0}(s), e_2(s), \dots, e_h(t)) = (e_1(s), e_2(s), \dots, e_{i_0}(s), \dots, e_h(t))$ . Obviously,  $e_{i_0}(s) = e_1(s)$ . Also  
 652  $e_1(t) = e_2(s)$  implies  $e_{i_0}(t) = e_1(t)$ . This shows that  $e_{i_0}$  and  $e_1$  are associated to the  
 653 same edge in  $E$ . Therefore, given a 2-sequence, the choice of a corresponding Eulerian  
 654 path correspond to the choice of  $\sigma = (\tau_1, \dots, \tau_{|E|})$  where  $\tau_e$  is a permutation of  $\{1, \dots, \pi_e\}$ .  
 655 Therefore  $\#\mathcal{E} = (\#\mathcal{S}) \prod_{e \in E} \pi_e!$ .

656 If  $G$  is undirected, the proof is still valid, but the operators  $e \mapsto e(s)$  and  $e \mapsto e(t)$  are  
 657 now induced the natural direction of the considered Eulerian path. ◀

658 Counting the number of Eulerian paths in a undirected graph has been proven to be a  
 659  $\#P$ -complete problem [4]. Since  $G \mapsto \psi(G)$  is bijective, counting the number of 2-admissible  
 660 sequences is also  $\#P$ -complete. Finally, counting Eulerian trails of weighted digraphs has  
 661 been well studied, hence the following proposition:

662 ► **Proposition 19.** If  $G = (V, E)$  is a weighted digraph, with  $\Pi(G) \in \mathcal{M}_d(\mathbb{N})$ . Then, if  $\deg(v)$   
 663 is the indegree of a vertex  $v$ , the number  $p_2$  of 2-admissible sequences is

$$664 \quad p_2 = \frac{t(\psi(G))}{\prod_{e \in E} \pi_e!} \prod_{v \in V} (\deg_{\psi(G)}(\psi(v)) - 1)! \quad (15)$$

665 where  $t(G)$  is the number of spanning trees of a graph  $G$ . If  $L$  is the Laplacian matrix of  $G$ ,  
 666 then  $t(G)$  is given by

$$667 \quad t(G) = \prod_{\substack{\lambda_i \in Sp(L) \\ \lambda_i \neq 0}} \lambda_i \quad (16)$$

668 **Proof.** Direct consequence of BEST Theorem [8]) and Matrix tree theorem [5]) ◀

669 To use formula 15,  $\deg_{\psi(G)}(\psi(v))$  can be obtained using the following formula:  $\deg_{\psi(G)}(\psi(v)) =$   
 670  $\sum_{n \in V} \pi_{nv} + \sum_{n \in V} \pi_{vn}$ .

## 671 **C Proofs section 3.2 ( $w \geq 3$ )**

672 **Proof of Proposition 3.** Let  $x = x_1, \dots, x_p$  be a  $w$ -admissible sequence of  $G$ . Let  $P$  be a walk  
 673 on  $H^{(w-2)}$ , and  $P[i]$  be the  $i$ -th element of  $P$ ,  $P[i] \in H^{(w-2)}$ :  $P[i] = (P[i]_1, \dots, P[i]_{w-1})$ .

Let us suppose that  $w \leq p$  (which we can always do), and let us show the following property by induction on  $k$ :

$\forall k \in \{w-1, \dots, p\}$ ,  $\exists$  walk  $P$  on  $H^{(w-2)}$  such that :

$$x_{1:k} = P[1]_1, P[2]_1, \dots, P[k - (w-1)]_1, P[k+1 - (w-1)]_{1:(w-1)}$$

- Initialisation:  $k = w-1$ . By construction of  $H^{(w-2)}$ ,  $x_{1:w-1}$  is the authentic sequence of "static walk":  $P = P[1] = x_{1:w-1} \in H^{(w-2)}$ .
- Induction: let us suppose the property is verified for  $k \in \{w-1, \dots, p-1\}$ , i.e there exists a walk  $P$  on  $H^{(w-2)}$  such that:

$$x_{1:k} = P[1]_1, P[2]_2, \dots, P[k - (w-1)]_1, P[k+1 - (w-1)]_{1:(w-1)}$$

Since  $x$  is  $w$ -admissible, then by definition:

$$\forall i \in \{k+1 - (w-1), \dots, k\}, \forall j \in \{i+1, \dots, \min\{k+1, i+w-1\}\} : (x_i, x_j) \in E$$

674 Therefore, by definition of  $H^{(w-2)}$ ,  $\xi^{k+1} = x_{k+1-(w-1)}, \dots, x_{k+1} \in H^{(w-2)}$ .

Let  $P[k+2 - (w-1)] \hat{=} \xi^{k+1}$ , then

$$P[k+2 - (w-1)]_{1:(w-1)} = x_{k+1-(w-1)}, \dots, x_{k+1}$$

Besides, from the induction assumption:  $\forall i \in \{1, \dots, k - (w-1)\}$ ,  $P[i]_1 = x_i$ . This ensures that:

$$x_{1:(k+1)} = P[1]_1, P[2]_1, \dots, P[k+1 - (w-1)]_1, P[k+2 - (w-1)]_{1:(w-1)}$$

675 which ends the induction and the proof. ◀

676 **Proof of Lemma 5.** Let  $P = P[1], \dots, P[r]$  a walk on  $H^{(w-2)}$  going through a strongly  
 677 connected component  $C$ , with an arbitrary ordering of its vertices, i.e  $C = \{c_1, \dots, c_m\}$ . This  
 678 means  $\exists (m_0, i_0) \in \{1, \dots, m\} \times \{1, \dots, r-1\}$  s.t  $P[i_0] = c_{m_0}$  and  $(c_{m_0}, P[i_0+1]) \in E^{(w-2)}$ .  
 679 Let  $\mathcal{P}_C = c_{m_0}, c_{j_1}, \dots, c_{j_v}$  be a path in  $C$  with  $(c_{j_v}, P[i_0+1]) \in E^{(w-2)}$ . Let  $Q$  be the new

680 path:  $Q = P[1], \dots, P[i_0], c_{j_1}, \dots, c_{j_v}, P[i_0 + 1], \dots, P[r]$ . By construction of  $H^{(w-2)}$ , the edges  
 681 (between elements of  $V$ ) created by any walk on  $H^{(w-2)}$  are in  $E$ , so  $Q$  is still admissible.

682 Let us label every node of  $R(H^{(w-2)})$  representing a strongly connected component of  
 683  $H^{(w-2)}$  by any 2-admissible sequence (one exists thanks to Prop. 9). A walk on  $H^{(w-2)}$ :  
 684  $x_1, \dots, x_p$  can be met by a walk on  $R(H^{(w-2)})$  using the following procedure:

685 For  $i \in \{1, \dots, p-1\}$ :

- 686 ■ if  $x_i, x_{i+1} \in E^{(w-2)}$ , we keep  $x_i$  and  $x_{i+1}$
- if  $x_i$  is a vertex of  $H^{(w-2)}$  and  $x_{i+1}$  is in a strongly connected component of  $H^{(w-2)}$  (but  
 a node of  $R(H^{(w-2)})$ ), represented by  $c_1, \dots, c_{C_i}$ , then a path from  $x_{i+1}$  to  $c_1$  exists since  
 the component is strongly connected:  $x_{i+1}, p_1, \dots, p_m, c_1$ . We keep

$$x_i, x_{i+1}, p_1, \dots, p_m, c_1, \dots, c_{C_i}$$

687 Using the aforementioned result, this does not perturb admissibility.

- 688 ■ if  $x_{i+1}$  is a vertex of  $H^{(w-2)}$  and  $x_i$  is in a strongly connected component of  $H^{(w-2)}$ , we  
 689 proceed similarly ( $x_i$  and  $x_{i+1}$  are swapped).
- 690 ■ if both  $x_{i+1}$  and  $x_i$  are strongly connected components of  $H^{(w-2)}$ , we add intermediary  
 691 nodes to both components similarly.

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