

Sequence Graphs: Characterization and Counting of Admissible Elements

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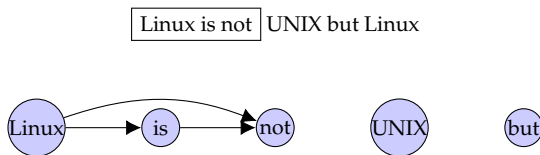


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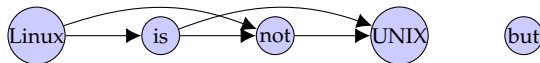


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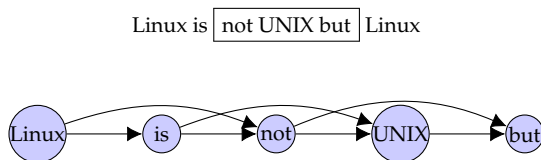


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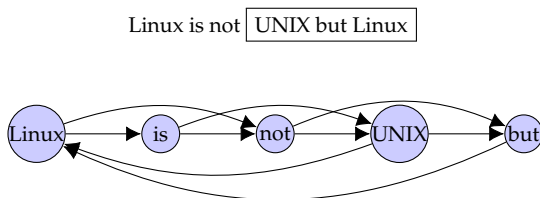


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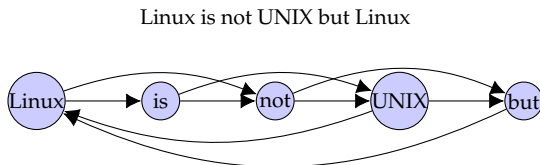
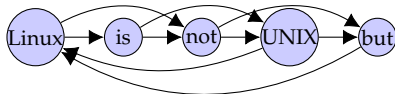


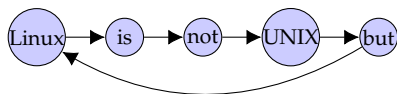
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- Such models still induce ambiguity due to the fact that several sequences can *a priori* create the same graph.



(a) No ambiguity ($w = 3$)



(b) Ambiguity ($w = 2$)

Figure: In case (b), the sequence graph is ambiguous: any circular permutation of the words admits the same representation.

- Popular models (word2vec, Glove, fastText, Latent random walks) use co-occurrence statistics
- What is their level of ambiguity?
- Difference with other Language models (e.g. LSTMs)?

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x is a w -realization of G

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- Correspondence between the monoid X^* into the graph set \mathcal{G} :

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- The degree of ambiguity of a representation is given by:

$$\text{Card Im } \phi_w^{-1}(G)$$

When G is a given graph.

Sequence Graphs: REALIZABLE_w and NUMREALIZATIONS_w

Problem 1 (REALIZABLE_w)

Parameters: Window size w

Input: Graph G (and optional matrix weights Π)

Output: True if (G, Π) is the w -sequence graph of some sequence x , False otherwise.

Problem 2 (NUMREALIZATIONS_w)

Parameters: Window size w

Input: Graph G (and optional matrix weights Π)

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

2-sequence Graphs: $w = 2$

First results: The case $w = 2$ leads to simple characterization and algorithmic treatment:

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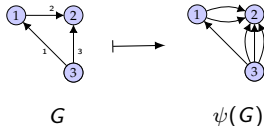
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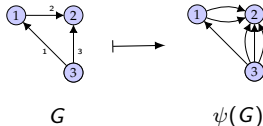


- Eulerian reductions.

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Table: Complexity for various instances ($w = 2$)

Data Instance	NUMREALIZATIONS ₂		REALIZABLE ₂	
	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	$R^+(G)$ straight line with unit weights
Weighted digraph	P	\mathbb{N} (BEST Theorem)	P	$\psi(G)$ (semi)Eulerian

General Case: $w \geq 3$

No trivial reduction. We propose 3 different approaches:

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 - with polynomial time complexity in the unweighted and undirected case
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 - Suffers from a large number of constraints.
- c) A dynamic programming formulation for NUMREALIZATIONS_w
 - with exponential time average complexity but much better than worst-case scenario.

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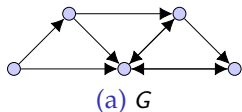
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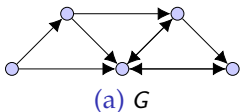


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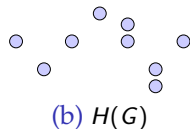
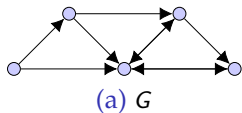


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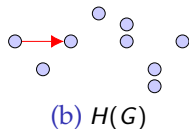
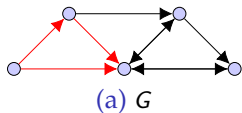


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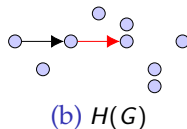
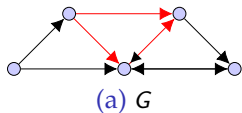


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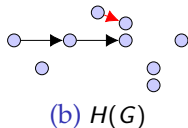
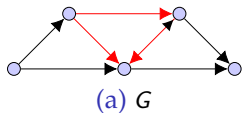


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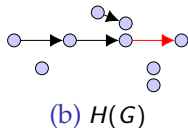
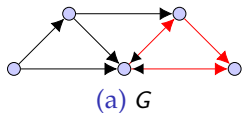


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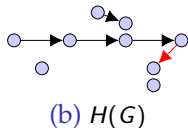
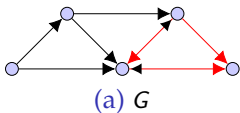


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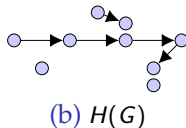
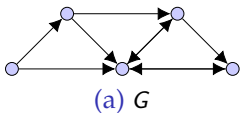


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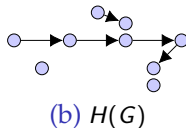
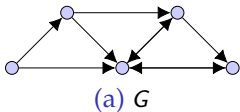
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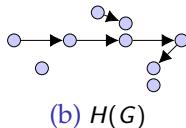
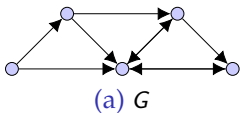


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→ If $w = 3$, a realization of G is a walk in $H(G)$

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Let $x = x_1, \dots, x_p$ be a w -realization of a graph $G = (V, E)$. If $w \leq p$, x , then x corresponds to a walk of length $p - w + 1$ on $H^{(w-2)}$.

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Theorem 3.2 (Khalife, 2020)

Let G a graph and $w \in \mathbb{N}^* - \{1, 2\}$. If G is undirected then REALIZABLE_w is in P .

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Let G a graph and $w \in \mathbb{N}^* - \{1, 2\}$. If G is undirected then REALIZABLE_w is in P .

Proof. Extract connected components of $H^{(w-2)}$. For each of them, there exists a walk covering all vertices at least once. A potential realization cannot generate more edges than these walks. Use the definition to compute the realizations from the walks and compare.

General Case: Direct Formulation and Digraphs

- Digraphs: the analogue procedure enumerates all paths in the DAG $R(H^{(w-2)})$, where the operator R is the contraction in strongly connected components.

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Example

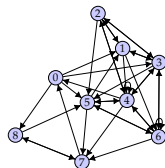
$$x_{\text{init}} = 0, 3, 1, 2, 3, 4, 4, 2, 5, 1, 4, 6, 3, 5, 6, 6, 4, 7, 0, 8, 5, 7$$

For $P \in \mathbb{N}^*$, let $x \in \mathbb{N}^{22P}$:

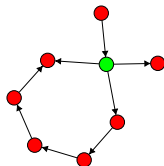
$$\forall i \in \{0, \dots, 22P - 1\} \quad x_i = x_{\text{init}}[i] + 10 \left\lfloor \frac{i}{22} \right\rfloor$$

Claim: With $w = 3$, $R(H(x))$ has at least 2^P paths.

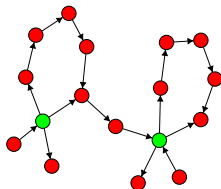
General Case: Direct Formulation and Digraphs



(a) $G = \phi_3(x_{\text{init}})$



(b) $R(H(x))$ ($P = 1$)



(c) $R(H(x))$ ($P = 2$)

Figure: Direct approach has exponential complexity in the worst case

- For digraphs and weighted graphs, the complexity classes characterizations of NUMREALIZATIONS_w and REALIZABLE_w remain opened ($w \geq 3$).

General Case: Integer Programming Formulation

Khalife S. & Ponty Y. (2020). *Sequence graphs realizations and ambiguity in language models (hal-02495333, v2)*

REALIZABLE_w can be formulated as an *Linear integer program*.

Decision variable $X \in \mathbb{M}_{n,p}(\{0, 1\})$ where $X_{i,j} = 1 \iff x_j = i$

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→ $w = 3$ (window size), $n = 20$ (vocabulary size), $p = 10$ (sequence length): 7600 constraints. Not solvable in practice with Branch and Bound.

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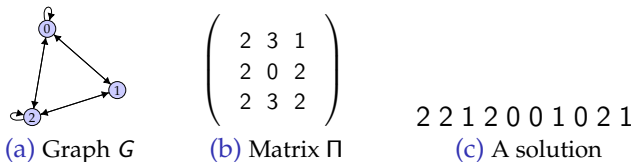


Figure: Example of instance solved using the Linear Integer Programming formulation ($n = 3, p = 10, w = 3$).

General Case: Dynamic Programming Formulation

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$N_w [\Pi, \rho, \mathbf{u}]$ number of realizations:

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Initialisation

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

The total number of admissible sequences is $N_w[\Pi, p, \varepsilon]$, ε being the empty prefix.

Dynamic Programming Formulation: Complexity Study

Proposition 4.1 (Khalife, 2020)

Comparison of the worst case complexity \mathcal{W}_C with Average complexity \mathcal{A}_C :

$$\frac{2^{w p}}{\mathcal{U}(w p, \alpha^2 p^2)} \leq \frac{\mathcal{W}_C}{\mathcal{A}_C}$$

$$\text{where } \mathcal{U}(m, r) = \frac{1}{\binom{m+r-1}{r-1}} \sum_{m_z=1}^{\min(r, m)} \binom{r}{m_z} \binom{m-1}{m_z-1} \left(\frac{m}{m_z} + 1\right)^{m_z}$$

Dynamic Programming Formulation: Complexity Study

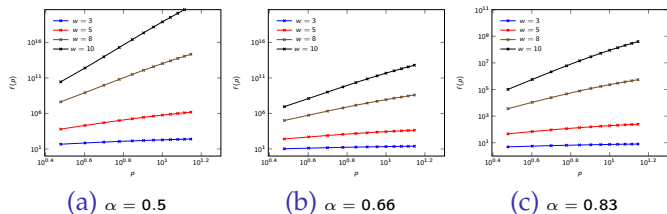
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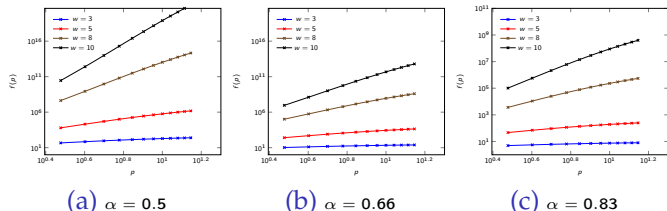
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- Good average complexity compared to worst-case
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Experiment 1: Ambiguity w.r.t window size

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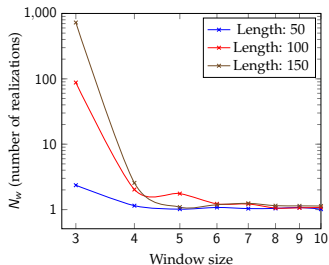


Figure: Estimation of the average number of realizations N_w .
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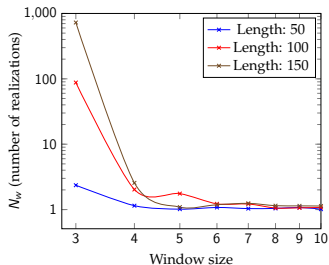


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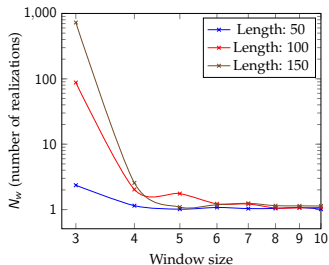


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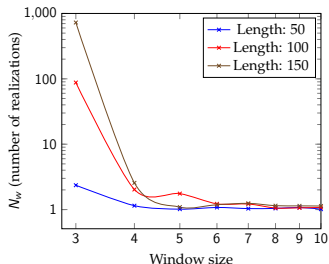


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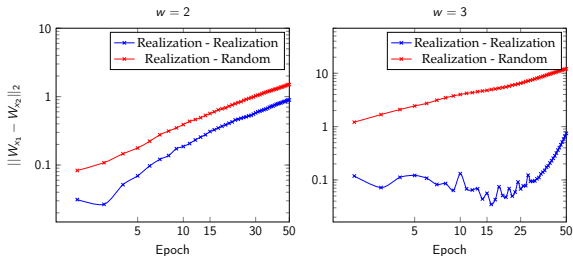


Figure: $\|W_{x_1} - W_{x_2}\|_2 = f(\text{Epoch})$ - LSTM, log – log scale

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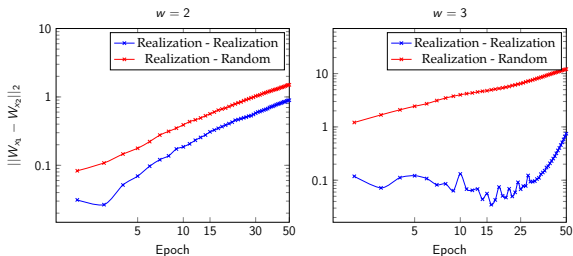


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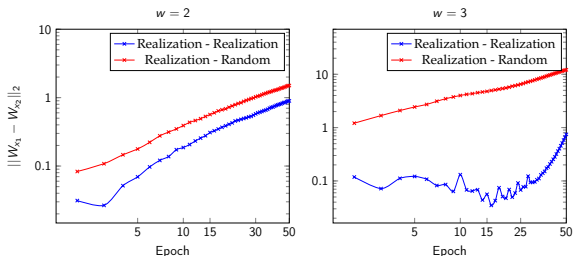


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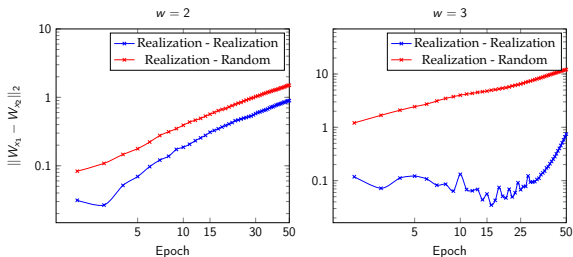


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Conclusion

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- Allows ambiguity measurement in co-occurrence based models
- Ambiguity is not shared with a recurrent neural network (LSTMs)

2-sequence Graphs

Proposition 6.1

Let $G = (V, E)$ a directed acyclic graph (DAG). G is a 2-sequence graph if and only if it is a straight line (directed tree where each node has at most one child). In this case, G has a unique realization.

Theorem 6.2

Let $G = (V, E)$ a unweighted digraph.

G is a 2-sequence graph $\iff R^+(G)$ is a 2-sequence graph $\iff R^+(G)$ is a straight line and its weights are all equal to 1.

where $R^+(G)$ is the DAG obtained by weighted contraction of G in strongly connected components. Proofs by contradiction.

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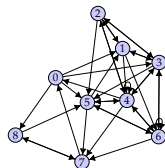
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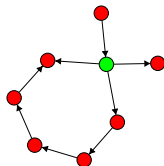
$$\forall i \in \{0, \dots, 22P - 1\} \quad x_i = x_{\text{init}}[i] + 10 \left\lfloor \frac{i}{22} \right\rfloor \quad (2)$$

Claim: With $w = 3$, $R(H(x))$ has at least 2^P paths.

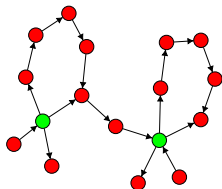
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General Case: Integer Programming Formulation

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

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

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

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

General Case: Integer Programming Formulation

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

- Branch and bound methods available

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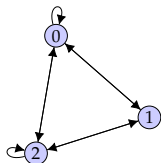
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(a) Graph G

$$\begin{pmatrix} 2 & 3 & 1 \\ 2 & 0 & 2 \\ 2 & 3 & 2 \end{pmatrix}$$

(b) Matrix Π

$$2 \ 2 \ 1 \ 2 \ 0 \ 0 \ 1 \ 0 \ 2 \ 1$$

(c) A solution

Figure: Example of instance solved using the Linear Integer Programming formulation ($w = 3$).

General Case: Direct Formulation

Idea: For $w > 3$, recursively iterate the process for $k \leq w - 2$:

$$E^{(k)} = \{u_{1:(k+1)} \in V^{k+1} \mid u_{1:k} \in E^{(k-1)}, u_{2:(k+1)} \in E^{(k-1)} \\ \text{s.t.}(u_1, u_{k+1}) \in E\}$$

$$H^{(k)} \hat{=} (E^{(k)}, E^{(k+1)})$$

Proposition 6.3

Let $x = x_1, \dots, x_p$ be a w -realization of a graph $G = (V, E)$. If $w \leq p$, x , then x corresponds to a walk of length $p - w + 1$ on $H^{(w-2)}$.

→ Proof by induction on $k \in \{1, \dots, p\}$

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- of the graph with weights matrix Π
 - of length ρ with starting pattern \mathbf{u}

Recursion

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Π' is an update of Π following:

$$\Pi'_{(\mathbf{u}, v)} := (\pi_{ij} - \#\{k \in \{1, \dots, |\mathbf{u}|\} \mid (u_k, v) = (i, j)\})_{(i, j) \in V^2}$$

General Case: Dynamic Programming Formulation

Initialisation

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

The total number of admissible sequences is $N_w[\Pi, p, \varepsilon]$, ε being the empty prefix.

Dynamic Programming Formulation: Complexity Study

Proposition 6.4

Dynamic programming formulation: Estimation of the Worst case complexity \mathcal{W}_C and Average complexity \mathcal{A}_C .

$$\mathcal{W}_C = n^w 2^{wp} \quad \mathcal{A}_C = n^w \mathcal{E}_C$$

$$\mathcal{L}(wp, n^2) \leq \mathcal{E}_C \leq \mathcal{U}(wp, n^2)$$

○ n number of words, w window size, p sequence length

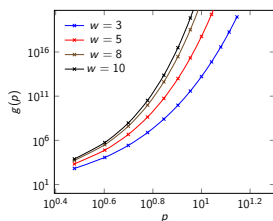
$$\circ \mathcal{L}(m, r) = \frac{1}{\binom{m+r-1}{r-1}} \sum_{m_z=1}^{\min(r,m)} \binom{r}{m_z} \binom{m-1}{m_z-1} 2^{m_z-1} (m - m_z + 2)$$

$$\circ \mathcal{U}(m, r) = \frac{1}{\binom{m+r-1}{r-1}} \sum_{m_z=1}^{\min(r,m)} \binom{r}{m_z} \binom{m-1}{m_z-1} \left(\frac{m}{m_z} + 1\right)^{m_z}$$

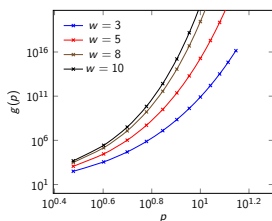
A lower bound of the ratio $\frac{\mathcal{W}_C}{\mathcal{A}_C}$ is given by $\frac{2^{wp}}{\mathcal{U}(wp, \alpha^2 p^2)}$.

Dynamic Programming Formulation: Complexity Study

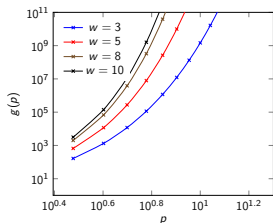
Lower bound of average complexity \mathcal{A}_C of the dynamic programming formulation, for several values of w and α (ratio of distinct words over ρ) in log – log scale.



(a) $\alpha = 0.5$



(b) $\alpha = 0.66$



(c) $\alpha = 0.83$

■ Still suffers from exponential complexity

Identification: use the Knowledge Graph

Algorithm 1: Feature extraction with knowledge graph and ontology

Data: Knowledge Graph \mathbf{G} , Query \mathbf{q} , Entity candidate \mathbf{e} with initial score s^0 , Types $(t_j)_{1 \leq j \leq \tau}$

Result: Entity candidate representation

- 1 $\mathbf{X}^{q,e} = [s^0]$;
 - 2 Get neighbor nodes of \mathbf{e} ;
 - 3 **for** $j = 1$ **to** τ **do**
 - 4 Aggregate text description of neighbors of type t_j ;
 - 5 Compute score s_{t_j} between $\mathcal{N}_{t_j}(\mathbf{e})$ and the query \mathbf{q} ;
 - 6 Append s_{t_j} to $\mathbf{X}^{q,e}$;
 - 7 **end**
 - 8 Return Score vectors $(\mathbf{X}^{q,e})_{1 \leq j \leq \tau+1}$
-

Sum up: Graph-based Comparison

Algorithm 2: Named entity identification (Inference)

Data: Knowledge base \mathbf{B} and its graph \mathbf{G}_B , queries $(\mathbf{q}_i)_{1 \leq i \leq M}$, scoring threshold \mathbf{K} , trained predictor $\hat{\mathbf{F}}$

Result: Entity candidate representation

- 1 **for** $i = 1$ to M **do**
 - 2 Use filtering with query \mathbf{q}_i , get list of \mathbf{K} top ranked entities $(\mathbf{e}_h^1)_{1 \leq h \leq \mathbf{K}}$
 - 3 Use algorithm 1 to return \mathbf{K} entity candidates new representations;
 - 4 Evaluate $\hat{\mathbf{F}}$ on each vector score and use maximum a posteriori to infer estimated gold entity $\hat{\mathbf{g}}_i$;
 - 5 **end**
 - 6 Return $(\hat{\mathbf{g}}_i)_{1 \leq i \leq M}$ (list of estimated gold entities);
-