Walk Aggregation Graph Networks

with Applications to Molecules

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Qualifying Presentation

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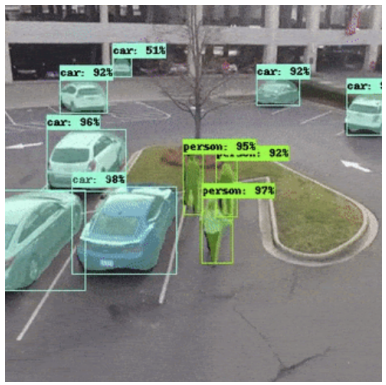
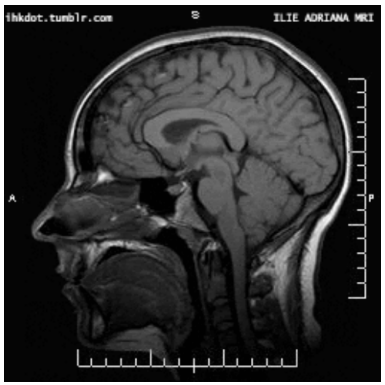
Overview

1. Molecular Property Prediction and Representations for Molecules
2. Existing Approaches to Building Representations for Molecules
3. Our Approach I: N-gram Graph
4. Our Approach II: AWARE

Machine Learning Everywhere

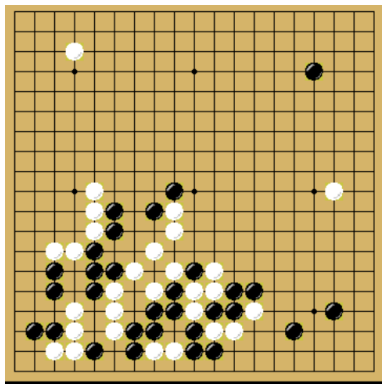


Computer Vision



Medical Imaging

NLP

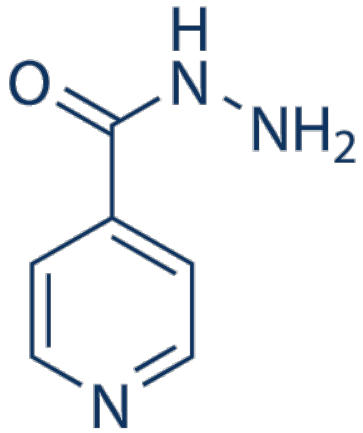


Game Playing

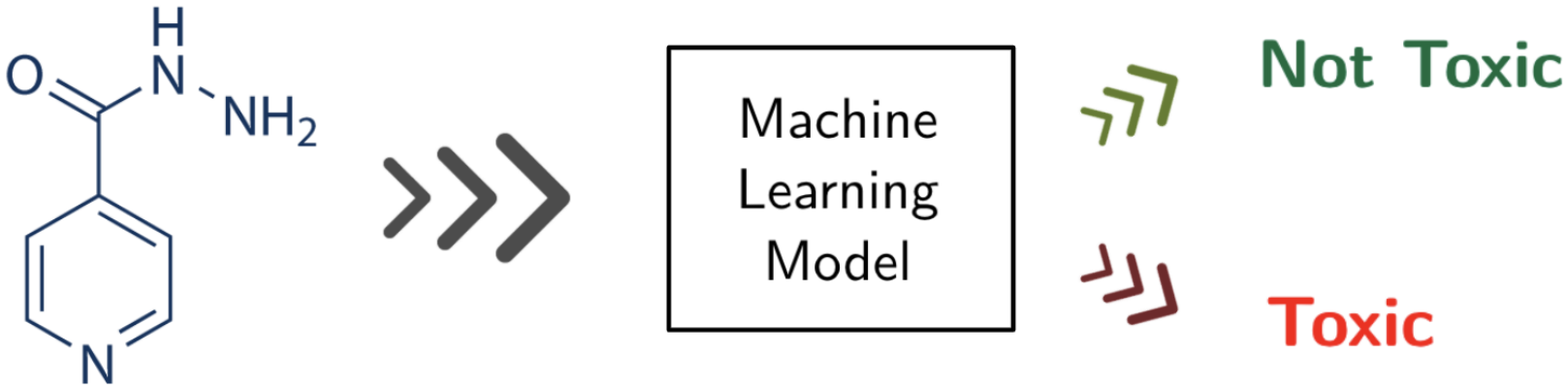
And more!

Molecules?

What about molecules?



Molecular Property Prediction



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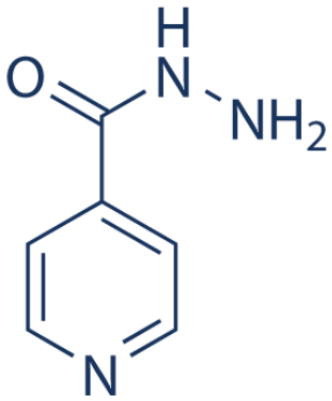

HOW?

Machine Learning Model

Not Toxic

Toxic

Challenge: Representation

Input to traditional machine learning models: **vectors**

How to represent a molecule as a vector?

- Fingerprints *e.g.* Morgan fingerprints
- Graph kernels *e.g.* WL-kernel
- Graph neural networks (GNN): GCN, Weave

Fingerprints/kernels are unsupervised and fast to compute.
GNNs are end-to-end supervised, more expensive; but powerful.

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N-gram Graph

Our previous work [1] is inspired by the **N-gram approach in NLP**.

- Unsupervised
- Fast to compute
- Overall better performance than traditional methods

[1] Liu, Shengchao, **Mehmet F. Demirel**, and Yingyu Liang. "N-gram graph: Simple unsupervised representation for graphs, with applications to molecules." Advances in Neural Information Processing Systems. 2019.

N-gram approach in NLP

n-gram is a contiguous sequence of n words from a given sentence.

"I love living in Madison"

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n-gram is a contiguous sequence of n words from a given sentence.

"I love living in Madison"

- **1-grams:** "I", "love", "living", "in ", "Madison"
- **2-grams:** "I love", "love living", "living in", "in Madison"
- **3-grams:** "I love living", "love living in", "living in Madison"

⋮

N-gram approach in NLP

n-gram is a contiguous sequence of n words from a given sentence

N-gram count vector $c_{(n)}$ is a numeric representation vector:

- its coordinates correspond to all n-grams
- its coordinate values are the number of times the corresponding n-gram shows up in the sentence

Notice that $c_{(1)}$ is just the histogram of the words in the sentence.

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Solution: Dimensionality reduction by word embeddings: $f_{(1)} = W c_{(1)}$

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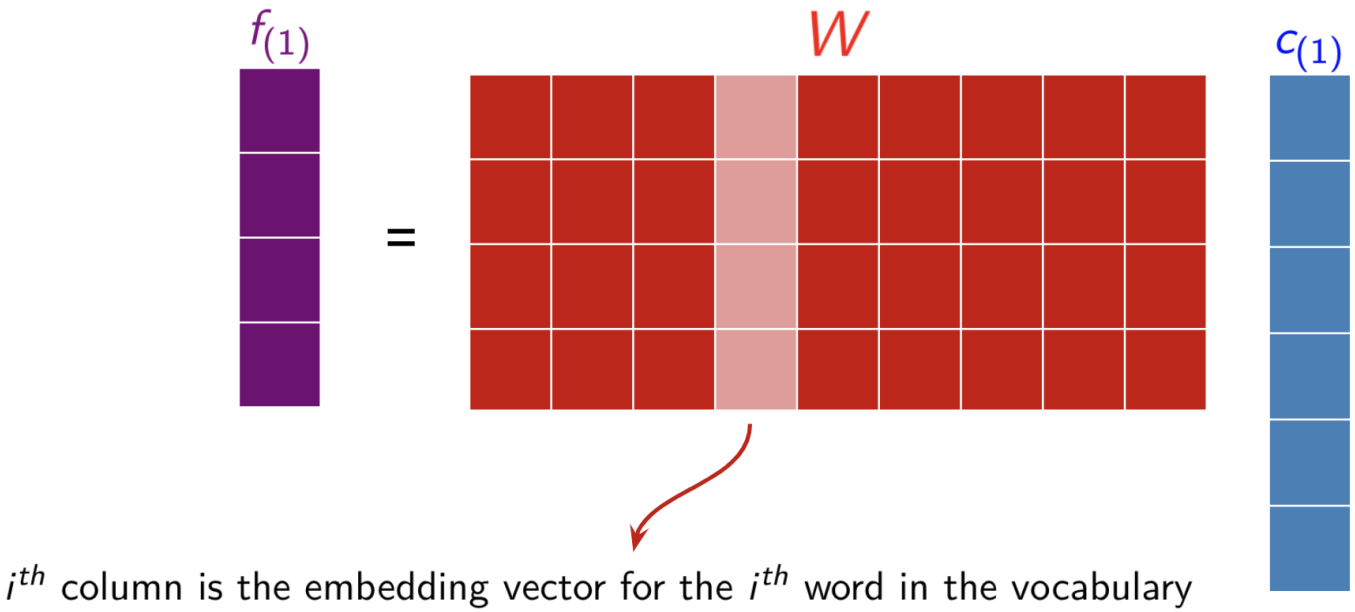

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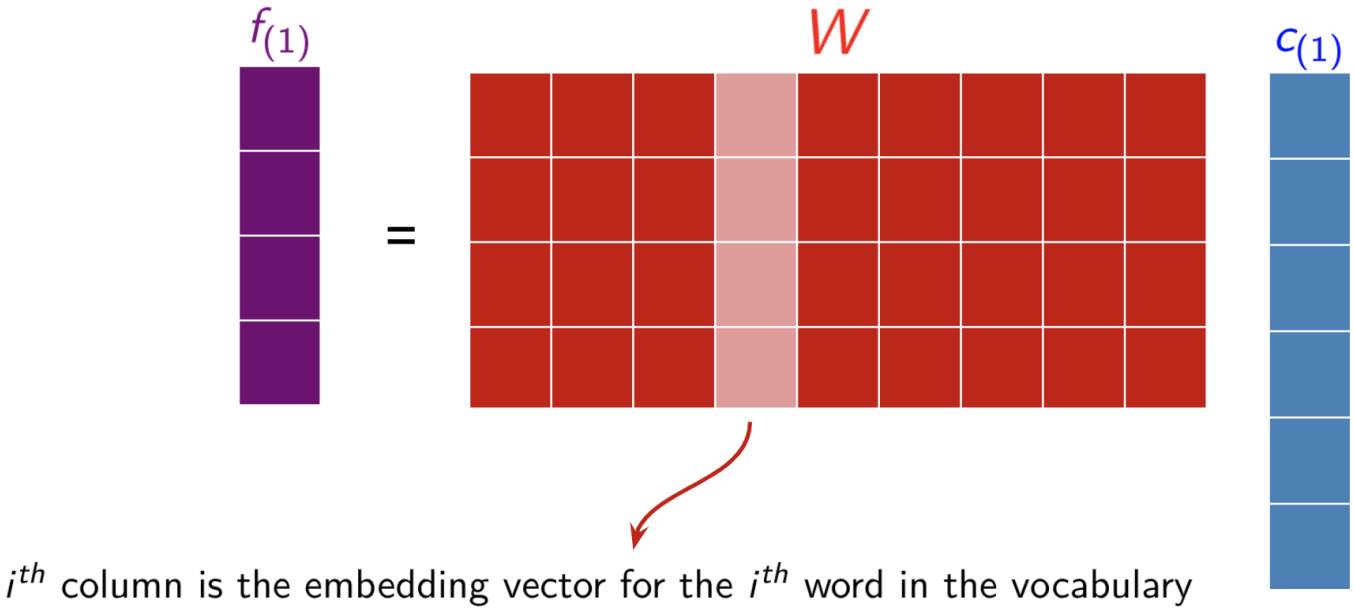

$f_{(1)}$ is just the sum of the word vectors in the sentence!

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Solution: Dimensionality reduction by word embeddings: $f_{(1)} = W c_{(1)}$

For general n:

- Embedding of an n-gram is the entry-wise product of its word vectors.
- $f_{(n)}$ is the sum of the embeddings of the n-grams in the sentence.

N-gram *graphs*?

Sentences are linear graphs on words.
Molecules are graphs on atoms with attributes!

- atom symbol, atom degree, is-acceptor, ...

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Molecules are graphs on atoms with attributes!

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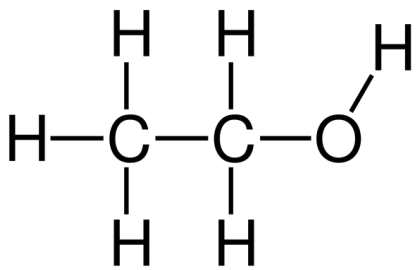
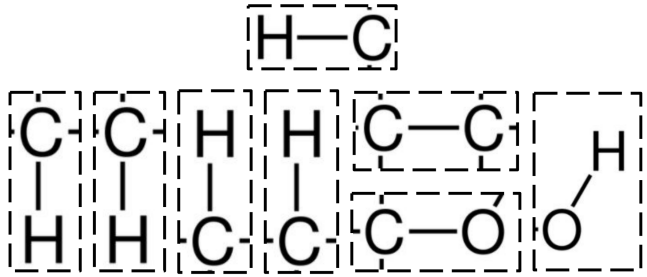
We can view:

- atoms with different attributes as different words
- walks of length n as n-grams.



A molecule



Its 2-grams

N-gram Graph algorithm

Sentences are linear graphs on words.
Molecules are graphs on atoms with attributes!

Given the embeddings for the atoms (vertex vectors):

- Enumerate all n-grams (walks of length n)
- Embedding of an n-gram: entry-wise product of its vertex vectors
- $f_{(n)}$: sum of embeddings of all n-grams
- Final N-gram Graph embedding f_G: concatenation of $f_{(1)}, f_{(2)}, \ldots, f_{(T)}$

N-gram Graph as simple GNN

GNN keeps a vector h_i for each vertex in the graph and uses some neighborhood aggregation strategy that iteratively updates by aggregating those of its neighbors.

$$f_i^{(k)} = \textbf{AGGREGATE}^{(k)}\left(\{h_j^{(k-1)} : j \in \text{Neighbor(i)}\}\right)$$
$$h_i^{(k)} = \textbf{COMBINE}^{(k)}\left(h_i^{(k-1)}, f_i^{(k)}\right)$$

N-gram Graph as simple GNN

Given vectors f_i for vertices i and graph adjacency matrix $\mathcal{A}$:

$F_{(1)} = F = [f_1, \ldots, f_m], f_{(1)} = F_{(1)}\mathbf{1}$
for each $n \in [2, T]$ **do**
  $F_{(n)} = (F_{(n-1)}\mathcal{A}) \odot F$
  $f_{(n)} = F_{(n)}\mathbf{1}$
end for
$f_G = [f_{(1)}; \ldots; f_{(T)}]$

Equivalent to a simple GNN without any parameters!

Experimental Results

60 tasks on 10 datasets from MoleculeNet [2].

Methods:

- WL-Kernel + SVM
- Morgan FP + RF or XGB
- Graph CNN (GCNN), Weave Neural Network, Graph Isomorphism Network (GIN)

- N-gram Graph + RF or XGB
- Vertex embedding dimension $r = 100$ and $T = 6$

[2] Wu, Zhenqin, et al. "MoleculeNet: a benchmark for molecular machine learning." Chemical science 9.2 (2018): 513-530

Experimental Results

N-gram Graph + XGB: top-1 in 21 and top-3 in 48 out of 60 tasks
Overall better performance than other methods

Table 2: Performance overview: (# of tasks with top-1 performance, # of tasks with top-3 performance) is listed for each model and each dataset. For cases with no top-3 performance on that dataset are left blank. Some models are not well tuned or too slow and are left in "-".

Dataset	# Task	Eval Metric	WL SVM	Morgan RF	Morgan XGB	GCNN	Weave	GIN	N-Gram RF	N-Gram XGB
Delaney	1	RMSE					1, 1	–	0, 1	0, 1
Malaria	1	RMSE		1, 1				–	0, 1	0, 1
CEP	1	RMSE		1, 1				–	0, 1	0, 1
QM7	1	MAE					0, 1	–	0, 1	1, 1
QM8	12	MAE		1, 4	0, 1	7, 12	2, 6	–	0, 2	2, 11
QM9	12	MAE	–		0, 1	4, 7	1, 8	–	0, 8	7, 12
Tox21	12	ROC-AUC	0, 2	0, 7		0, 2	0, 1		3, 12	9, 12
clintox	2	ROC-AUC	0, 1			1, 2	0, 1			1, 2
MUV	17	PR-AUC	4, 12	5, 11	5, 11			0, 7	2, 4	1, 6
HIV	1	ROC-AUC		1, 1					0, 1	0, 1
Overall	60		4, 15	9, 25	5, 13	12, 23	4, 18	0, 7	5, 31	**21, 48**

Assumptions.

- Each vertex has $S = 1$ attribute and it takes values from a set of size K. $W \in \mathbb{R}^{r \times K}$ is the vertex embedding matrix.
- Assume for simplicity that no two vertices in a walk p can have the same attribute value.

Idea: There exists a linear mapping $W^{[n]}$ such that $f_{(n)} = W^{[n]} c_{(n)}$.

- For $S = 1$, $W^{[n]}$ is the n-way column Hadamard product of W.
- There are a wide family of prior distributions on W such that $W^{[n]}$ has RIP with high probability.

  $\Longrightarrow$ With sparse $c_{(n)}$, $c_{(n)}$ can efficiently be recovered from $f_{(n)}$.
- A linear classifier learned on $f_{(n)}$ is comparable to the best linear classifier on $c_{(n)}$.

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Current Work: AWARE

Parametrization of the N-gram graph algorithm:
Attentive **W**alk **A**ggregation G**R**aph N**E**twork

The N-gram graph algorithm has no parameters and requires no training. Therefore, it is efficient in computation. However:

- Huge design space for adding trainable parameters.
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Weighted Features

The downstream learning tasks may prefer certain directions both in the vertex embedding space and final embedding space.

Given vectors $F = [f_1, \ldots, f_m]$ for m vertices and graph adjacency matrix $\mathcal{A}$:

$F_{(1)} = F$, $f_{(1)} = F_{(1)}\mathbf{1}$
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Then for a vertex embedding f_i, $W_1 f_i$ will stretch its components along W_1's larger singular vectors while relatively shrink the components along the smaller ones.

Same idea for W_3.

Attentive Messages

Some nodes have more impact on their neighbors.

- Weighted sum of latent vectors from neighbors (with attention).

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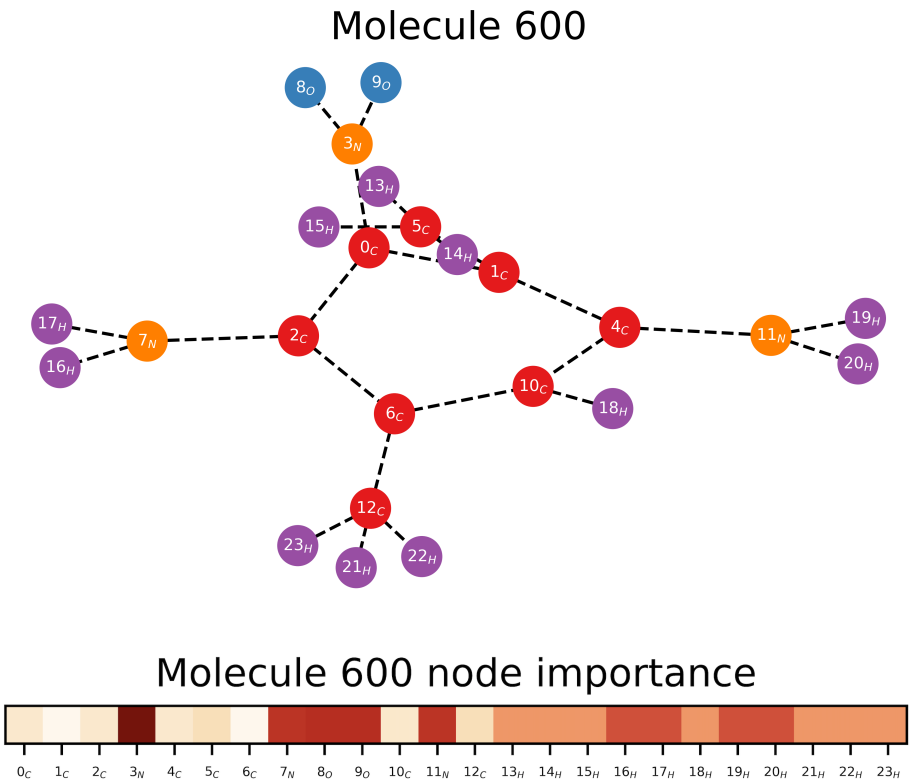
$$[s_{(n-1)}]_{ji} = [F_{(n-1)}]_j^\top W_2 [F_{(n-1)}]_i$$

$$[\bar{S}_{(n-1)}]_{ji} = \frac{\exp([s_{(n-1)}]_{ji})}{\sum_{k \in \text{neighbors of } i} \exp([s_{(n-1)}]_{ki})}$$

Attentive Messages: Visualization

Mutagenicity dataset: NO_2 and NH_2 atom groups are known to have a mutagenic effect in a molecule.



AWARE performs top-1 in 27 and top-3 in 48 out of 60 tasks
Overall better performance than other methods, including N-gram Graph

Table 3. Overall performance: (# of tasks with top-1 performance, # of tasks with top-3 performance) is listed for each model and each dataset. For cases with no top-3 performance on that dataset are left blank. Some models are not well tuned or too slow and are left in "-".

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HIV	1	ROC	1,1	0,1					0,1		
MUV	17	ROC	1,7	1,7	3,5	1,9	0,1	1,2	1,4	0,2	9,14
Total	60		3,13	1,10	3,7	9,24	1,2	8,18	7,41	1,18	**27,48**

Theoretical Analysis

Assumption. Each vertex has $S = 1$ attribute and it takes values from a set of size K. $W \in \mathbb{R}^{r \times K}$ is the vertex embedding matrix. Also assume that $W_1 = W_3 = I$ and σ is linear.

Idea: There exists a linear mapping $W^{[n]}$ such that $f_{(n)} = W^{[n]} \Lambda_{(n)} c_{(n)}$ where $\Lambda_{(n)}$ is a diagonal weighting matrix that depends on the scoring matrix $\bar{S}$.

- A similar analysis can be applied to $\Lambda_{(n)} c_{(n)}$ instead of $c_{(n)}$.
- Benefit of weighting: If $\Lambda_{(n)}$ emphasizes important features for prediction, then better to learn over $\Lambda_{(n)} c_{(n)}$ rather than $c_{(n)}$. Thus, we can learn over $f_{(n)} = W^{[n]} \Lambda_{(n)} c_{(n)}$.

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Thank you!

Appendix

Theorem 1 *If* $r = \Omega(ns_n^3 \log K)$ *where* s_n *is the sparsity of* $c_{(n)}$*, then there is a prior distribution over* W *so that* $f_{(n)} = T_{(n)}c_{(n)}$ *for a linear mapping* $T_{(n)}$*. If additionally* $c_{(n)}$ *is the sparsest vector satisfying* $f_{(n)} = T_{(n)}c_{(n)}$*, then with probability* $1 - O(S\exp(-(r/S)^{1/3}))$*,* $c_{(n)}$ *can be efficiently recovered from* $f_{(n)}$*.*

Appendix

Prediction Power. Consider a prediction task and let $\ell_{\mathcal{D}}(g)$ denote the risk of a prediction function g over the data distribution $\mathcal{D}$.

Theorem 2 *Let g_c be a prediction function on the count statistics $c_{[T]}$. In the same setting as in Theorem 1, with probability $1 - O(TS\exp(-(r/S)^{1/3}))$, there is a function g_f on the N-gram graph embeddings f_G with risk $\ell_{\mathcal{D}}(g_f) = \ell_{\mathcal{D}}(g_c)$.*

Consider the binary classification task with the logistic loss function $\ell(g, y)$ where g is the prediction and y is the true label. Let $\ell_{\mathcal{D}}(\theta) = \mathbb{E}_{\mathcal{D}}[\ell(g_\theta, y)]$ denote the risk of a linear classifier g_θ with weight vector θ over the data distribution $\mathcal{D}$. Let θ^* denote the weight of the classifier over $c_{[n]}$ minimizing $\ell_{\mathcal{D}}$. Suppose we have a dataset $\{(G_i, y_i)\}_{i=1}^M$ i.i.d. sampled from $\mathcal{D}$, and $\hat{\theta}$ is the weight over f_G which is learned via ℓ_2-regularization with regularization coefficient λ:

$$\hat{\theta} = \arg\min_\theta \frac{1}{M} \sum_{i=1}^{M} \ell(\langle \theta, f_{G_i} \rangle, y_i) + \lambda \|\theta\|_2. \tag{4}$$

Theorem 3 *Assume that f_G is scaled so that $\|f_G\|_2 \leq 1$ for any graph from $\mathcal{D}$. There exists a prior distribution over W, such that with $r = \Omega(\frac{n s_{\max}^3}{\epsilon^2} \log K)$ for $s_{\max} = \max\{s_n : 1 \leq n \leq T\}$ and appropriate choice of regularization coefficient, with probability $1 - \delta - O(TS \exp(-(r/S)^{1/3}))$, the $\hat{\theta}$ minimizing the ℓ_2-regularized logistic loss over the N-gram graph embeddings f_{G_i}'s satisfies*

$$\ell_{\mathcal{D}}(\hat{\theta}) \leq \ell_{\mathcal{D}}(\theta^*) + O\left(\|\theta^*\|_2 \sqrt{\epsilon + \frac{1}{M} \log \frac{1}{\delta}} \right). \tag{5}$$

Theorem 4 (Restatement of Theorem 1.1 in [12]) *Suppose A is $(2k, \epsilon)$-RIP for an $\epsilon < \sqrt{2} - 1$. Let $\hat{x}$ denote the solution to (9), and let x_k denote the vector x with all but the k-largest entries set to zero. Then*

$$\|\hat{x} - x\|_1 \leq C_0 \|x_k - x\|_1$$

and

$$\|\hat{x} - x\|_2 \leq C_0 k^{-1/2} \|x_k - x\|_1.$$

In particular, if x is k-sparse, the recovery is exact.

Furthermore, it has been shown that A is (k, ϵ)-RIP with overwhelming probability when $d = \Omega(k \log \frac{N}{k})$ and $\sqrt{d} A_{ij} \sim \mathcal{N}(0, 1)(\forall i, j)$ or $\sqrt{d} A_{ij} \sim \mathcal{U}\{-1, 1\}(\forall i, j)$.

Definition 3 (ℓ-way Column Hadamard Product) *Let A be a $d \times N$ matrix, and let ℓ be a natural integer. The ℓ-way column Hadamard-product of A is a $d \times \binom{N}{\ell}$ matrix denoted as $A^{(\ell)}$, whose columns indexed by a sequence $1 \leq i_1 < i_2 \cdots < i_\ell \leq d$ is the element-wise product of the $i_1, i_2, \ldots, i_\ell$-th columns of A, i.e., $(i_1, i_2, \ldots, i_\ell)$-th column in $A^{(\ell)}$ is $A_{i_1} \odot A_{i_2} \odot \cdots \odot A_{i_\ell}$ where A_j for $j \in [N]$ is the j-th column in A.*

We have the following theorems:

Theorem 5 (Restatement of Theorem 4.1 in [32]) *Let X be an $n \times d$ matrix, and let A be a $d \times N$ random matrix with independent entries R_{ij} such that $\mathbb{E}[R_{ij}] = 0, \mathbb{E}[R_{ij}] = 1$, and $|R_{ij}| \leq \tau$ almost surely. Let $\epsilon \in (0, 1)$, and let k be an integer satisfying $sr(X) \geq \frac{C\tau^8}{\epsilon^2} k^2 \log \frac{N^2}{k\epsilon}$ for some universal constant $C > 0$. Then with probability at least $1 - \exp(-c\epsilon^2 sr(X)/(k^2\tau^8))$ for some universal constant $c > 0$, the matrix $XA^{(\ell)}/\|X\|_F$ is (k, ϵ)-RIP.*

Here, $\mathrm{sr}(X) = \|X\|_F^2/\|X\|^2$ is the stable rank of X. In our case, we will apply the theorem with X being $\mathbf{I}_{d\times d}/\sqrt{d}$ where $\mathbf{I}_{d\times d} \in \mathbb{R}^{d\times d}$ is the identity matrix.

Theorem 6 (Restatement of Theorem 4.3 in [32]) *Let X be an $n \times d$ matrix, and let A be a $d \times N$ random matrix with independent entries R_{ij} such that $\mathbb{E}[R_{ij}] = 0, \mathbb{E}[R_{ij}] = 1$, and $|R_{ij}| \leq \tau$ almost surely. Let $\ell \geq 3$ be a constant. Let $\epsilon \in (0, 1)$, and let k be an integer satisfying $sr(X) \geq \frac{C\tau^{4\ell}}{\epsilon^2} k^3 \log \frac{N^\ell}{k\epsilon}$ for some universal constant $C > 0$. Then with probability at least $1 - \exp(-c\epsilon^2 sr(X)/(k^2\tau^{4\ell}))$ for some universal constant $c > 0$, the matrix $XA^{(\ell)}/\|X\|_F$ is (k, ϵ)-RIP.*

Appendix

Theorem 7 (Restatement of Theorem 4.2 in [3]) *Suppose A is $(\Delta\mathcal{X}, \epsilon)$-RIP. Then with probability at least $1-\delta$,*

$$\ell_{\mathcal{D}}^{A}(\hat{\theta}_A) \leq \ell_{\mathcal{D}}(\theta^*) + O\left(\lambda_\ell B\|\theta^*\|\sqrt{\epsilon + \frac{1}{M}\log\frac{1}{\delta}}\right)$$

for appropriate choice of C. Here, $\Delta\mathcal{X} = \{x - x' : x, x' \in \mathcal{X}\}$ for any $\mathcal{X} \subseteq \mathbb{R}^N$.

Definition 3 (Walk Weights). *Define the weight for one attribute value v as $w(v) = 1$, and define the weight for a sequence of attribute values $(v_0, \ldots, v_{n-1})$ with $n > 1$ as:*

$$w(v_0, \ldots, v_{n-1}) := \prod_{i=0}^{n-2} S(F_{(1)}(v_i), F_{(1)}(v_{i+1})) \quad (4)$$

where $S(\cdot, \cdot)$ is the score function in Eq (2), $F_{(1)}(v_i) = Wh(v_i)$, and $h(v_i)$ is the one-hot vector for the attribute value v_i.

Theorem 1. *The embedding $f_{(n)}$ is a linear mapping of the walk statistics $c_{(n)}$:*

$$f_{(n)} = W^{[n]} \Lambda_{(n)} c_{(n)} \tag{5}$$

where $W^{[n]}$ is the n-way column products of W, and $\Lambda_{(n)}$ is a K^n-dimensional diagonal matrix, whose columns correspond to all possible length-n sequences of attribute values, with the diagonal entry in the column indexed by a sequence of attribute values $(v_0, \ldots, v_{n-1})$ being its weight $w(v_0, \ldots, v_{n-1})$. Then

$$f_{[T]} := \mathcal{M} \Lambda c_{[T]} \tag{6}$$

where $\mathcal{M}$ is a block-diagonal matrix with diagonal blocks $W, W^{[2]}, \ldots, W^{[T]}$, and Λ a block-diagonal matrix with diagonal blocks $\Lambda_{(1)}, \Lambda_{(2)}, \ldots, \Lambda_{(T)}$.

The intuition for the benefit of appropriate weighting is simple. Suppose that the label is given by a linear function on $c_{[T]}$ with parameter θ^*, i.e., $y = \langle \theta^*, c_{[T]} \rangle$. When we learn over the weighted features $\Lambda c_{[T]}$, if the support of the diagonal entries $\mathrm{diag}(\Lambda)$ contains the support of θ^* (i.e., if $\theta^*_i \neq 0$ then $\Lambda_{ii} \neq 0$), the parameter $\Lambda^\dagger \theta^*$ on $\Lambda c_{[T]}$ has the same predictions and loss as θ^* on $c_{[T]}$. So we only need to learn $\Lambda^\dagger \theta^*$ on $\Lambda c_{[T]}$, which can require fewer data samples for learning (equivalently, smaller loss for a fixed amount of samples). Learning over $f_{[T]}$ is learning over a compressed version of $\Lambda c_{[T]}$, which shares the same intuition.

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{M} \sum_{i=1}^{M} \ell(\langle \theta, f_{[T]}(G_i) \rangle, y_i) + \lambda \|\theta\|_2. \quad (7)$$

Theorem 2. *Assume that $\mathcal{M}$ satisfies the $(2s, \epsilon)$-RIP, and $c_{[T]}$ is s-sparse. Also assume that the support of $diag(\Lambda)$ contains the support of θ^*. For any $\delta \in (0, 1)$, the $\hat{\theta}$ minimizing the ℓ_2-regularized logistic loss over the embeddings $f_{[T]}(G_i)$'s satisfies with probability at least $1 - \delta$:*

$$\ell_{\mathcal{D}}(\hat{\theta}) \leq \ell_{\mathcal{D}}(\theta^*) + O\left(B_\Lambda \sqrt{\epsilon + \frac{1}{M} \log \frac{1}{\delta}} \right) \quad (8)$$

for an appropriate choice of regularization coefficient λ. Here the term B_Λ is defined as

$$B_\Lambda := \|\Lambda^\dagger \theta^*\|_2 \max_{G \sim \mathcal{D}} \|\Lambda c_{[T]}(G)\|_2 \quad (9)$$

and $\Lambda^\dagger$ is the pseudo-inverse of Λ.

Definition 7 (Walk Statistics for the General Case). *Given a walk $p = (i_1, \ldots, i_n)$ of length n, the vector $\mathbf{e}_p \in \{0,1\}^{(\prod_j k_j)^n}$ is defined as the one-hot vector for the attribute value sequence $(\mathcal{V}_{i_1}, \ldots, \mathcal{V}_{i_n})$ along the walk. The walk statistics vector $c_{(n)}(G) = \sum_p \mathbf{e}_p$ with the sum over all walks p of length n in the graph G. Furthermore, let the walk statistics $c_{[T]}(G)$ be the concatenation of $c_{(1)}(G), \ldots, c_{(T)}(G)$. When G is clear from the context, we write $c_{(n)}$ and $c_{[T]}$ for short.*

So the definition is similar to that for the case with $S = 1$, except that now it is in dimension $K_n = (\prod_{j=0}^{S-1} k_j)^n$.

To describe the linear mapping from $c_{(n)}$ to $f_{(n)}$, we need to introduce the following notation.

Definition 8. *Let $(W_1 W)^{\{n\}}$ be a matrix with K_n column corresponding to all possible length-n sequences of attribute values, with the column indexed by a sequence of attribute values $(v_0, \ldots, v_{n-1})$ being $(W_1 W h(v_0)) \odot (W_1 W h(v_1)) \odot \cdots \odot (W_1 W h(v_{n-1}))$, where $h(v_i) = [h(v_i^0), \ldots, h(v_i^{S-1})]$ and $h(v_i^j)$ is the one-hot vector for the attribute value v_i^j for the j-th attribute in v_i.*

The following theorem then shows that $f_{(n)}$ can be a compressed version of the walk statistics, weighted by the weighting parameter matrix W_1, W_3 and also by the attention scores $\bar{S}$.

Theorem 6. *The embedding $f_{(n)}$ is a linear mapping of the walk statistics $c_{(n)}$:*

$$f_{(n)} = W_3 (W_1 W)^{\{n\}} \Lambda_{(n)} c_{(n)}. \tag{40}$$