Sketch-GNN: Scalable Graph Neural Networks with Sublinear Training Complexity

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Abstract

Graph Neural Networks (GNNs) are widely applied to graph learning problems such as node classification. When scaling up the underlying graphs of GNNs to a larger size, we are forced to either train on the complete graph and keep the full graph adjacency and node embeddings in memory (which is often infeasible) or mini-batch sample the graph (which results in exponentially growing computational complexities with respect to the number of GNN layers). Various sampling-based and historical-embedding-based methods are proposed to avoid this exponential growth of complexities. However, none of these solutions eliminates the linear dependence on graph size. This paper proposes a sketch-based algorithm whose training time and memory grow sublinearly with respect to graph size by training GNNs atop a few compact sketches of graph adjacency and node embeddings. Based on polynomial tensor-sketch (PTS) theory, our framework provides a novel protocol for sketching non-linear activations and graph convolution matrices in GNNs, as opposed to existing methods that sketch linear weights or gradients in neural networks. In addition, we develop a locality sensitive hashing (LSH) technique that can be trained to improve the quality of sketches. Experiments on large-graph benchmarks demonstrate the scalability and competitive performance of our Sketch-GNNs versus their full-size GNN counterparts.

1 Introduction

Graph Neural Networks (GNNs) have achieved the state-of-the-art graph learning in numerous applications, including classification [26], clustering [3], recommendation systems [42], social networks [16] and more, through representation learning of target nodes using information aggregated from neighborhoods in the graph. The manner in which GNNs utilize graph topology, however, makes it challenging to scale learning to larger graphs or deeper models with desirable computational and memory efficiency. Full-batch training that stores the Laplacian of the complete graph suffers from a memory complexity of $\mathcal{O}(m + ndL + d^2L)$ on an n-node, m-edge graph with node features of dimension d when employing an L-layer graph convolutional network (GCN). This linear memory complexity dependence on n and the limited memory capacity of GPUs make it difficult to train on large graphs with millions of nodes or more. As an example, the *MAG240M-LSC* dataset [21] is a node classification benchmark with over 240 million nodes that takes over 202 GB of GPU memory when fully loaded.

To address the memory constraints, two major lines of research are proposed: (1) Sampling-based approaches [18, 11, 12, 14, 44] based on the idea of implementing message passing only between the neighbors within a sampled mini-batch; (2) Historical-embedding based techniques, such as GNNAutoScale [17] and VQ-GNN [15]), which maintain the expressive power of GNNs on sampled subgraphs using historical embeddings. However, all of these methods require the number of mini-batches to be proportional to the size of the graph for fixed memory consumption. In other words,

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they significantly increase computational time complexity in exchange for memory efficiency when scaling up to large graphs. For example, training a 4-layer GCN with just 333K parameters (1.3 MB) for 500 epochs on *ogbn-papers100M* can take more than 2 days on a powerful AWS p4d.24x large instance [21].

We seek to achieve efficient training of GNNs with time and memory complexities sublinear in graph size without significant accuracy degradation. Despite the difficulty of this goal, it should be achievable given that (1) the number of learnable parameters in GNNs is independent of the graph size, and (2) training may not require a traversal of all local neighborhoods on a graph, but rather only the most representative ones (thus sublinear in graph size) as some neighborhoods may be very similar. In addition, commonly-used GNNs are typically small and shallow with limited model capacity and expressive power, indicating that a modest proportion of data may suffice.

This paper presents *Sketch-GNN*, a framework for training GNNs with sublinear time and memory complexity with respect to graph size. Using the idea of sketching, which maps high-dimensional data structures to a lower dimension through entry hashing, we sketch the $n \times n$ adjacency matrix and the $n \times d$ node feature matrix to a few $c \times c$ and $c \times d$ sketches respectively before training, where c is the sketch dimension. While most existing literature focuses on sketching linear weights or gradients, we introduce a method for sketching non-linear activation units using polynomial tensor sketch theory [19]. This preserves prediction accuracy while avoiding the need to "unsketch" back to the original high dimensional graph-node space n, thereby eliminating the dependence of training complexity on the underlying graph size n. Moreover, we propose to learn and update the sketches in an online manner using learnable locality sensitive hashing (LSH) [9]. This reduces the performance loss by adaptively enhancing the sketch quality while incurring minor overhead sublinear in graph size. In practice, we find that the sketch-ratio c/n required to maintain "full-graph" model performance drops as n increases; as a result, our Sketch-GNN enjoys sublinear training scalability.

Sketch-GNN applies sketching techniques to GNNs to achieve training complexity sublinear to the *data* size. This is fundamentally different from the few existing works which sketch the weights or gradients [29, 13, 25, 28, 36] to reduce the memory footprint of the model and speed up optimization. Our approach is flexible to architecture and has the potential to be generalized to other neural networks and data types, e.g., CNNs on gigapixel images. To the best of our knowledge, *Sketch-GNN* is the first sub-linear complexity training algorithm for GNNs based on LSH and tensor sketching. The sublinear efficiency obtained applies not only to GNNs with a fixed convolution matrix, such as GCN [26] and GraphSAGE [18], but also to GNNs with learnable convolution matrices, such as GAT [38].

Experiments on several large graph datasets, such as *ogbn-product* [21] with 2.45M nodes, demonstrate that *Sketch-GNNs* can match the performance of the standard model trained on the complete graph, while requiring significantly reduced computations and memory for both fixed (GCN, GraphSAGE) and learnable convolution (GAT) models. For instance, SketchGCN on *ogbn-arxiv* [21] is 72% and 55% faster than the corresponding full-graph and sampling-based (GraphSAINT [44]) baselines, while the pre-processing time is just 14% of overall reduction (when running 500 epochs).

2 Preliminaries

Basic Notations. Consider a graph with n nodes and m edges. Connectivity is given by the adjacency matrix $A \in \{0,1\}^{n \times n}$ and features on nodes are represented by the matrix $X \in \mathbb{R}^{n \times d}$, where d is the number of features. Given a matrix C, let $C_{i,j}$, $C_{i,:}$, and $C_{:,j}$ denote its (i,j)-th entry, i-th row, and j-th column, respectively. $\odot$ denotes the element-wise (Hadamard) product, whereas $C^{\odot k}$ represents the k-th order element-wise power. $\|\cdot\|_F$ is the symbol for the Frobenius norm. $I_n \in \mathbb{R}^{n \times n}$ denotes the identity matrix, whereas $\mathbf{1}_n \in \mathbb{R}^n$ is the vector whose elements are all ones. $\mathsf{Med}\{\cdot\}$ represents the element-wise median over a set of matrices. Superscripts are used to indicate multiple instances of the same kind of variable; for instance, $X^{(l)} \in \mathbb{R}^{n \times d_l}$ are the node representations on layer l.

Unified Framework of GNNs. A *Graph Neural Network (GNN)* layer receives the node representation of the preceding layer $X^{(l)} \in \mathbb{R}^{n \times d}$ as input and outputs a new representation $X^{(l+1)} \in \mathbb{R}^{n \times d}$, where $X = X^{(0)} \in \mathbb{R}^{n \times d}$ are the input features. Although GNNs are designed following different guiding principles, such as neighborhood aggregation (GraphSAGE), spatial convolution (GCN), self-attention (GAT), and Weisfeiler-Lehman (WL) alignment (GIN [43]), the great majority of GNNs can be interpreted as performing message passing on node features, followed by feature

transformation and an activation function. The update rule of these GNNs can be summarized as [15]

$$X^{(l+1)} = \sigma\Big(\textstyle\sum_q C^{(q)} X^{(l)} W^{(l,q)} \Big). \tag{1}$$

Where $C^{(q)} \in \mathbb{R}^{n\times n}$ denotes the q-th convolution matrix that defines the message passing operator, $q \in \mathbb{Z}_+$ is index of convolution, $\sigma(\cdot)$ is some choice of nonlinear activation function, and $W^{(l,q)} \in \mathbb{R}^{d_l \times d_{l+1}}$ denotes the learnable linear weight matrix for the l-th layer and q-th filter. GNNs under this paradigm differ from each other by their choice of convolution matrices $C^{(q)}$, which can be either fixed (GCN and GraphSAGE) or learnable (GAT). In Appendix A.1, we re-formulate a number of well-known GNNs under this framework. Unless otherwise specified, we assume $q = 1$ and $d = d_l$ for every layer $l \in [L]$ for notational convenience.

Count Sketch and Tensor Sketch. **(1)** *Count sketch* [7, 40] is an efficient dimensionality reduction method that projects an n-dimensional vector $\boldsymbol{u}$ into a smaller c-dimensional space using a random hash table $h : [n] \to [c]$ and a binary Rademacher variable $s : [n] \to \{\pm 1\}$, where $[n] = \{1, \ldots, n\}$. Count sketch is defined as $\mathsf{CS}(\boldsymbol{u})_i = \sum_{h(j)=i} s(j)\boldsymbol{u}_j$, which is a linear transformation of $\boldsymbol{u}$, i.e., $\mathsf{CS}(\boldsymbol{u}) = R\boldsymbol{u}$. Here, $R \in \mathbb{R}^{c\times n}$ denotes the so-called *count sketch matrix*, which has exactly one non-zero element per column. **(2)** *Tensor sketch* [31] is proposed as a generalization of count sketch to the tensor product of vectors. Given $\boldsymbol{z} \in \mathbb{R}^n$ and an order k, consider a k number of i.i.d. hash tables $h^{(1)}, \ldots, h^{(k)} : [n] \to [c]$ and i.i.d. binary Rademacher variables $s^{(1)}, \ldots, s^{(k)} : [n] \to \{\pm 1\}$. Tensor sketch also projects vector $\boldsymbol{z} \in \mathbb{R}^n$ into $\mathbb{R}^c$, and is defined as $\mathsf{TS}_k(\boldsymbol{z})_i = \sum_{h(j_1,\cdots,j_k)=i} s^{(1)}(j_1)\cdots s^{(k)}(j_k)\boldsymbol{z}_{j_1}\cdots\boldsymbol{z}_{j_k}$, where $h(j_1, \cdots, j_k) = (h^{(1)}(j_1) + \cdots + h^{(k)}(j_k)) \bmod c$. By definition, a tensor sketch of order $k = 1$ degenerates to count sketch; $\mathsf{TS}_1(\cdot) = \mathsf{CS}(\cdot)$. **(3)** We define *count sketch of a matrix* $U \in \mathbb{R}^{d\times n}$ as the count sketch of each row vector individually, i.e., $\mathsf{CS}(U) \in \mathbb{R}^{d\times c}$ where $[\mathsf{CS}(U)]_{i,:} = \mathsf{CS}(U_{i,:})$. The *tensor sketch of a matrix* is defined in the same way. Pham and Pagh [31] devise a fast computation of tensor sketch of $U \in \mathbb{R}^{d\times n}$ (sketch dimension c and order k) using count sketches and the Fast Fourier Transform (FFT):

$$\mathsf{TS}_k(U) = \mathsf{FFT}^{-1}\Big(\textstyle\bigodot_{p=1}^{k} \mathsf{FFT}\big(\mathsf{CS}^{(p)}(U)\big) \Big), \tag{2}$$

where $\mathsf{CS}^{(p)}(\cdot)$ is the count sketch with hash function $h^{(p)}$ and Rademacher variable $s^{(p)}$. $\mathsf{FFT}(\cdot)$ and $\mathsf{FFT}^{-1}(\cdot)$ are the FFT and its inverse applied to each row of a matrix.

Locality Sensitive Hashing. The definition of count sketch and tensor sketch is based on hash table(s) that only requires a data independent uniformity, i.e., with high probability the hash-buckets are of similar size. In contrast, locality sensitive hashing (LSH) is a hashing scheme that uses locality-sensitive hash function $H : \mathbb{R}^d \to [c]$ to ensure that nearby vectors are hashed into the same bucket (out of c buckets in total) with high probability while distant ones are not. *SimHash* achieves the locality-sensitive property by employing random projections [8]. Given a random matrix $P \in \mathbb{R}^{c/2\times d}$, SimHash defines a locality-sensitive hash function

$$H(\boldsymbol{u}) = \arg\max\left([P\boldsymbol{u} \parallel -P\boldsymbol{u}]\right), \tag{3}$$

where $[\cdot \parallel \cdot]$ denotes concatenation of two vectors and $\arg\max$ returns the index of the largest element. SimHash is efficient for large batches of vectors [1]. In this paper, we apply a learnable version of SimHash that is proposed by Chen et al. [9], in which the projection matrix P is updated using gradient descent; see Section 3.3 for details.

3 Sketch-GNN Framework via Polynomial Tensor Sketch

Problem and Insights. We intend to develop a "sketched counterpart" of GNNs, where training is based solely on (dimensionality-reduced) compact sketches of the convolution and node feature matrices, the sizes of which can be set independently of the graph size n. In each layer, Sketch-GNN receives some sketches of the convolution matrix C and node representation matrix $X^{(l)}$ and outputs some sketches of the node representations $X^{(l+1)}$. As a result, the memory and time complexities are inherently independent of n. The bottleneck of this problem is estimating the nonlinear activated product $\sigma(CX^{(l)}W^{(l)})$, where $W^{(l)}$ is the learnable weight of the l-th layer.

Before considering the nonlinear activation, as a first step, we approximate the linear product $CX^{(l)}W^{(l)}$, using dimensionality reduction techniques such as random projections and low-rank decompositions. As a direct corollary of the (distributional) Johnson–Lindenstrauss (JL) lemma [24], there exists a projection matrix $R \in \mathbb{R}^{c\times n}$ such that $CX^{(l)}W^{(l)} \approx \left(CR^\intercal\right)\left(RX^{(l)}W^{(l)}\right)$ [15].

Tensor sketch is one of the techniques that can achieve the JL bound [2]; for an error bound, see Lemma 1 in Appendix B.

Count sketch offers a good estimation of a matrix product, $CX^{(l)}W^{(l)} \approx \mathsf{CS}(C)\mathsf{CS}((X^{(l)}W^{(l)})^\mathsf{T})^\mathsf{T}$. While tensor sketch can be used to approximate the power of matrix product, i.e., $(CX^{(l)}W^{(l)})^{\odot k} \approx \mathsf{TS}_k(C)\mathsf{TS}_k((X^{(l)}W^{(l)})^\mathsf{T})^\mathsf{T}$, where $(\cdot)^{\odot k}$ is the k-th order element-wise power. If we combine the estimators of element-wise powers of $CX^{(l)}W^{(l)}$, we can approximate the (element-wise) activation $\sigma(\cdot)$ on $CX^{(l)}W^{(l)}$. This technique is known as a *polynomial tensor sketch (PTS)* and is discussed in [19]. In this paper, we apply PTS to sketch the message passing of GNNs, including the nonlinear activations.

3.1 Sketch-GNN: Approximated Update Rules

Polynomial Tensor Sketch. Our goal is to approximate the update rule of GNNs (Eq. (1)) in each layer. We first expand the element-wise non-linearity σ as a power series, and then approximate the powers using count/tensor sketch, i.e.,

$$X^{(l+1)} = \sigma(CX^{(l)}W^{(l)}) \approx \sum\nolimits_{k=1}^{r} c_k \left(CX^{(l)}W^{(l)}\right)^{\odot k} \approx \sum\nolimits_{k=1}^{r} c_k \, \mathsf{TS}_k(C) \, \mathsf{TS}_k\big((X^{(l)}W^{(l)})^\mathsf{T}\big)^\mathsf{T}, \quad (4)$$

where the $k = 0$ term always evaluates to zero as $\sigma(0) = 0$. In Eq. (4), coefficients c_k are introduced to enable learning or data-driven selection of the weights when combing the terms of different order k. This allows for the approximation of a variety of nonlinear activation functions, such as sigmoid and ReLU. The error of this approximation relies on the precise estimation of the coefficients $\{c_k\}_{k=1}^r$. To identify the coefficients, Han et al. [19] design a coreset-based regression algorithm, which requires at least $O(n)$ additional time and memory. Since the coefficients $\{c_k\}_{k=1}^r$ that achieve the best performance for the classification tasks do not necessarily approximate a known activation, we propose learning the coefficients $\{c_k\}_{k=1}^r$ to optimize the classification loss directly using gradient descent with simple L_2 regularization. Experiments indicate that the learned coefficients can approximate the sigmoid activation with relative errors comparable to those of the coreset-based method; see Fig. 1a in Section 5.

Approximated Update Rules. The remaining step is to approximate the operations of GNNs using PTS (Eq. (4)) on sketches of convolution matrix C and node representation matrix $X^{(l)}$. Consider r pairwise-independent count sketches $\{\mathsf{CS}^{(k)}(\cdot)\}_{k=1}^r$ with sketch dimension c, associated with hash tables $h^{(1)}, \ldots, h^{(r)}$ and binary Rademacher variables $s^{(1)}, \ldots, s^{(r)}$, defined prior to training an L-layer *Sketch-GNN*. Using these hash tables and Rademacher variables, we may also construct tensor sketches $\{\mathsf{TS}_k(\cdot)\}_{k=2}^r$ up to the maximum order r.

In *Sketch-GNN*, sketches of node representations (instead of the $O(n)$ standard representation) are propagated between layers. To get rid of the dependence on n, we count sketch both sides of Eq. (4)

$$\begin{aligned} S_X^{(l+1,k')} &:= \mathsf{CS}^{(k')}\big((X^{(l+1)})^\mathsf{T}\big) \approx \mathsf{CS}^{(k')}\big(\textstyle\sum_{k=1}^{r} c_k^{(l)} \mathsf{TS}_k\big((X^{(l)}W^{(l)})^\mathsf{T}\big)\mathsf{TS}_k(C)^\mathsf{T}\big) \\ &= \textstyle\sum_{k=1}^{r} c_k^{(l)} \, \mathsf{TS}_k\big((X^{(l)}W^{(l)})^\mathsf{T}\big)\mathsf{CS}^{(k')}\big(\mathsf{TS}_k(C)^\mathsf{T}\big) \\ &= \textstyle\sum_{k=1}^{r} c_k^{(l)} \mathsf{FFT}^{-1}\Big(\bigodot_{p=1}^{k} \mathsf{FFT}\big((W^{(l)})^\mathsf{T} S_X^{(l,p)}\big)\Big) \, S_C^{(l,k,k')}, \end{aligned} \quad (5)$$

where $S_X^{(l+1,k')} = \mathsf{CS}^{(k')}((X^{(l+1)})^\mathsf{T}) \in \mathbb{R}^{d\times c}$ is the transpose of column-wise count sketch of $X^{(l+1)}$, and the superscripts of $S_X^{(l+1,k')}$ indicate that it is the k'-th count sketch of $X^{(l+1)}$ (i.e., sketched by $CS^{(k)}(\cdot)$). In the second line of Eq. (5), we can move the matrix, $c_k^{(l)}\mathsf{TS}_k((X^{(l)}W^{(l)})^\mathsf{T})$, multiplied on the left to $\mathsf{TS}_k(C)^\mathsf{T}$ out of the count sketch function $\mathsf{CS}^{(k')}(\cdot)$, since the operation of row-wise count sketch $\mathsf{CS}^{(k')}(\cdot)$ is equivalent to multiplying the associated count sketch matrix $R^{(k')}$ on the right, i.e., for any $U \in \mathbb{R}^{n\times n}$, $\mathsf{CS}^{(k')}(U) = UR^{(k')}$. In the third line of Eq. (5), we denote the "two-sided sketch" of the convolution matrix as $S_C^{(l,k,k')} := \mathsf{CS}^{(k')}(\mathsf{TS}_k(C)^\mathsf{T}) \in \mathbb{R}^{c\times c}$ and expand the tensor sketch $\mathsf{TS}_k((X^{(l)}W^{(l)})^\mathsf{T})$ using the FFT-based formula (Eq. (2)).

Eq. (5) is the (recursive) **update rule** of *Sketch-GNN*, which approximates the operation of the original GNN and learns the sketches of representations. Looking at the both ends of Eq. (5), we obtain a formula that approximates the sketches of $X^{(l+1)}$ using the sketches of $X^{(l)}$ and C, with learnable weights $W^{(l)} \in \mathbb{R}^{d\times d}$ and coefficients $\{c_k^{(l)} \in \mathbb{R}\}_{k=1}^r$. The forward-pass and backward-propagation between the input sketches $\{S_X^{(0,k)}\}_{k=1}^r$ and the sketches of the final layer representations $\{S^{(L,k)}\}_{k=1}^r$ take $O(c)$ time and memory (see Section 3.3 for complexity details).

3.2 Error Bound on Estimated Representation

Based on Lemma 1 and the results in [19], we establish an error bound on the estimated final layer representation $\widetilde{X}^{(L)}$ for GCN; see Appendix B for the proof and discussions.

Theorem 1. *For a Sketch-GNN with L layers, the estimated final layer representation is $\widetilde{X}^{(L)} = \mathsf{Med}\{R^{(k)} S_X^{(L,k)} \mid k = 1, \cdots, r\}$, where the sketches are recursively computed using Eq. (5). For $\Gamma^{(l)} = \max\{5\|X^{(l)}W^{(l)}\|_F^2, (2+3^r)\sum_i(\sum_j [X^{(l)}W^{(l)}]_{i,j})^r\}$, it holds that $\mathbf{E}(\|X^{(L)} - \widetilde{X}^{(L)}\|_F^2)/\|X^{(L)}\|_F^2 \leq \prod_{l=1}^{L}(1 + 2/(1 + c{\lambda^{(l)}}^2/nr\Gamma^{(l)})) - 1$, where $\lambda^{(l)} \geq 0$ is the smallest singular value of the matrix $Z \in \mathbb{R}^{nd\times r}$ and $Z_{:,k}$ is the vectorization of $(CX^{(l)}W^{(l)})^{\odot k}$. Moreover, if $(c(\lambda^{(l)})^2/nr\Gamma^{(l)}) \gg 1$ holds true for every layer, the relative error is $O(L(n/c))$, which is proportional to the depth of the model, and inversely proportional to the sketch ratio (c/n).*

Remarks. Despite the fact that in Theorem 1 the error bound grows for smaller sketch ratios c/n, we observe in experiments that the sketch-ratio required for competitive performance decreases as n increases; see Section 5. As for the number of independent sketches r, we know from Lemma 1 that the dependence of r on n is $r = \Omega(3^{\log_c n})$ which is negligible when n is not too small; thus, in practice $r = 3$ is used.

The theoretical framework may not completely correspond to reality. Experimentally, the coefficients $\{\{c_k^{(l)}\}_{k=1}^r\}_{l=1}^L$ with the highest performance do not necessarily approximate a known activation. We defer the challenging problem of bounding the error of sketches and coefficients learned by gradients to future studies. Although the error bound is in expectation, we do not train over different sketches per iteration due to the instability caused by randomness. Instead, we introduce learnable locality sensitive hashing (LSH) in the next section to counteract the approximation limitations caused by the fixed number of sketches.

3.3 A Practical Implementation: Learning Sketches using LSH

Motivations of Learnable Sketches. In Section 3, we apply polynomial tensor sketch (PTS) to approximate the operations of GNNs on sketches of the convolution and feature matrices. Nonetheless, the pre-computed sketches are fixed during training, resulting in **two major drawbacks**: **(1)** The performance is limited by the quality of the initial sketches. For example, if the randomly-generated hash tables $\{h^{(k)}\}_{k=1}^r$ have unevenly distributed buckets, there will be more hash collisions and consequently worse sketch representations. The performance will suffer because only sketches are used in training. **(2)** More importantly, when multiple Sketch-GNN layers are stacked, the input representation $X^{(l)}$ changes during training (starting from the second layer). Fixed hash tables are not tailored to the "changing" hidden representations.

We seek a method for efficiently constructing high-quality hash tables tailored for each hidden embedding. Locality sensitive hashing (LSH) is a suitable tool since it is data-dependent and preserves data similarity by hashing similar vectors into the same bucket. This can significantly improve the quality of sketches by reducing the errors due to hash collisions.

Combining LSH with Sketching. At the time of sketching, the hash table $h^{(k)} : [n] \to [c]$ is replaced with an LSH function $H^{(k)} : \mathbb{R}^d \to [c]$, for any $k \in [r]$. Specifically, in the l-th layer of a Sketch-GNN, we hash the i-th node to the $H^{(k)}(X_{i,:}^{(l)})$-th bucket for every $i \in [n]$, where $X_{i,:}^{(l)}$ is the embedding vector of node i. As a result, we define a data-dependent hash table

$$h^{(l,k)}(i) = H^{(k)}(X_{i,:}^{(l)}) \tag{6}$$

that can be used for computing the sketches of $S_X^{(l,k)}$ and $S_C^{(l,k,k')}$. This LSH-based sketching can be directly applied to sketch the fixed convolution matrix and the input feature matrix. If SimHash is used, i.e., $H^{(k)}(\boldsymbol{u}) = \arg\max\left(\left[P^{(k)}\boldsymbol{u} \parallel -P^{(k)}\boldsymbol{u}\right]\right)$ (Eq. (3)), an additional $O(ncr(\log c + d))$ computational overhead is introduced to hash the n nodes for the r hash tables during preprocessing; see Appendix F more information. SimHash(es) are implemented as simple matrix multiplications that are practically very fast.

In order to employ LSH-based hash functions customized to each layer to sketch the hidden representations of a Sketch-GNN (i.e., $l = 2, \ldots, L-1$), we face **two major challenges**: **(1)** Unless we explicitly unsketch in each layer, the estimated hidden representations $\widetilde{X}^{(l)}(l = 2, \ldots, L-1)$ cannot be accessed and used to compute the hash tables. However, unsketching any hidden representation, i.e., $\widetilde{X}^{(l)} = \mathsf{Med}\{R^{(k)} S_X^{(l,k)} \mid k = 1, \cdots, r\}$, requires $O(n)$ memory and time. We need to come

up with an efficient algorithm that updates the hash tables without having to unsketch the complete representation. **(2)** It's unclear how to change the underlying hash table of a sketch across layers without unsketching to the n-dimensional space, even if we know the most up-to-date hash tables suited to each layer.

The **challenge (2)**, i.e., changing the underlying hash table of across layers, can be solved by maintaining a sparse $c \times c$ matrix $T^{(l,k)} := R^{(l,k)}(R^{(l+1,k)})^\mathsf{T}$ for each $k \in [r]$, which only requires $O(cr)$ memory and time overhead; see Appendix C for more information and detailed discussions. We focus on **challenge (1)** for the remainder of this section.

Online Learning of Sketches. To learn a hash table tailored for a hidden layer using LSH without unsketching, we develop an efficient algorithm to update the LSH function using only a size-$|B|$ subset of the length-n unsketched representations, where B denotes a subset of nodes we select. This algorithm, which we term *online learning of sketches*, is made up of two key parts: *(Part 1)* select a subset of nodes $B \subseteq [n]$ to effectively update the hash table, and *(Part 2)* update the LSH function $H(\cdot)$ with a triplet loss computed using this subset.

(1) Selection of subset B: Because model parameters are updated slowly during neural network training, the data-dependent LSH hash tables also changes slowly (this behavior was detailed in [9]). The amount of updates to the hash table drops very fast along with training, empirically verified in Fig. 1b (left) in Section 5. Based on this insight, we only need to update a small fraction of the hash table during training. To identify this subset $B \in [n]$ of nodes, gradient signals can be used. Intuitively, a node representation vector hashed into the wrong bucket will be aggregated with distant vectors and lead to larger errors and subsequently larger gradient signals. Specifically, we propose finding the candidate set B of nodes by taking the union of the several buckets with the largest gradients, i.e., $B = \{i \mid h^{(l,k)}(i) = \arg\max_j [S_X^{(l,k)}]_{j,:} \text{ for some } k\}$. The memory and overhead required to update the entries in B in the hash table is $O(|B|)$.

(2) Update of LSH function: In order to update the projection matrix P that defines a SimHash $H^{(k)} : \mathbb{R}^d \to [c]$ (Eq. (3)), instead of the $O(n)$ full triplet loss introduced by [9], we consider a sampled version of the triplet loss on the candidate set B with $O(|B|)$ complexity, namely

$$\mathcal{L}(H, \mathcal{P}_+, \mathcal{P}_-) = \max\left\{0, \textstyle\sum_{(\boldsymbol{u},\boldsymbol{v})\in\mathcal{P}_-} \cos(H(\boldsymbol{u}), H(\boldsymbol{v})) - \sum_{(\boldsymbol{u},\boldsymbol{v})\in\mathcal{P}_+} \cos(H(\boldsymbol{u}), H(\boldsymbol{v})) + \alpha\right\}, \quad (7)$$

where $\mathcal{P}_+ = \{(\widetilde{X}_{i,:}, \widetilde{X}_{j,:}) \mid i, j \in B, \langle \widetilde{X}_{i,:}, \widetilde{X}_{j,:}\rangle > t_+\}$ and $\mathcal{P}_- = \{(\widetilde{X}_{:,i}, \widetilde{X}_{:,j}) \mid i, j \in B, \langle \widetilde{X}_{:,i}, \widetilde{X}_{:,j}\rangle < t_-\}$ are the similar and dissimilar node-pairs in the subset B; $t_+ > t_-$ and $\alpha > 0$ are hyper-parameters. This triplet loss $\mathcal{L}(H, \mathcal{P}_+, \mathcal{P}_-)$ is used to update P using gradient descent, as described in [9], with a $O(c|B|d + |B|^2)$ overhead. Experimental validation of this LSH update mechanism can be found in Fig. 1b in Section 5.

Avoiding $O(n)$ in Loss Evaluation. We can estimate the final layer representation using the r sketches $\{S^{(L,k)}\}_{k=1}^r$, i.e., $\widetilde{X}^{(L)} = \mathsf{Med}\{R^{(k)} S_X^{(L,k)} \mid k = 1, \cdots, r\}$ and compute the losses of all nodes for node classification (or some node pairs for link prediction). However, the complexity of loss evaluation is $O(n)$, proportional to the number of ground-truth labels. In order to avoid $O(n)$ complexity completely, rather than un-sketching the node representation for all labeled nodes, we employ the locality sensitive hashing (LSH) technique again for loss calculation so that only a subset of node losses are evaluated based on a set of hash tables. Specifically, we construct an LSH hash table for each class in a node classification problem, which indexes all of the labeled nodes of this class and can be utilized to choose the nodes with poor predictions by leveraging the locality property. This technique, introduced in [10], is known as sparse forward-pass and back-propagation, and we defer the descriptions to Appendix C.

One-time Preprocessing. If the convolution matrix C is fixed (GCN, GraphSAGE), the "two-sided sketch" $S_C^{(l,k,k')} = \mathsf{CS}^{(k')}(\mathsf{TS}_k(C)^\mathsf{T}) \in \mathbb{R}^{c\times c}$ is the same in each layer and may be denoted as $S_C^{(k,k')}$. In addition, all of the r^2 sketches of C, i.e., $\{\{S_C^{(k,k')} \in \mathbb{R}^{c\times c}\}_{k=1}^r\}_{k'=1}^r$ can be computed during the preprocessing phase. If the convolution matrix C is sparse (which is true for most GNNs following Eq. (1) on a sparse graph), we can use the sparse matrix representations for the sketches $\{\{S_C^{(k,k')} \in \mathbb{R}^{c\times c}\}_{k=1}^r\}_{k'=1}^r$, and the total memory taken by the r^2 sketches is $O(r^2 c(m/n))$ where $(2m/n)$ is the average node degree (see Appendix F for details). We also need to compute the r count sketches of the input node feature matrix $X = X^{(0)}$, i.e., $\{S_X^{(0,k)}\}_{k=1}^r$ during preprocessing, which

requires $O(rcd)$ memory in total. In this regard, we have substituted the input data with compact graph-size independent sketches (i.e., $O(c)$ memory). Although the preprocessing time required to compute these sketches is $O(n)$, it is a one-time cost prior to training, and it is widely known that sketching is practically very fast.

Complexities of Sketch-GCN. The theoretical complexities of Sketch-GNN is summarized as follows, where for simplicity we assume bounded maximum node degree, i.e., $m = O(n)$. **(1) Training Complexity**: *(1a) Forward and backward propagation*: $O(Lcrd(\log(c) + d + m/n)) = O(c)$ time and $O(Lr(cd + rm/n)) = O(c)$ memory. *(1b) Hash and sketch update*: $O(Lr(c + |B|d)) = O(c)$ time and memory. **(2) Preprocessing**: $O(r(rm + n + c)) = O(n)$ time and $O(rc(d + rm/n)) = O(c)$ memory. **(3) Inference**: $O(Ld(m + nd)) = O(n)$ time and $O(m + Ld(n + d)) = O(n)$ memory (the same as a standard GCN). We defer a detailed summary of the theoretical complexities of Sketch-GNN to Appendix F.

We generalize Sketch-GNN to more GNN models in Appendix D and the pseudo-code which outlines the complete workflow of Sketch-GNN can be find in Appendix E.

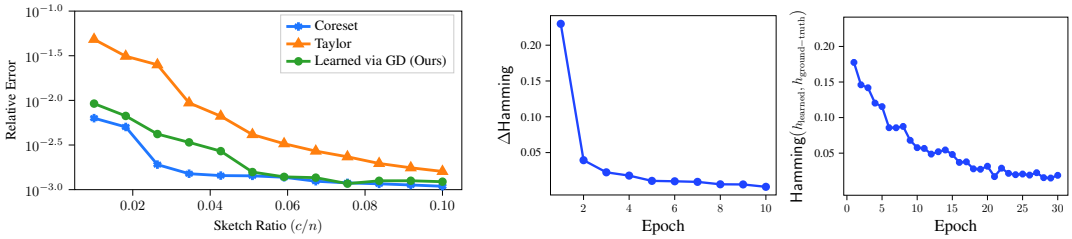
4 Related Work

Scalable methods for GNNs can be categorized into four classes, all of them still require linear training complexities. **(A)** On a large sparse graph with n nodes and m edges, the "full-graph" training of a L-layer GCN with d-dimensional (hidden) features per layer requires $O(m+ndL+d^2L)$ memory and $O(mdL + nd^2L)$ epoch time. **(B)** Sampling-based methods sample mini-batches from the complete graph following three schemes: (1) node-wisely sample a subset of neighbors in each layer to reduce the neighborhood size; (2) layer-wisely sample a set of nodes independently in each layer; (3) subgraph-wisely sample a subgraph directly and simply forward-pass and back-propagate on that subgraph. **(B.1)** GraphSAGE [18] samples r neighbors for each node while ignoring messages from other neighbors. $O(br^L)$ nodes are sampled in a mini-batch (where b is the mini-batch size), and the epoch time is $O(ndr^L)$; therefore, GraphSAGE is impractical for deep GNNs on a large graph. FastGCN [12] and LADIES [46] are layer-sampling methods that apply importance sampling to reduce variance. **(B.2)** The subgraph-wise scheme has the best performance and is most prevalent. Cluster-GCN [14] partitions the graph into many densely connected subgraphs and samples a subset of subgraphs (with edges between subgraphs added back) for training per iteration. GraphSAINT [44] samples a set of nodes and uses the induced subgraph for mini-batch training. Both Cluster-GCN and GraphSAINT require $O(mdL + nd^2L)$ epoch time, which is the same as "full-graph" training, although Cluster-GCN also needs $O(m)$ pre-processing time. **(C)** Apart from sampling strategies, historical-embedding-based methods propose mitigating sampling errors and improving performance using some stored embeddings. GNNAutoScale [17] keeps a snapshot of all embeddings in CPU memory, leading to a large $O(ndL)$ memory overhead. VQ-GNN [15] maintains a vector quantized data structure for the historical embeddings, whose size is independent of n. **(D)** Linearized GNNs [41, 4, 32] replace the message passing operation in each layer with a one-time message passing during preprocessing. They are practically efficient, but the theoretical complexities remain $O(n)$. Linearized models usually over-simplify the corresponding GNN and limit its expressive power.

Towards sublinear GNNs. Nearly all existing scalable methods focus on mini-batching the large graph and resolving the memory bottleneck of GNNs, without reducing the epoch training time. Few recent work focus on graph compression [22, 23] can also achieve sublinear training time by coarsening (e.g., using [30]) the graph during preprocessing and training GNNs on the coarsened graph with fewer nodes and edges. Nevertheless, this strategy suffers from **two issues**: **(1)** Although graph coarsening is a one-time cost, the memory and time overheads are often worse than $O(n)$ and can be prohibitively large on graphs with over 100K nodes. Even the fastest graph coarsening algorithm used by [22] takes more than 68 minutes to process the 233K-node *Reddit* graph [44]; see Table 1. The long preprocessing time renders any training speedups meaningless. **(2)** The test performance of a model trained on the coarsened graph highly depends on the GNN type. Although the performance of [22] on GCN is good, significant performance degradations are observed on GraphSAGE and GAT; see Section 5.

We defer discussion of more scalable GNN papers and the broad literature of sketching and LHS for neural networks to Appendix G.

5 Experiments



(a) Error of PTS (b) Learnable LSH

Figure 1: **Figure 1a** Relative errors when applying polynomial tensor sketch (PTS) to the nonlinear unit $\sigma(CXW)$ following Eq. (4). The dataset used is Cora [33]. σ is the sigmoid activation. We set $r = 5$ and test on a GCN with fixed $W = I_d \in \mathbb{R}^{d\times d}$. The coefficients $\{c_k\}_{k=1}^r$ can be computed by a coreset regression [19] (blue), by a Taylor expansion of $\sigma(\cdot)$ (orange), or learned from gradient descent proposed by us (green). **Figure 1b** The left plot shows the Hamming distance changes of the hash table in the 2nd layer during the training of a 2-layer *Sketch-GCN*, where the hash table is constructed from the unsketched representation $\widetilde{X}^{(1)}$ using SimHash. The right plot shows the Hamming distances between the hash table learned using our algorithm and the hash table constructed directly from $\widetilde{X}^{(1)}$.

Table 1: Time and memory efficiencies of Sketch-GNN versus other scalable methods.

Benchmark	*ogbn-arxiv*			*Reddit*		
Efficiency Measure	Preprocessing Time	Epoch Time	Train Memory	Preprocessing Time	Epoch Time	Train Memory
"Full-Graph" (oracle)	—	0.49 s	983 MB	—	OOM[1]	OOM
GraphSAINT	—	0.30 s	31.4 MB	—	2.09 s	977 MB
VQ-GNN	—	0.37 s	48.9 MB	—	2.16 s	1281 MB
Coarsening	358 s	0.20 s	22.1 MB	4123 s	1.04 s	530 MB
Sketch-GNN (ours)	27 s	0.13 s	38.7 MB	141 s	0.81 s	748 MB

[1] "OOM" refers to "out of memory".

Table 2: Performance of Sketch-GNN in comparison to Graph Coarsening [22] on *ogbn-arxiv*.

Benchmark	*ogbn-arxiv*								
GNN Model	GCN			GraphSAGE			GAT		
"Full-Graph" (oracle)	.7174 ± .0029			.7149 ± .0027			.7233 ± .0045		
Sketch Ratio (c/n)	0.1	0.2	0.4	0.1	0.2	0.4	0.1	0.2	0.4
Coarsening	.6508 ± .0091	.6665 ± .0010	.6892 ± .0035	.5264 ± .0251	.5996 ± .0134	.6609 ± .0061	.5177 ± .0028	.5946 ± .0027	.6307 ± .0041
Sketch-GNN (ours)	.6913 ± .0154	.7004 ± .0096	.7028 ± .0087	.6929 ± .0194	.6963 ± .0056	.7048 ± .0080	.6967 ± .0067	.6910 ± .0135	.7053 ± .0034

Table 3: Performance of Sketch-GNN versus SGC [41], GraphSAINT [44], and VQ-GNN [15].

Benchmark	*ogbn-arxiv*			*Reddit*			*ogbn-product*		
SGC	.6944 ± .0005			.9464 ± .0011			.6683 ± .0029		
GNN Model	GCN	GraphSAGE	GAT	GCN	GraphSAGE	GAT	GCN	GraphSAGE	GAT
"Full-Graph" (oracle)	.7174 ± .0029	.7149 ± .0027	.7233 ± .0045	OOM	OOM +/	OOM	OOM	OOM	OOM
GraphSAINT	.7079 ± .0057	.6987 ± .0039	.7117 ± .0032	.9225 ± .0057	.9581 ± .0074	.9431 ± .0067	.7602 ± .0021	.7908 ± .0024	.7971 ± .0042
VQ-GNN	.7055 ± .0033	.7028 ± .0047	.7043 ± .0034	.9399 ± .0021	.9449 ± .0024	.9438 ± .0059	.7524 ± .0032	.7809 ± .0019	.7823 ± .0049
Sketch Ratio (c/n)	0.4			0.3			0.2		
Sketch-GNN (ours)	.7028 ± .0087	.7048 ± .0080	.7053 ± .0034	.9280 ± .0034	0.9485 ± .0061	.9326 ± .0063	.7659 ± .0086	.7851 ± .0071	.7797 ± .0101

In this section, we evaluate the proposed *Sketch-GNN* algorithm and compare it with the (oracle) "full-graph" training baseline, a graph-coarsening based method (**Coarsening** [22]) which has sublinear training time, and other scalable methods including: a sampling-based method (**GraphSAINT** [44]), a historical-embedding based method (**VQ-GNN** [15]), and a linearized GNN (**SGC** [41]). We test on several large graph benchmarks including *ogbn-arxiv* (169K nodes, 1.2M edges), *Reddit* (233K nodes, 11.6M edges), and *ogbn-products* (2.4M nodes, 61.9M edges) from [20, 44]. See Appendix H for the implementation details.

Proof-of-Concept Experiments: (1) Errors of gradient-learned PTS coefficients: In Fig. 1a, we train the PTS coefficients to approximate the sigmoid activated $\sigma(CXW)$ to evaluate its approximation power to the ground-truth activation. The relative errors are comparable to those of the coreset-based method. **(2) Slow-change phenomenon of LSH hash tables**: In Fig. 1b (left), we count the changes of the hash table constructed from an unsketched hidden representation for each epoch, characterized by the Hamming distances between consecutive updates. The changes drop rapidly as training progresses, indicating that apart from the beginning of training, the hash codes of most nodes do not change at each update. **(3) Sampled triplet loss for learnable LSH**: In Fig. 1b (right), we verify the effectiveness of our update mechanism for LSH hash functions, as the learned hash table gradually approaches the "ground truth", i.e., the hash table constructed from the unsketched hidden representation.

Efficiency of Sketch-GNNs. For efficiency measures, we are interested in the comparison to Coarsening, as both approaches achieve sublinear training time at the cost of some preprocessing overheads. We use a 3-layer GCN as the backbone and set the sketch ratios (c/n, ratio of sketch dimension c to graph size n) of both algorithms to $c/n = 0.1$, meaning that the coarsened graph contains $n/10$ nodes. We measure their preprocessing time, average epoch training time, and peak training memory, as reported in Table 1. Although not rigorously comparable, we also set the mini-batch size of GraphSAINT and VQ-GNN to $b = n/10$. We report the average epoch training time and peak training memory for each method and the "full-graph" training baseline. In addition to Table 1, the following are also recorded: (1) Coarsening requires 980 MB to preprocess *ogbn-arxiv*, whereas Sketch-GNN only requires 539 MB. (2) Our preprocessing on the largest dataset, *ogbn-product* (2.4M nodes), takes only 414s. (3) The wallclock time for the validation accuracy to reach 99% of its best is 88 ± 8s for SketchGCN, which is shorter than VQ-GNN's 103 ± 11s and GraphSAINT's 120 ± 4s.

From Table 1 and the aforementioned results, we can draw **four important conclusions**: **(1)** Sketch-GNN achieves the fastest average epoch time. The coarsened graph is typically much denser and increases the time required for message passing. **(2)** Sketch-GNN usually converges faster than GraphSAINT and VQ-GNN. **(3)** Our preprocessing time is significantly less than that of Coarsening. Coarsening suffers from an extremely long preprocessing time, rendering the training speed-ups meaningless. Moreover, our preprocessing time scales well with graph size and sparsity. **(4)** We also require less preprocessing memory as sketching is linear/multi-linear operation and usually preserves sparsity. **(5)** Sketch-GNN often requires more training memory than Coarsening in order to maintain the copies of sketches and additional data structures, although these memory overheads are small.

Performance of Sketch-GNNs. We first compare the performance of *Sketch-GNN* with Coarsening under various sketch ratios to understand how their performance is affected by the memory bottleneck. In Table 2, we report the test accuracy of both approaches on *ogbn-arxiv*, with a 3-layer GCN, GraphSAGE, or GAT as the backbone and a sketch ratio of 0.1, 0.2, or 0.4. We see there are significant performance degradations when applying Coarsening to GraphSAGE and GAT, even under sketch ratio 0.4, indicating that Coarsening may be compatible only with specific GNNs (GCN and APPNP as explained in [22]). In contrast, the performance drops of Sketch-GNN are always small across all architectures, even when the sketch ratio is 0.1. Therefore, our approach generalizes to more GNN architectures and consistently outperforms the Coarsening method.

We move on to compare Sketch-GNN with linearized GNNs (SGC), sampling-based (GraphSAINT), and historical-embedding-based (VQ-GNN) methods. In Table 3, we report the performance of SGC, the "full-graph" training (oracle), GraphSAINT and VQ-GNN with mini-batch size 50K (their performance is not affected by the choice of mini-batch size if it is not too small), and Sketch-GNN with appropriate sketch ratios (0.4 on *ogbn-arxiv*, 0.3 on *Reddit*, and 0.2 on *ogbn-product*). From Table 3, we confirm that, with an appropriate sketch ratio, the performance of *Sketch-GNN* is always close to the "full-graph" oracle and competitive with the other scalable approaches. Impressively, the needed sketch ratio c/n for Sketch-GNN to achieve competitive performance reduces as graph size grows. This further illustrates that, as previously indicated, the required training complexities (to get acceptable performance) are sublinear to the graph size.

Ablation Studies: (1) Dependence of sketch dimension c on graph size n. Although the theoretical approximation error increases under smaller sketch ratio c/n, we observe competitive experimental results with smaller c/n especially on large graphs. In practice, the sketch-ratio required to maintain "full-graph" model performance decreases with n, as verified in Table 3: $c/n = 0.4$ is needed on *ogbn-arxiv* with 169K nodes but $c/n = 0.2$ is adequate on *ogbn-product* with 2.45M nodes. **(2) Learned Sketches versus Fixed Sketches.** We find that learned sketches can improve the performance of all models and on all datasets. Under sketch-ratio $c/n = 0.2$, the Sketch-GCN with learned sketches achieves 0.7004 ± 0.0096 accuracy on *ogbn-arxiv* while fixed randomized sketches degrade performance to 0.6649 ± 0.0106.

6 Conclusion

We present *Sketch-GNN*, a sketch-based GNN training framework with sublinear training time and memory complexities. Our main contributions are (1) approximating nonlinear operations in GNNs using polynomial tensor sketch (PTS) and (2) updating sketches using learnable locality sensitive hashing (LSH). Our novel framework has the potential to be applied to other architectures and applications where the amount of data makes training even simple models impractical.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] See Section 1.
   (b) Did you describe the limitations of your work? [Yes] Currently, our work has two major limitations: (1) our theoretical assumptions and results may not perfectly correspond to the reality; see the theoretical remarks in Section 3, and (2) our implementation is not fully-optimized with the more advanced libraries; see the efficiency discussions in Section 5.

(c) Did you discuss any potential negative societal impacts of your work? [Yes] We see our work as a theoretical and methodological contribution toward more resource-efficient graph representation learning. Our methodological advances may enable larger-scale network analysis for societal good. However, progress in graph embedding learning may potentially inspire other hostile social network studies, such as monitoring fine-grained user interactions.

(d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...

   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Lemma 1 and Theorem 1.

   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendix B.

3. If you ran experiments...

   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Appendix H.

   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Appendix H.

   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See Section 5.

   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Appendix H.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...

   (a) If your work uses existing assets, did you cite the creators? [Yes] See Appendix H.

   (b) Did you mention the license of the assets? [Yes] See Appendix H.

   (c) Did you include any new assets either in the supplemental material or as a URL? [No]

   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [No]

   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [No]

5. If you used crowdsourcing or conducted research with human subjects...

   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]