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1. Block-wise quantization of GNNs
2. Variance minimization due to activation compression

# Overview 

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## Background

## Contributions

Block-wise Quantization
Variance Minimization

## Summary and Conclusions

## A Quick Introduction to GNNs

- Graph $\mathcal{G}=(\mathbf{X}, \mathbf{A})$ with $N$ nodes
- $\mathbf{X} \in \mathbb{R}^{N \times F}$ : Dense node feature matrix with $F$-dimensional features
- $\mathbf{A} \in\{0,1\}^{N \times N}$ : Sparse adjacency matrix
- $\mathbf{A}_{i, j}=1$ if an edge exists between nodes $i$ and $j$, otherwise $\mathbf{A}_{i, j}=0$


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- $\mathbf{A}_{i, j}=1$ if an edge exists between nodes $i$ and $j$, otherwise $\mathbf{A}_{i, j}=0$
- GNN Layer Update
- $\mathbf{H}^{(\ell+1)}=\sigma\left(\mathbf{A} \mathbf{H}^{(\ell)} \boldsymbol{\Theta}^{(\ell)}\right)$
- Initial node representations: $\mathbf{H}^{(0)}:=\mathbf{X}$
- Weights: $\Theta^{(\ell)} \in \mathbb{R}^{D \times D}$ at layer $\ell$
- Non-linearity: $\sigma(\cdot)$


Figure: Animation of message-passing.

## The Memory Bottleneck of GNNs

- Memory usage of activations
- During the forward-pass all intermediate results $\left(\mathbf{H}^{(\ell)} \mathbf{\Theta}^{(\ell)}\right) \in \mathbb{R}^{N \times D}$ and node embedding matrices $\mathbf{H}^{(\ell)} \in \mathbb{R}^{N \times D}$ are stored in memory.
- Results in $\mathcal{O}(L N D)$ space complexity, with $L$ being the number of layers.
- For this reason we focus on compressing activation maps.


## Random projection

- Projection of the activations into a lower-dimensional space
- $\mathbf{H}_{\text {proj }}^{(\ell)}=\operatorname{RP}\left(\mathbf{H}^{(\ell)}\right)=\mathbf{H}^{(\ell)} \mathbf{R}$ where $\mathbf{R} \in \mathbb{R}^{D \times R}$ is the normalized Rademacher matrix with $R<D$ (Achlioptas 2001).
- $\mathbf{R}$ has the following property: $\mathbb{E}\left[\mathbf{H}^{(\ell)} \mathbf{R} \mathbf{R}^{\top}\right]=\mathbb{E}\left[\mathbf{H}^{(\ell)} \mathbf{I}\right]=\mathbb{E}\left[\mathbf{H}^{(\ell)}\right]$


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- For this reason, $R$ defines the projected dimensionality.


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1. A shift and scale into $[0, B]$ :

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\overline{\mathbf{h}}=(\mathbf{h}-\min (\mathbf{h})) \frac{B}{\max (\mathbf{h})-\min (\mathbf{h})}
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Figure: Example histogram of some $\overline{\mathbf{h}}$ with $b=2$. Colors denote what integer a value most likely stochastically rounds to.

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2. A stochastic rounding (SR) operation denoted by $L \cdot 7$ :

$$
\mathbf{h}_{\mathrm{INT}}=\text { Quant }(\mathbf{h})=\lfloor\overline{\mathbf{h}}\rceil
$$



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- Stochastic rounding (SR) keeps $\hat{\mathbf{h}}$ unbiased, with rounding probability proportional to boundary proximity
- This also applies to non-integer rounding values.

Figure: Same $\overline{\mathbf{h}}$ as before, but with non-uniform bin widths (quantization boundaries).

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Block-wise Quantization
Variance Minimization

Summary and Conclusions

## Block-wise quantization

- Taking inspiration from Chen et al. 2021; Dettmers et al. 2021, we group the input tensor such that $G$ elements are quantized at a time.
- This is done with

$$
\mathbf{H}_{\mathrm{block}}^{(\ell)} \in \mathbb{R}^{\frac{N \cdot R}{G} \times G}:=\operatorname{reshape}\left(\mathbf{H}_{\mathrm{proj}}^{(\ell)}, G\right),
$$

where reshape denotes the reshape function as known from packages like Numpy or Pytorch.

- Since each quantization operation is done row-wise, this increases concurrency.


Figure: The matrix that has been reshaped to a lower row-count, also has fewer quantizations.

## Results of block-wise quantization

|  | G/R | Accuracy $\uparrow$ | S (e/s) $\uparrow$ | S Impr. (\%) | M (MB) $\downarrow$ | Impr. (\%) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |

## Results of block-wise quantization

| Quant. | G/R | Accuracy $\uparrow$ | $\mathbf{S}(\mathrm{e} / \mathrm{s}) \uparrow$ | S Impr. (\%) | M(MB) $\downarrow$ | M Impr. (\%) |
| :---: | :---: | :---: | :---: | ---: | :---: | ---: |
| FP32 | - | $71.95 \pm 0.16$ | 13.07 | - | 786.22 | - |
| INT2 | 1 | $71.16 \pm 0.21$ | 10.03 | - | 30.47 | - |
|  | 2 | $71.16 \pm 0.34$ | 10.23 | +2.00 | 27.89 | -8.47 |
|  | 4 | $71.17 \pm 0.22$ | 10.46 | +4.29 | 26.60 | -12.70 |
| INT2 | 8 | $71.21 \pm 0.39$ | 10.54 | +5.08 | 25.95 | -14.83 |
|  | 16 | $71.01 \pm 0.19$ | 10.55 | +5.18 | 25.72 | -15.59 |
|  | 32 | $70.87 \pm 0.29$ | 10.54 | +5.08 | 25.60 | -15.98 |
|  | 64 | $71.28 \pm 0.25$ | 10.54 | +5.08 | 25.56 | -16.11 |

Table: $G / R$ denotes the factor by which we increase the dimensionality via block-wise quantization.
Standard deviations of test accuracy is computed over 10 runs

## Variance minimization

- While stochastic rounding (SR) is not biased, it does induce some variance.
- If we can minimize this variance, we can minimize the expected quantization error.
- Done by finding the quantization boundaries that minimize the variance.


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- In order to do this we need three components:

1. The distribution of activations (probability density function or pdf)
2. The variance induced as a function of the activation $(\operatorname{Var}(\lfloor h\rceil))$
3. Through integration, we can use (1) and (2) to calculate the expected variance, which we then minimize as a function of the boundaries.

## Distribution of the activations

- SR is performed on the normalized activations $\overline{\mathbf{H}}_{\text {proj }}^{(\ell)}$, which are all of the activations transformed into the range $[0, B]$.


Figure: Histogram of observed and theorized $\overline{\mathbf{H}}_{\text {proj }}^{(1)}$ in a GNN model on the OGB-Arxiv data.

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## Distribution of the activations

- SR is performed on the normalized activations $\overline{\mathbf{H}}_{\text {proj }}^{(\ell)}$, which are all of the activations transformed into the range $[0, B]$.
- Two PDF's are hypothesized: $\mathcal{U}$ (EXACT) and $\mathcal{C N}$ (Ours).
- $\mathcal{C N}$ is the clipped normal distribution and is the result of clipping $\mathcal{N}$ such that the support lies in $[0, B]$.
- Empirically we have shown that we can define $\mathcal{C N}$ just from the dimensionality $D$, that is

$$
\begin{aligned}
& \mathcal{C N}_{[1 / D]} \text { is the pdf of } y \text { given, } \\
& \qquad y=\min (\max (0, X), B), \quad X \sim \mathcal{N}(\mu, \sigma), \\
& \text { where } \mu=B / 2 \text { and } \sigma=-\mu / \Phi^{-1}(1 / D)
\end{aligned}
$$



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## Distribution of SR variance

- Using Xia et al. 2020, we can estimate the variance induced by SR.
- This turns out to be

$$
\operatorname{Var}(\lfloor h\rceil)=\sum_{i=1}^{i=B}\left(\delta_{i}\left(h-\alpha_{i-1}\right)-\left(h-\alpha_{i-1}\right)^{2}\right),
$$

where $\delta_{i}$ is the width of the bin containing $h$, and $\alpha_{i}$ is the starting position of the bin.



Figure: SR variance as a function of second $(\alpha)$ and third $(\beta)$ boundary position.

## Using the distributions to lessen variance induced by SR

- By combining the PDF of activations and the variance induced as a function of an activations $(\operatorname{Var}(\lfloor h\rceil))$, we get:

$$
\left.\left.\begin{array}{rl}
\mathbb{E}[\operatorname{Var}(\lfloor h\rceil)] & =\int_{0}^{\alpha}\left(\alpha \cdot h-h^{2}\right) \mathcal{C \mathcal { N }} \\
{[1 / D]}
\end{array}(h) d h\right]^{\beta}\left((\beta-\alpha)(h-\alpha)-(h-\alpha)^{2}\right) \mathcal{C} \mathcal{N}_{[1 / D]}(h) d h ~(h-\beta)^{2}\right) \mathcal{C N}_{[1 / D]}(h) d h
$$

- Using numerical integration we can minimize the above w.r.t. $\alpha$ and $\beta$ (variance minimization), and cache the best boundaries for any $D$.


## Results of variance minimization

Dataset Layer $\quad \mathbf{R} \quad \mathcal{U} \quad \mathcal{C N}{ }_{[1 / D]} \quad$ Reduction Factor ( $\times$ ) $\quad$ Var. Reduction (\%)

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| Dataset | Layer | $\mathbf{R}$ | $\mathcal{U}$ | $\mathcal{C N}_{[1 / D]}$ | Reduction Factor $(\times)$ | Var. Reduction (\%) |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| Arxiv | layer 1 | 16 | 0.0495 | 0.0213 | 2.32 | 3.17 |
|  | layer 2 | 16 | 0.0446 | 0.0016 | 27.88 | 2.09 |
|  | layer 3 | 16 | 0.0451 | 0.0041 | 11.00 | 2.19 |
| Flickr | layer 1 | 63 | 0.0674 | 0.0017 | 39.65 | 6.14 |
|  | layer 2 | 32 | 0.0504 | 0.0033 | 15.27 | 4.37 |

Table: Jensen-Shannon divergence measure for Uniform and Clipped Normal distributions compared to the normalized activations $\overline{\mathbf{h}}$ at each layer of the GNN for Arxiv and Flickr datasets.

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| INT2 | 1 | $71.16 \pm 0.21$ | 10.03 | - | 30.47 | - |
| INT2+VM | 1 | $71.20 \pm 0.19$ | 9.16 | -8.67 | 30.47 | 0.00 |

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- Unfortunately they can suffer from poor memory scaling.
- EXACT (Liu et al. 2022) tries to alleviate this, via extreme activation compression
- We try to show that you can improve this further, even in an already very compressed activation space.


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- Non-uniform distribution of GNN activation maps demonstrated.
- Introduced variable and non-uniform bin widths in stochastic rounding to reduce quantization variance.
- Methods are model-agnostic: opportunities for applying these methods to other architectures and pre-trained networks.


## Bibliography

－Achlioptas，Dimitris（2001）．＂Database－Friendly Random Projections＂．In：Proceedings of the Twentieth ACM SIGMOD－SIGACT－SIGART Symposium on Principles of Database Systems．PODS＇01．Santa Barbara，California，USA：Association for Computing Machinery，pp．274－281．ISBN：1581133618．DOI： 10．1145／375551．375608．URL：https：／／doi．org／10．1145／375551．375608．
目 Chen，Jianfei et al．（2021）．ActNN：Reducing Training Memory Footprint via 2－Bit Activation Compressed Training．arXiv： 2104.14129 ［cs．LG］．
目 Dettmers，Tim et al．（2021）．＂8－bit Optimizers via Block－wise Quantization＂．In：CoRR abs／2110．02861．arXiv：2110．02861．URL：https：／／arxiv．org／abs／2110．02861．
目 Liu，Zirui et al．（2022）．＂EXACT：Scalable Graph Neural Networks Training via Extreme Activation Compression＂．In：International Conference on Learning Representations．URL： https：／／openreview．net／forum？id＝vkaMaq95＿rX．
目 Xia，Lu et al．（2020）．Improved stochastic rounding．arXiv： 2006.00489 ［math．NA］．

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