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Activation Compression of Graph Neural Networks using Block-Wise Quantization with Improved Variance Minimization

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

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Summary and Conclusions

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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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- GNN Layer Update
 - $\mathbf{H}^{(\ell+1)} = \sigma \left(\mathbf{A} \, \mathbf{H}^{(\ell)} \, \mathbf{\Theta}^{(\ell)} \right)$
 - Initial node representations: $\mathbf{H}^{(0)} := \mathbf{X}$
 - Weights: $\boldsymbol{\Theta}^{(\ell)} \in \mathbb{R}^{D \times D}$ at layer ℓ
 - 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 $(\mathbf{H}^{(\ell)}\mathbf{\Theta}^{(\ell)}) \in \mathbb{R}^{N \times D}$ and node embedding matrices $\mathbf{H}^{(\ell)} \in \mathbb{R}^{N \times D}$ are stored in memory.
 - Results in $\mathcal{O}(LND)$ 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
- $\mathbf{H}_{\text{proj}}^{(\ell)} = \text{RP}(\mathbf{H}^{(\ell)}) = \mathbf{H}^{(\ell)}\mathbf{R}$ where $\mathbf{R} \in \mathbb{R}^{D \times R}$ is the normalized Rademacher matrix with R < D (Achlioptas 2001).
- **R** has the following property: $\mathbb{E}[\mathbf{H}^{(\ell)}\mathbf{R}\mathbf{R}^{\top}] = \mathbb{E}[\mathbf{H}^{(\ell)}\mathbf{I}] = \mathbb{E}[\mathbf{H}^{(\ell)}]$

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- For this reason, R defines the projected dimensionality.

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

$$\bar{\mathbf{h}} = (\mathbf{h} - \min(\mathbf{h})) \frac{B}{\max(\mathbf{h}) - \min(\mathbf{h})}$$



Figure: Example histogram of some $\bar{\mathbf{h}}$ with b = 2. Colors denote what integer a value most likely stochastically rounds to.

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A stochastic rounding (SR) operation denoted by |·]:

$$\mathbf{h}_{\mathtt{INT}} = \mathsf{Quant}\left(\mathbf{h}
ight) = \left\lfloor ar{\mathbf{h}}
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- Property: $\mathbb{E}[\hat{\mathbf{h}}] = \mathbf{h}$
- Stochastic rounding (SR) keeps $\hat{\mathbf{h}}$ unbiased, with rounding probability proportional to boundary proximity
- This also applies to non-integer rounding values.



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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

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

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

Quant.	G/R	Accuracy ↑	S (e/s) ↑	S Impr. (%)	M (MB) ↓	M Impr. (%)
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Results of block-wise quantization

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

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- 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 $(Var(\lfloor h \rfloor))$
 - 3. Through integration, we can use (1) and (2) to calculate the expected variance, which we then minimize as a function of the boundaries.

SR is performed on the normalized activations H^(l)_{proj}, which are all of the activations transformed into the range [0, B].



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

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- SR is performed on the normalized activations H^(l)_{proj}, which are all of the activations transformed into the range [0, B].
- Two PDF's are hypothesized: $\mathcal U$ (EXACT) and \mathcal{CN} (Ours).
- \mathcal{CN} 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{CN} just from the dimensionality D, that is

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





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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

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

where δ_i is the width of the bin containing *h*, and α_i is the starting position of the bin.



Figure: SR variance as a function of second (α) and third (β) 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 (Var([h])), we get:

$$\mathbb{E}[\operatorname{Var}(\lfloor h \rceil)] = \int_0^{\alpha} (\alpha \cdot h - h^2) \mathcal{CN}_{[1/D]}(h) dh$$
$$+ \int_{\alpha}^{\beta} \left((\beta - \alpha)(h - \alpha) - (h - \alpha)^2 \right) \mathcal{CN}_{[1/D]}(h) dh$$
$$+ \int_{\beta}^{B} \left((B - \beta)(h - \beta) - (h - \beta)^2 \right) \mathcal{CN}_{[1/D]}(h) dh$$

• Using numerical integration we can minimize the above w.r.t. α and β (variance minimization), and cache the best boundaries for any *D*.

Results of variance minimization

	Dataset	Layer	R	\mathcal{U}	$\mathcal{CN}_{[1/D]}$	Reduction Factor (\times)	Var. Reduction $(\%)$
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Dataset	Layer	R	U	$\mathcal{CN}_{[1/D]}$	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 $\bar{\mathbf{h}}$ at each layer of the GNN for Arxiv and Flickr datasets.

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INT2+VM	1	71.20 ± 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

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- Check out carbontracker.info for advancing CO2e reduction in ML.



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