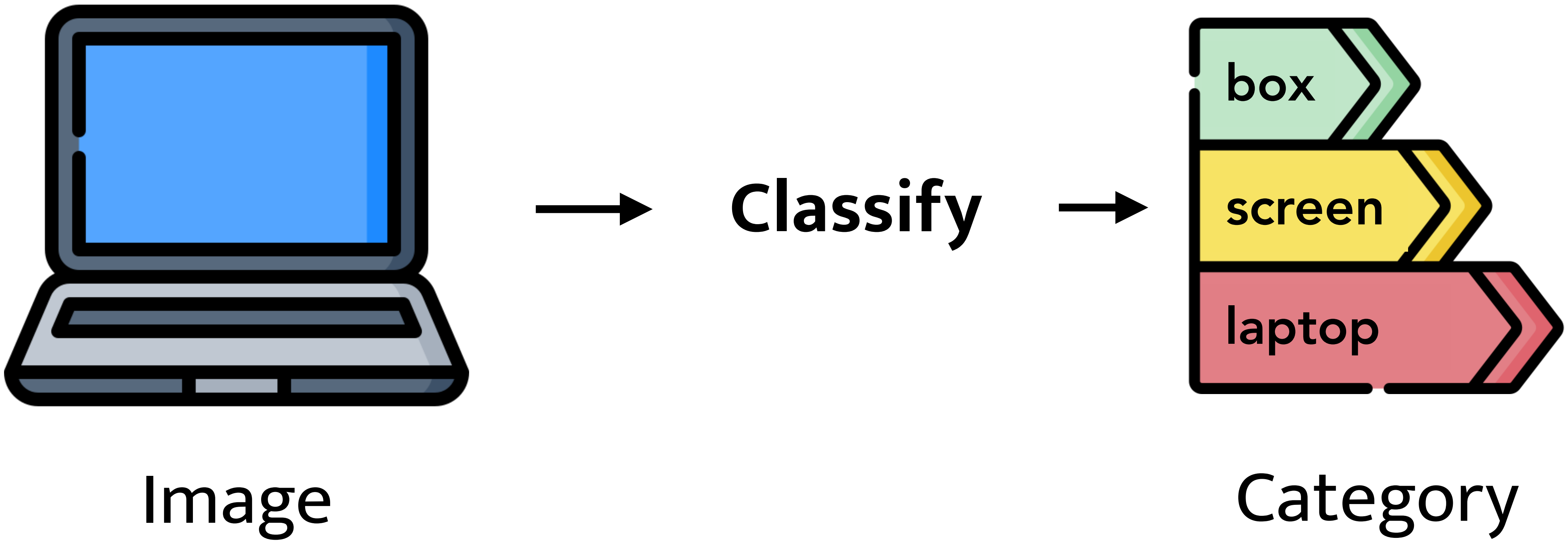
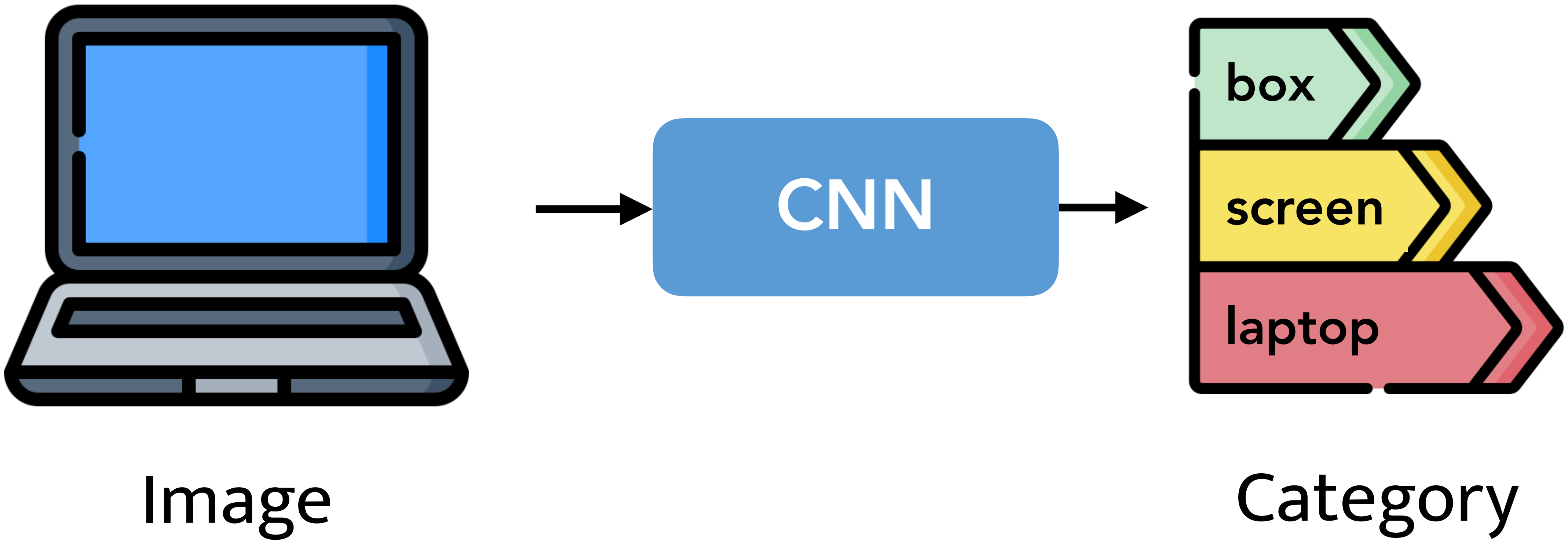
BNS-GCN: Efficient Full-Graph Training of Graph Convolutional Networks with Partition-Parallelism and Random Boundary Node Sampling

Cheng Wan*, **Youjie Li***, Ang Li, Nam Sung Kim, Yingyan Lin

MLSys 2022


Classify
box
screen
laptop
Image
Category



Convolutional Neural Networks (CNNs) are powerful in image classification

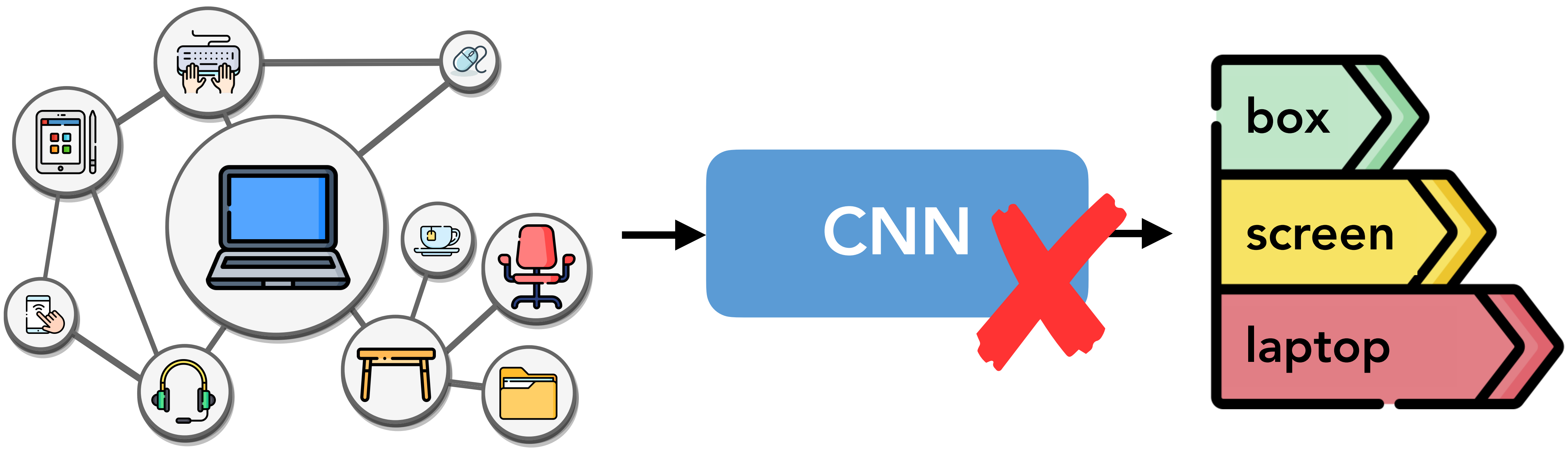


Image + **Relationship**
(e.g., co-purchase)

Category

How to incorporate **relationship** among data samples?

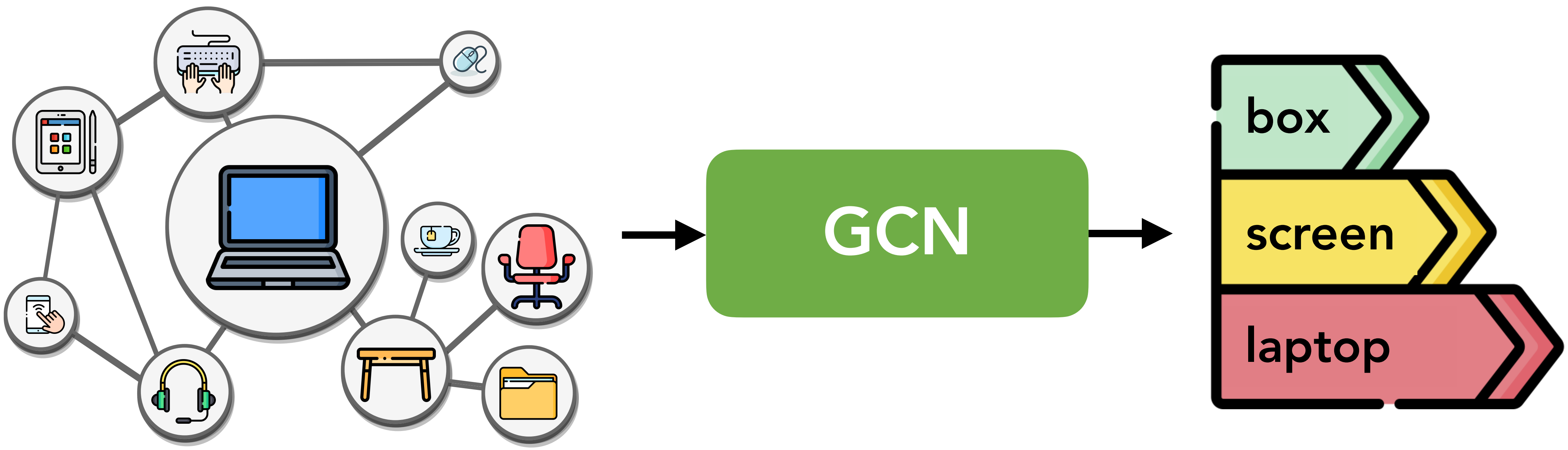


Image + **Relationship**
(e.g., co-purchase)

Category

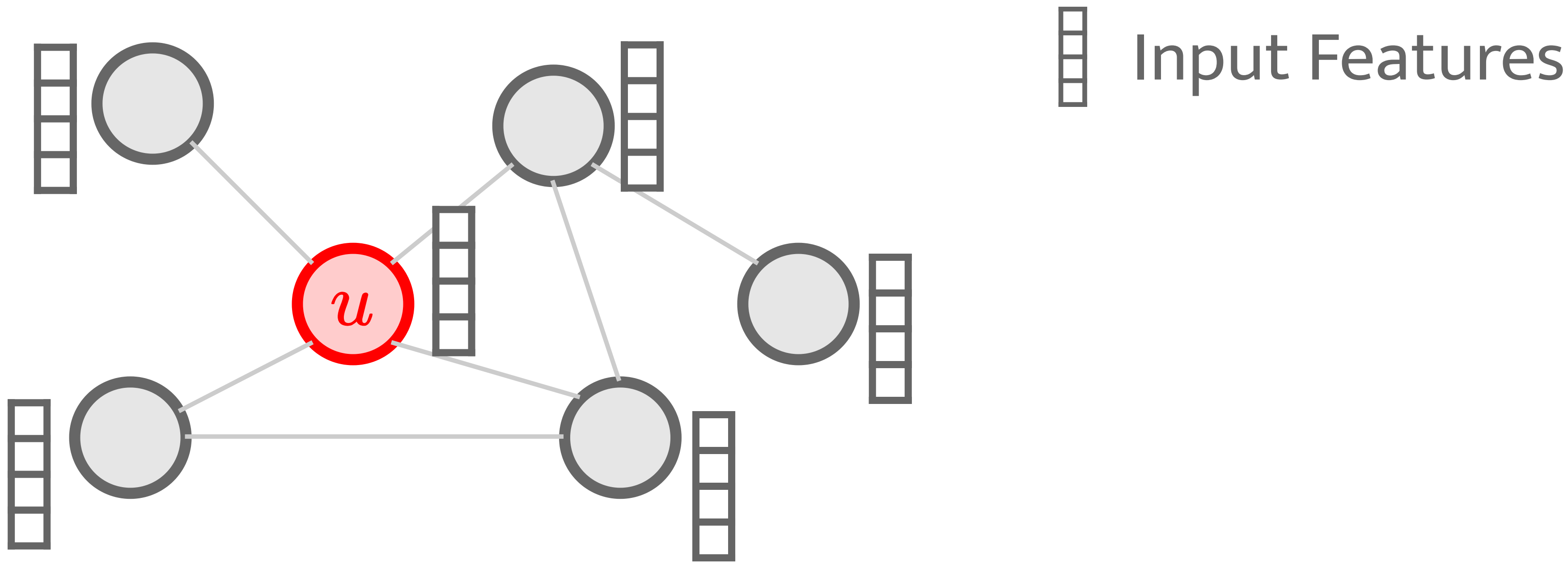
Graph Convolutional Network (GCN)

the SOTA model for capturing **relationship**

[1] Kipf and Welling. Semi-supervised classification with graph convolutional networks. *ICLR'17*

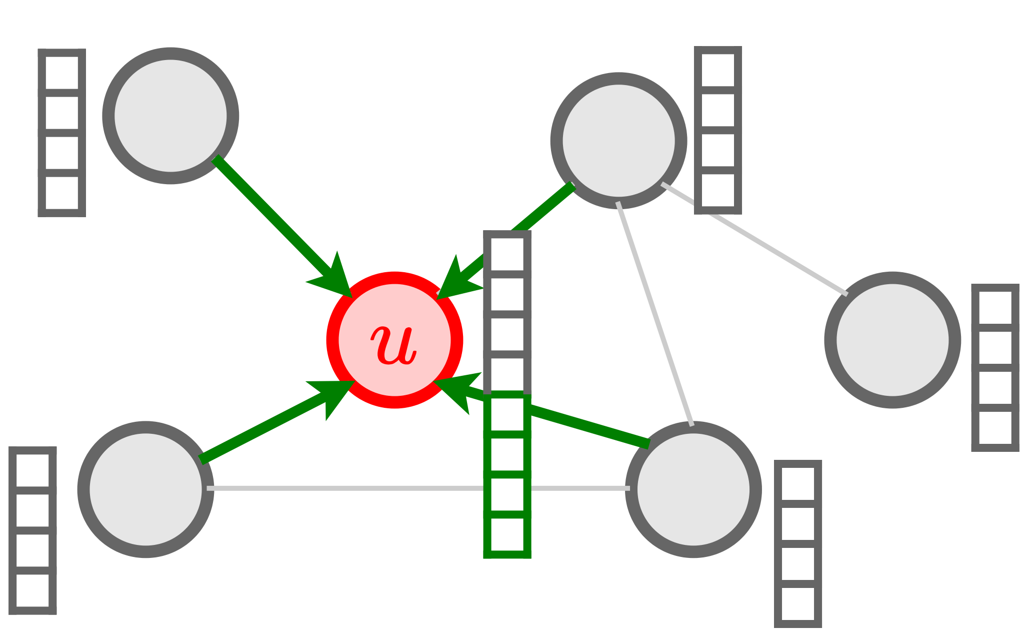
Graph Convolutional Network (GCN)

How to compute the embedding of node u?



Graph Convolutional Network (GCN)

How to compute the embedding of node u?

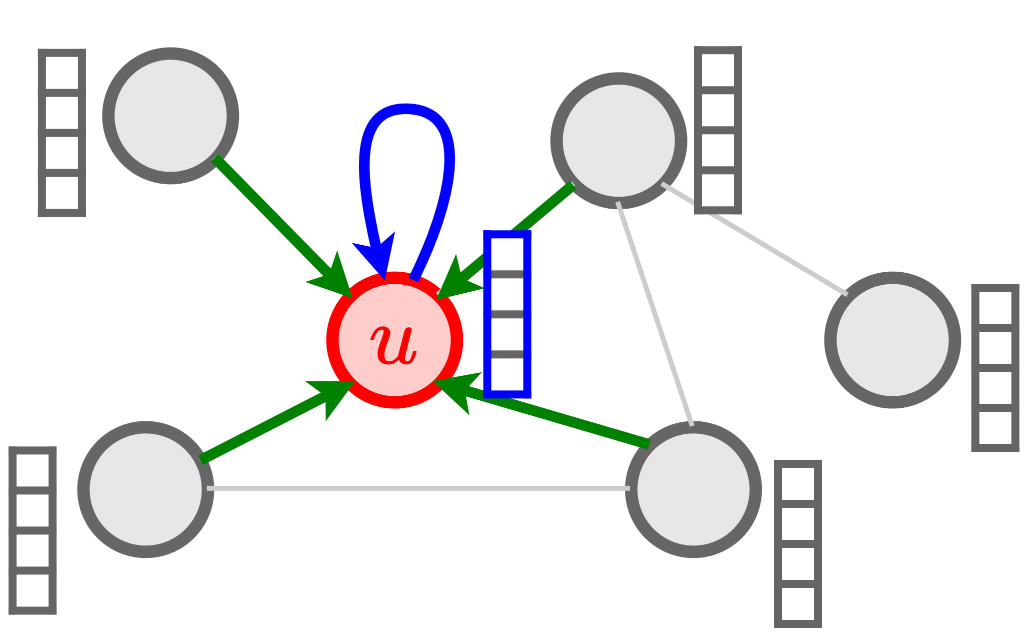


Input Features

① Neighbor Aggregation
(e.g., average pooling)

Graph Convolutional Network (GCN)

How to compute the embedding of node u?



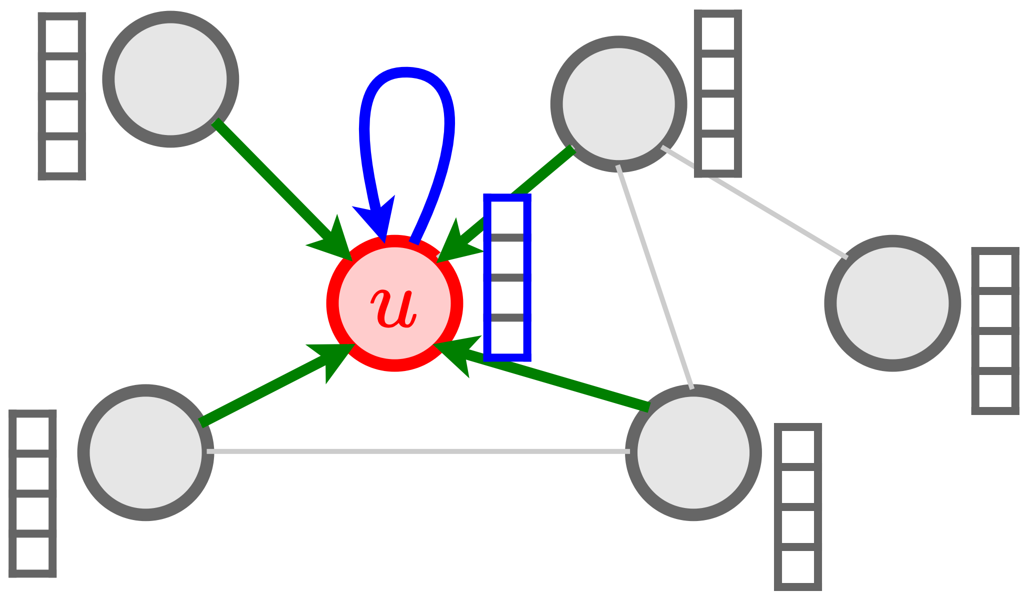
Input Features

① Neighbor Aggregation
(e.g., average pooling)

② Feature Update
(e.g., MLP)

Graph Convolutional Network (GCN)

How to compute the embedding of node u?



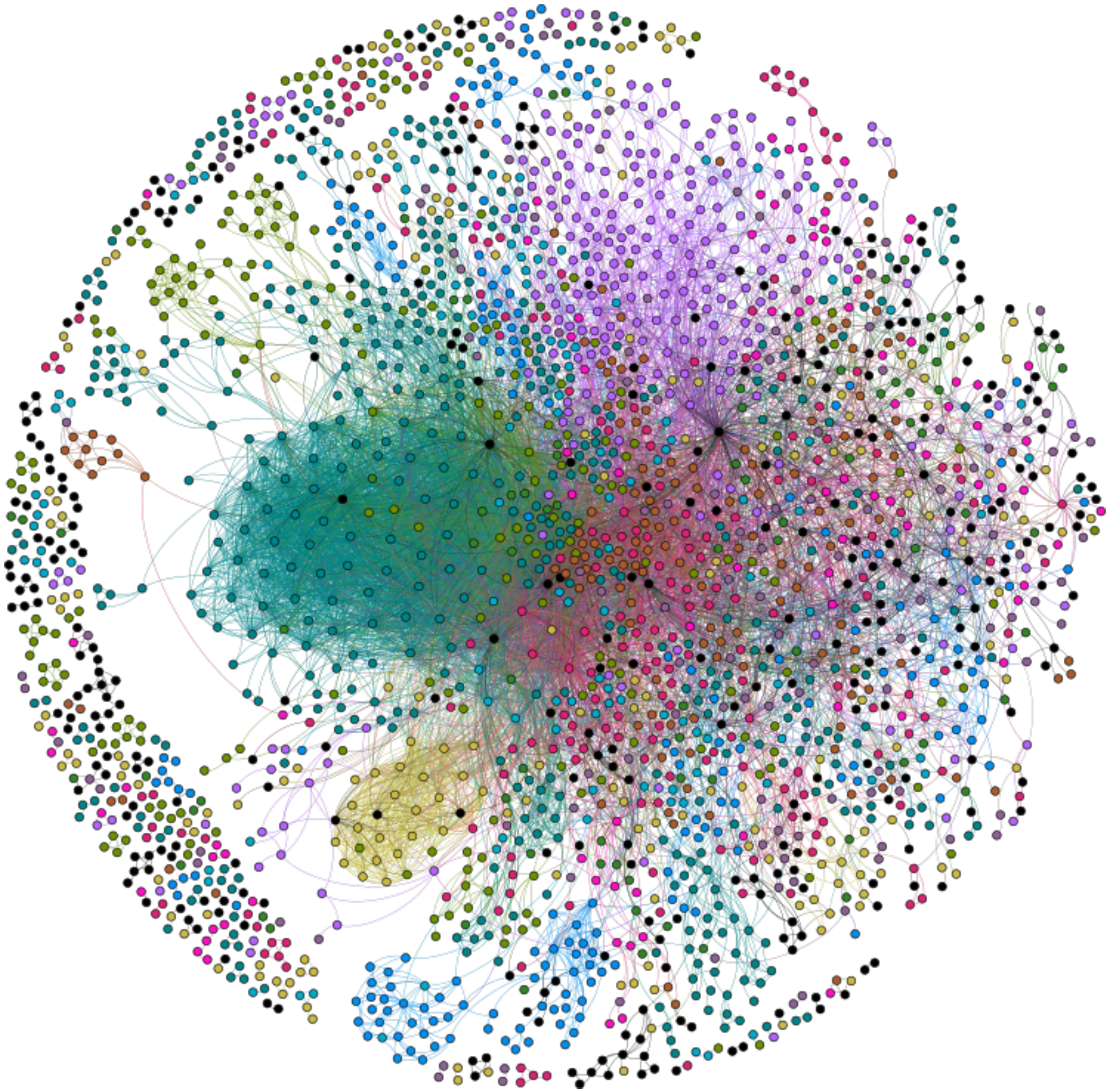
Input Features

① Neighbor Aggregation
(e.g., average pooling)

② Feature Update
(e.g., MLP)

Output embedding can be fed to the next GCN layer
or be used to downstream tasks
(e.g., node classification)

Challenge: **Giant** Graphs for GCNs



Amazon Co-Purchase Dataset [1,2]

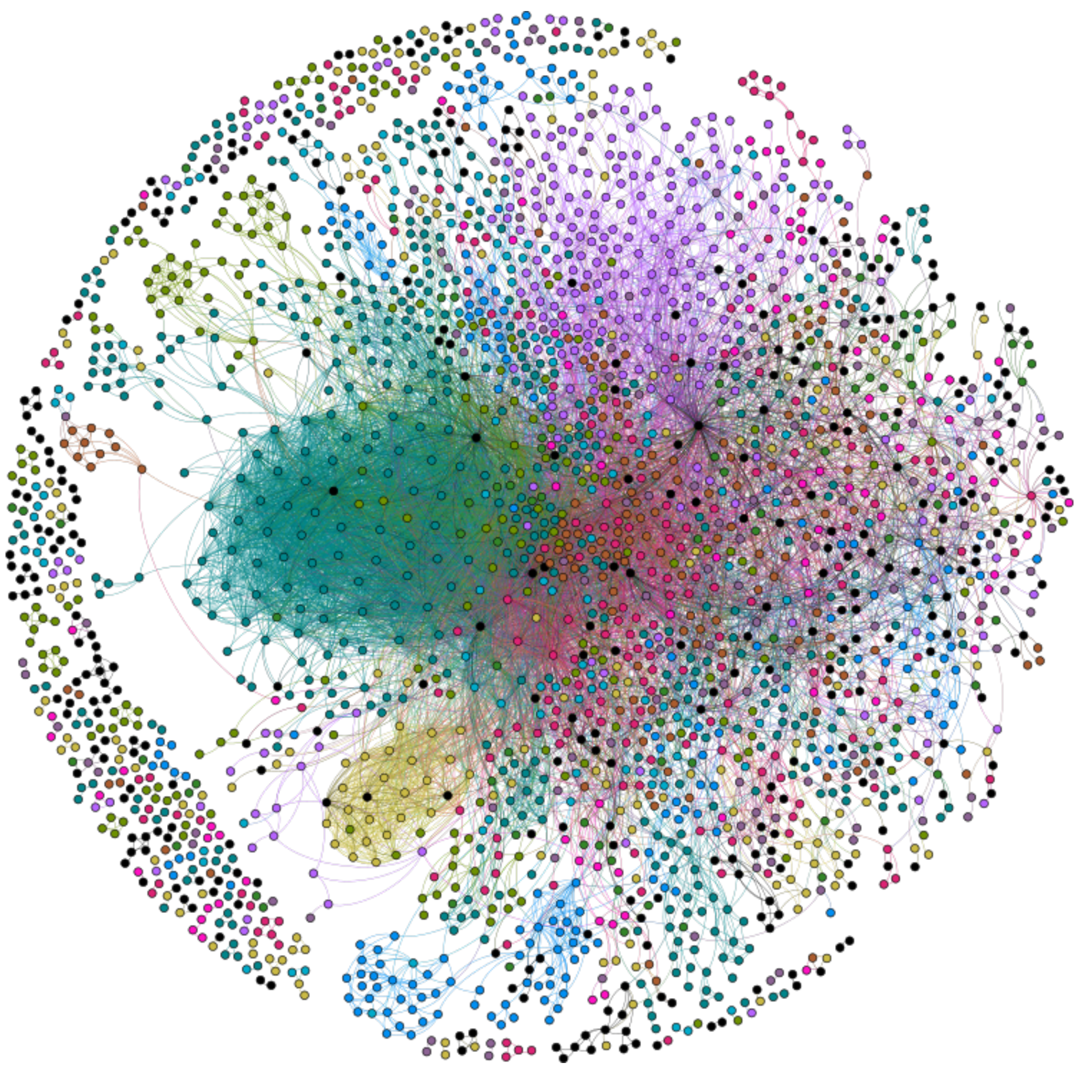
9.4M nodes

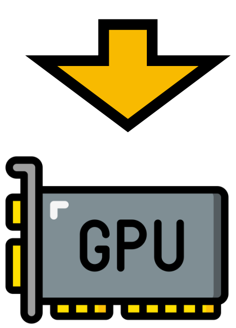
231M edges

>100GB memory for a 3-layer GCN

[1] Backman, Evans and Girke. Large-scale Bioactivity Analysis of the Small-molecule Assayed Proteome. *PLoS ONE'17*.
[2] McAuley et al. Image-based Recommendations on Styles and Substitutes. *SIGIR'15*.

Challenge: **Giant** Graphs for GCNs





>100GB training

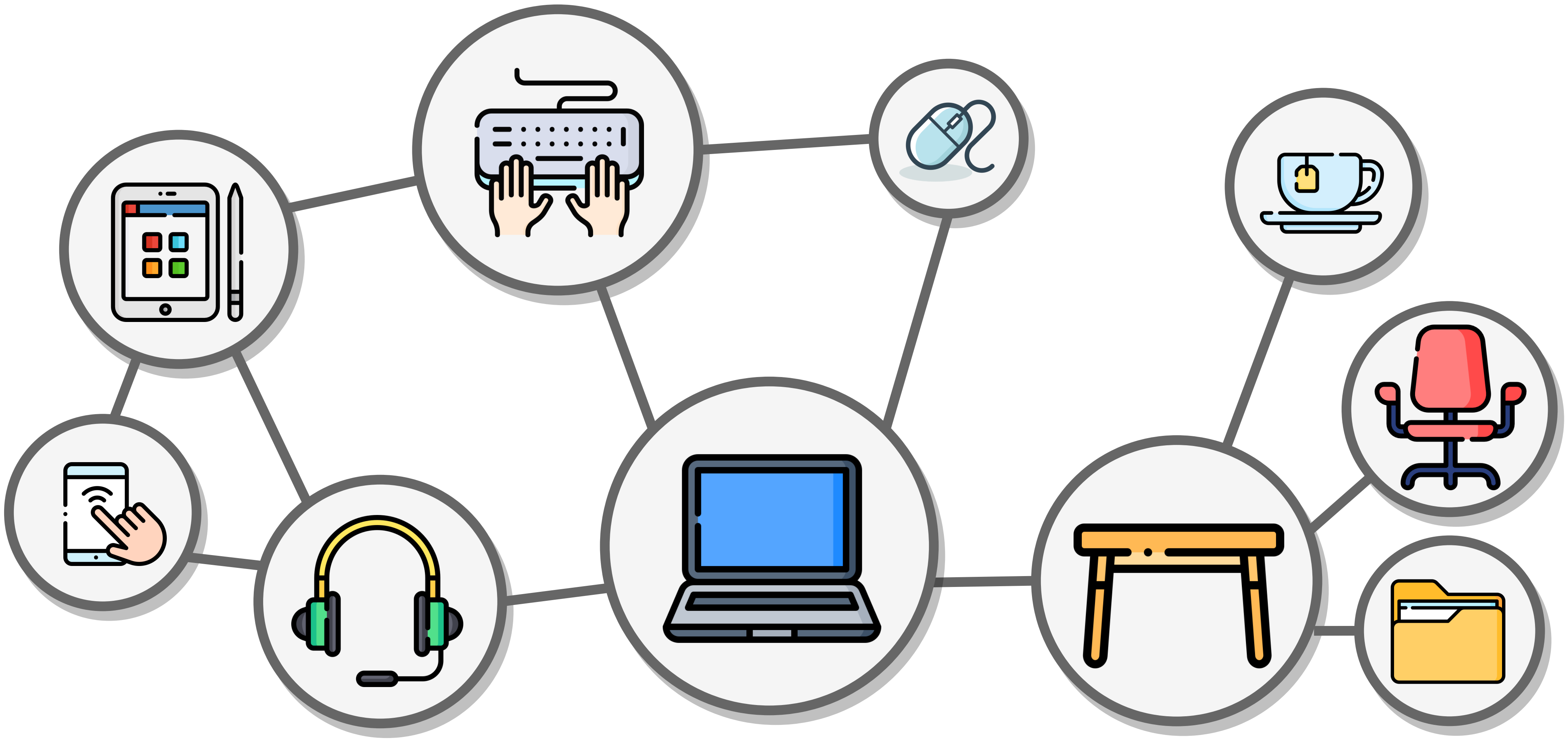
NOT fit

16GB V100

How to train a GCN at scale? Efficiently?

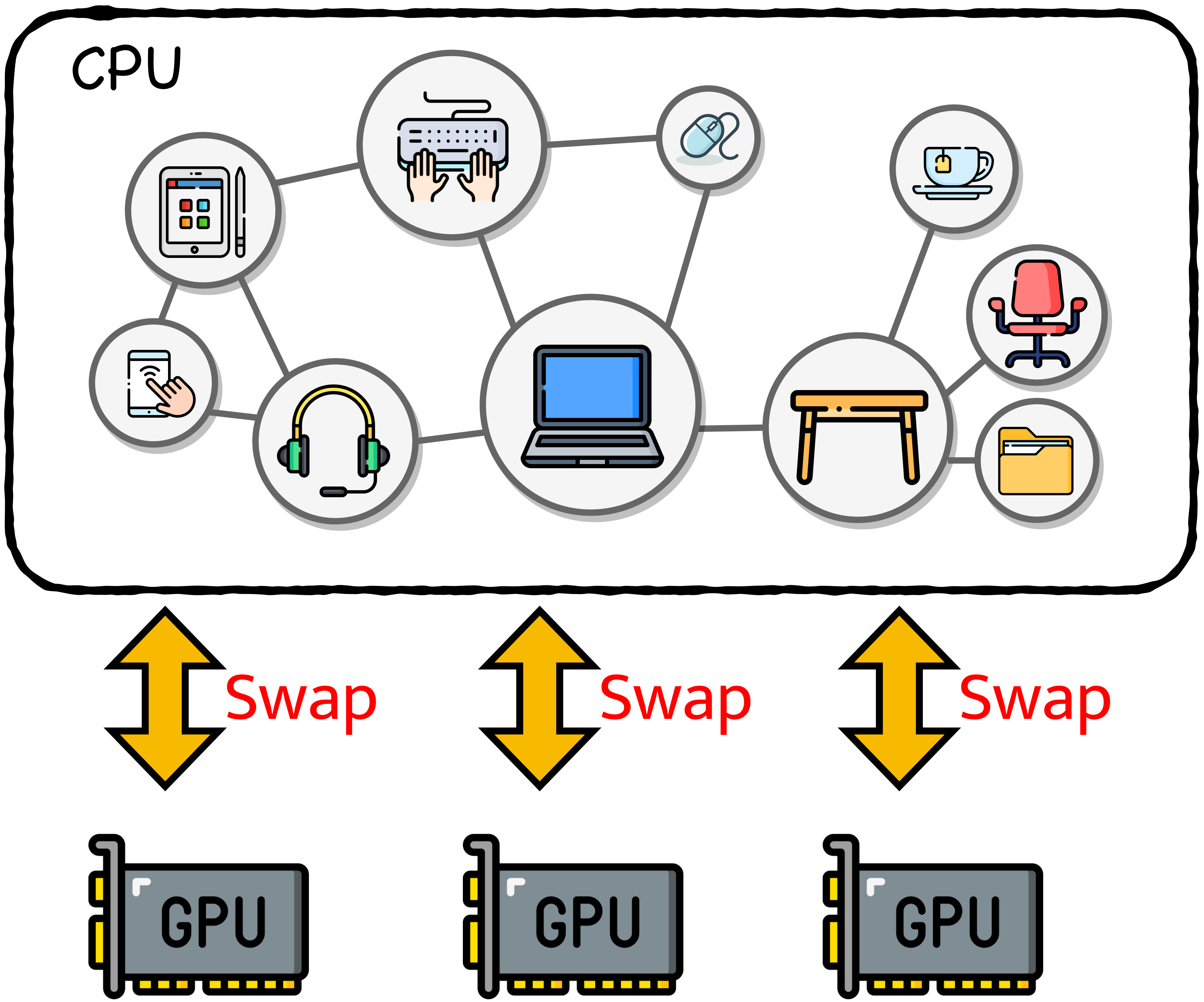
🤔

Category I

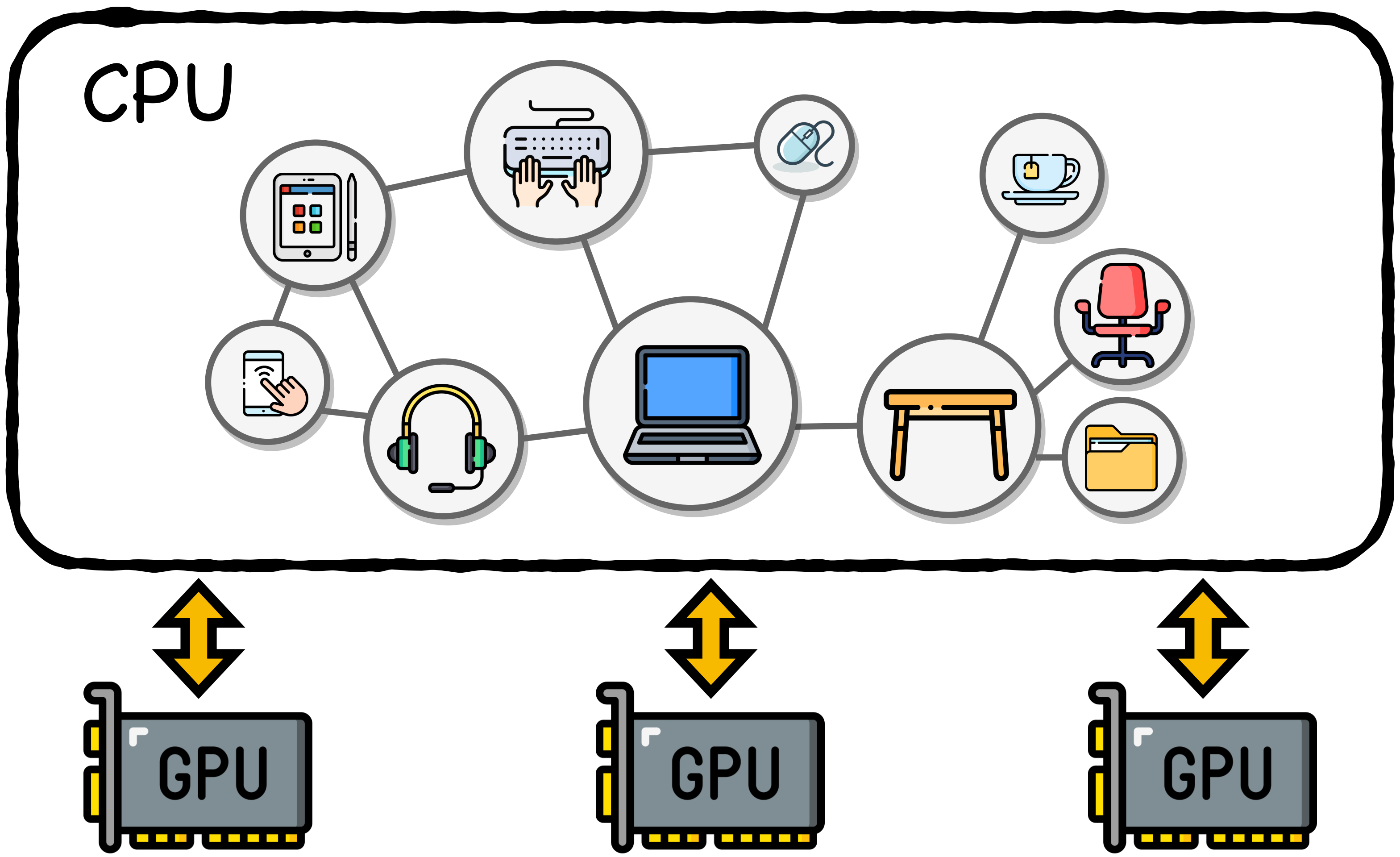


Storage in CPU

Training in GPU



Category I: Swap-Based Methods

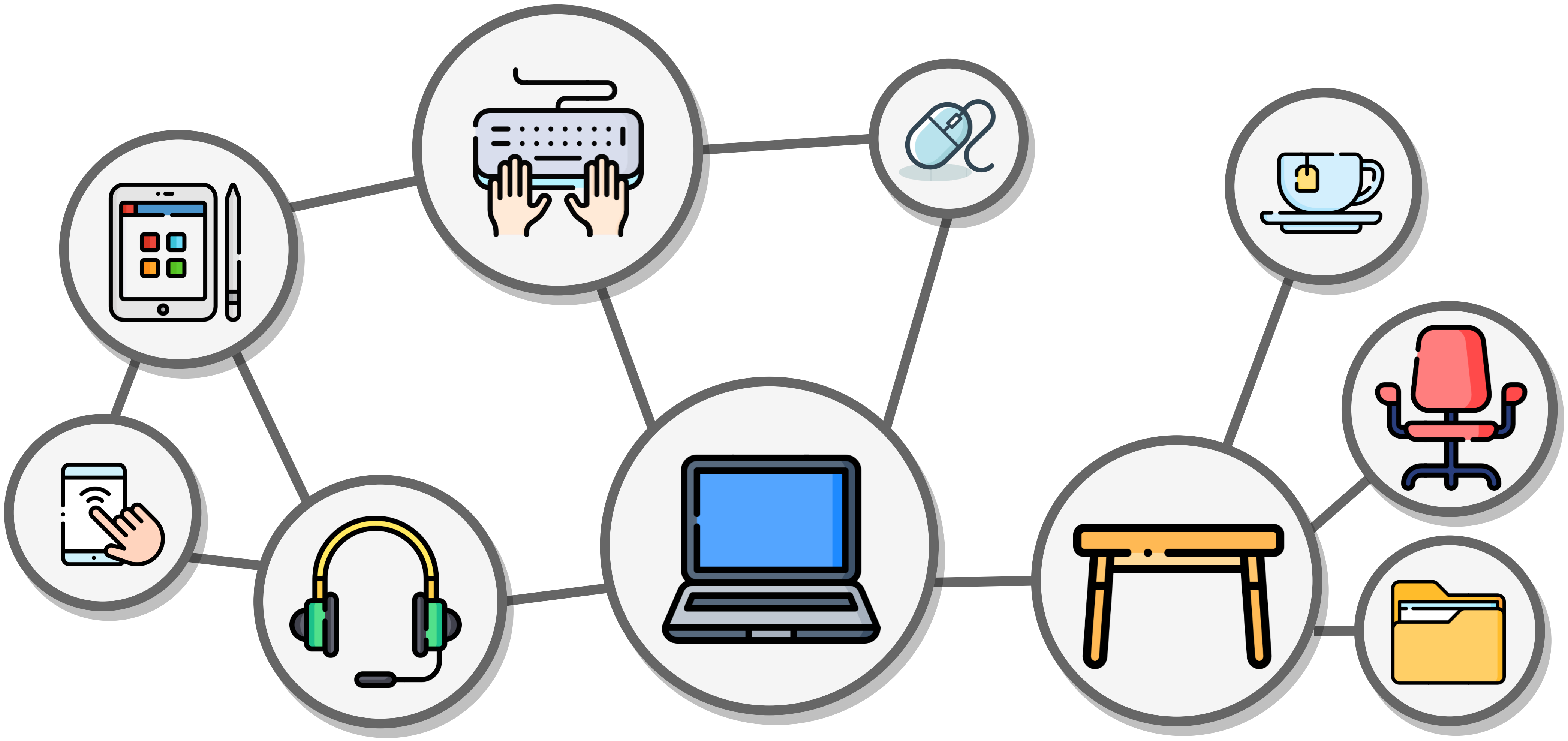


Pro: Scalability of Graph

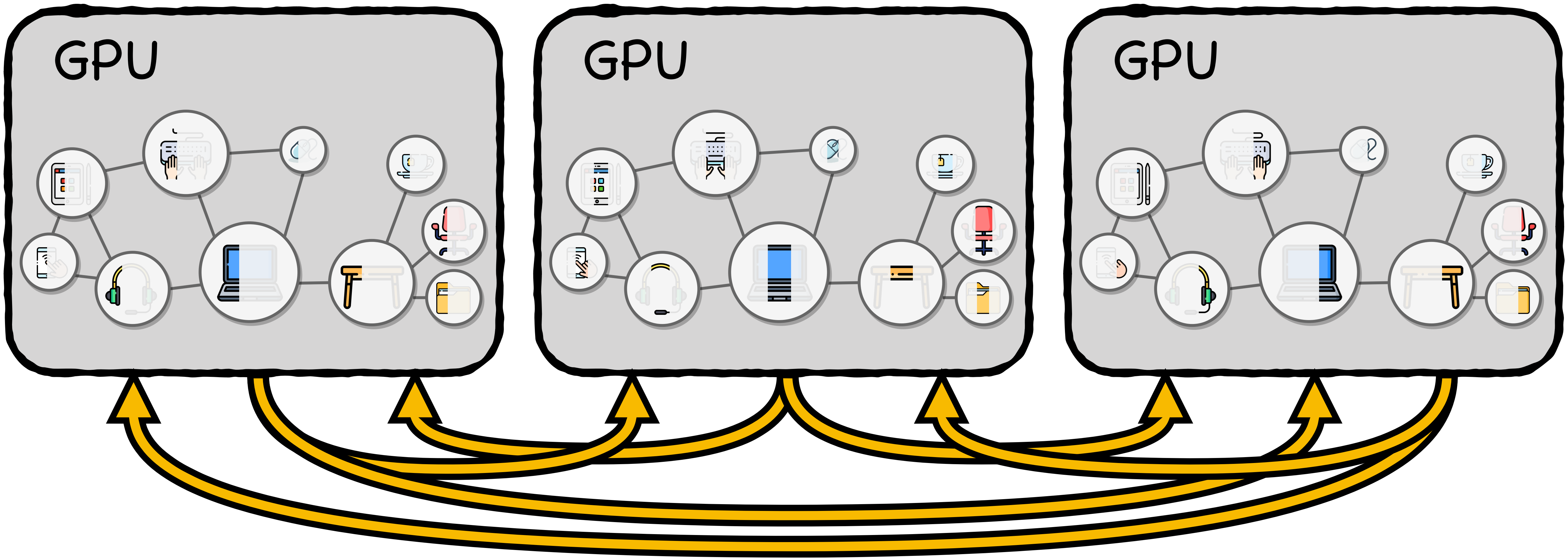
Con: Expensive CPU-GPU Swap

[1] Ma et al. NeuGraph: Parallel Deep Neural Network Computation on Large Graphs. *USENIX ATC'19*
[2] Jia et al. Improving the Accuracy, Scalability, and Performance of Graph Neural Networks with Roc. *MLSys'20*
[3] Fey et al. GNNAutoScale: Scalable and Expressive Graph Neural Networks via Historical Embeddings. *ICML'21*

Category II

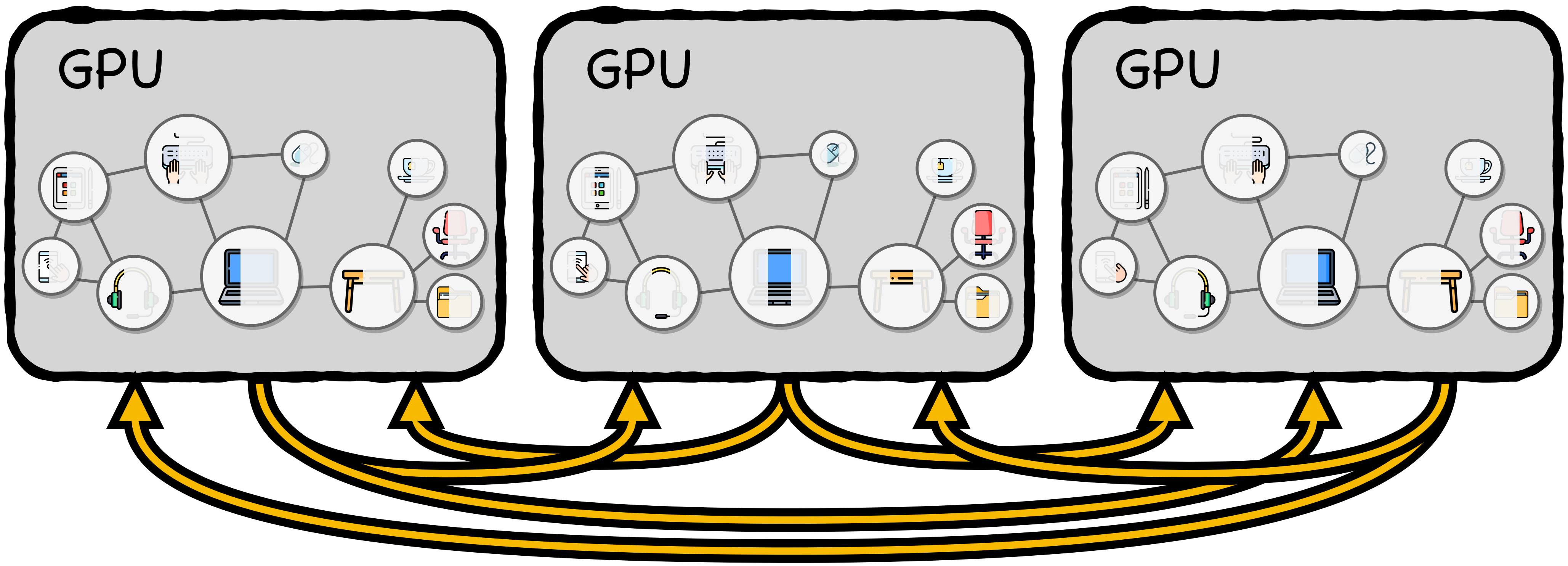


Slicing features across GPUs



Broadcast

Category II: Slice-Based Methods

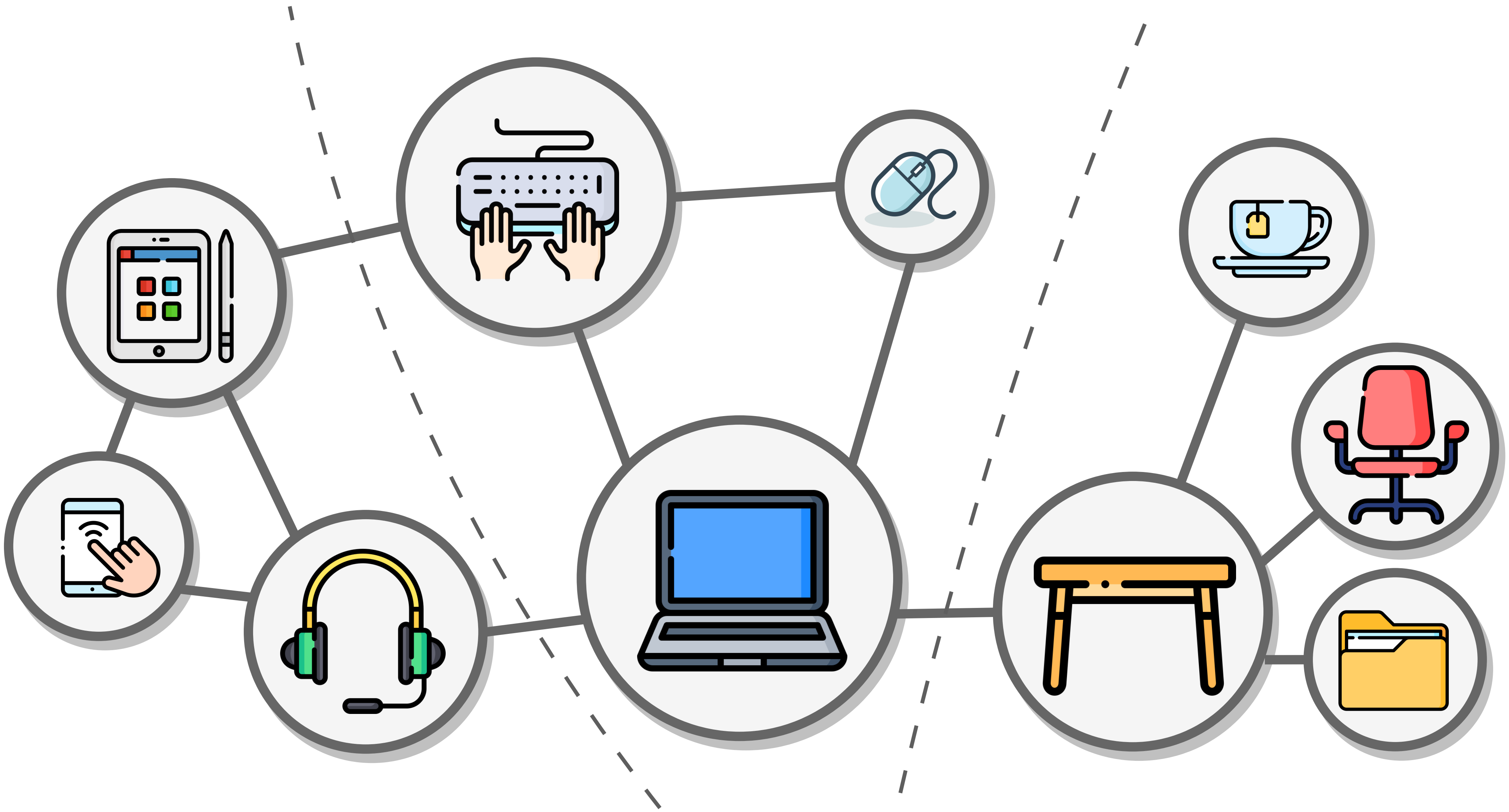


Pro: Balanced Workload

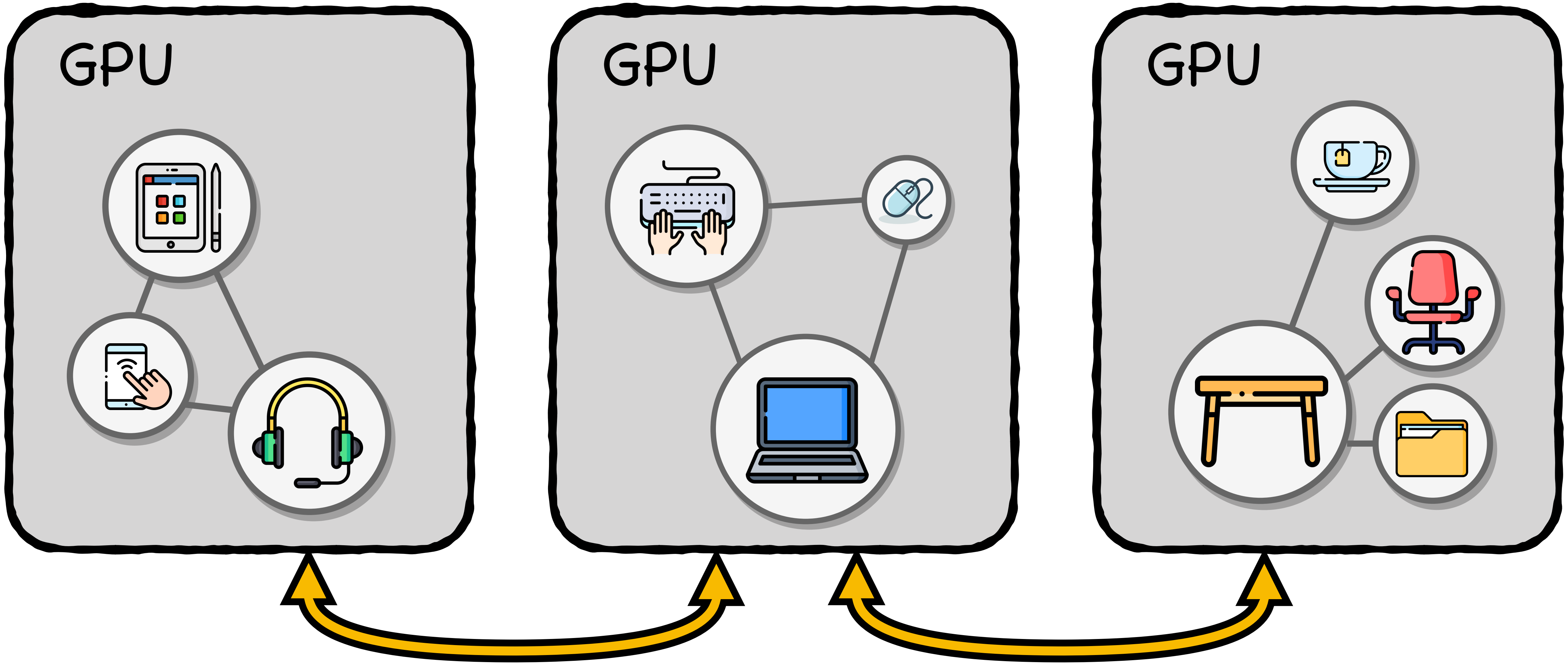
Con: Expensive Broadcast

[1] Tripathy, Yelick and Buluc. Reducing Communication in Graph Neural Network Training. *SC'20*

Category III

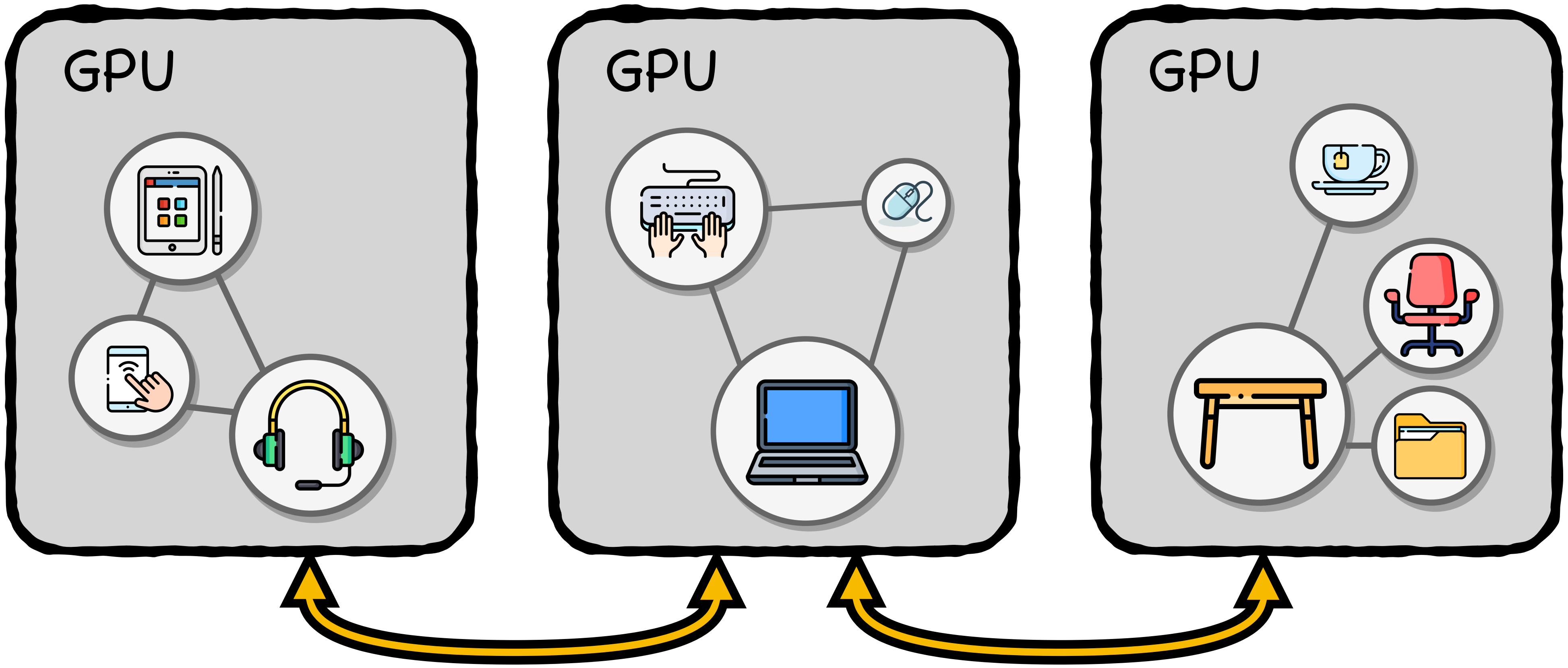


Assigning one partition to one GPU



Point-to-point

Category III: Partition-Based Methods



Pro: Reduced Communication

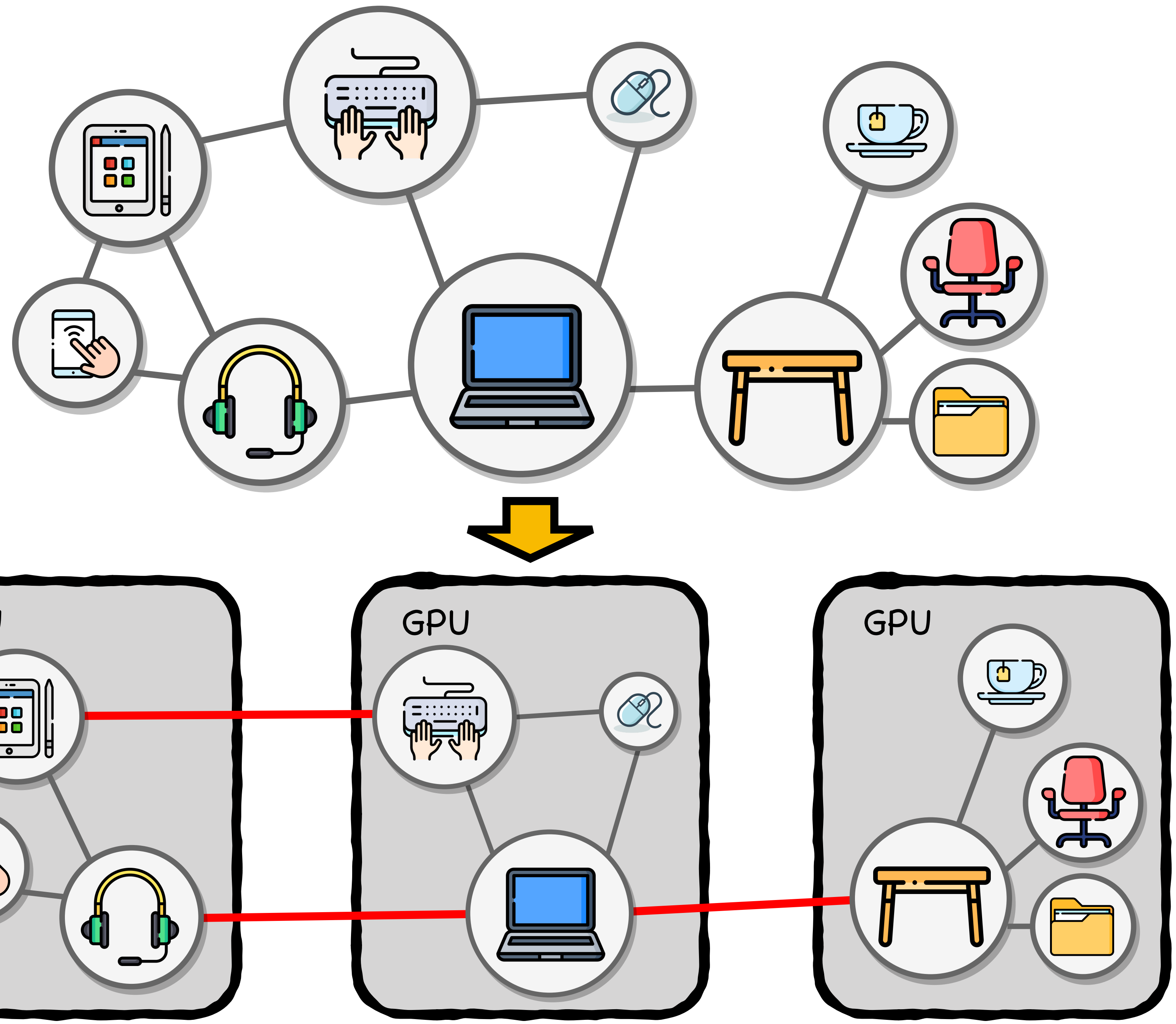
The drawback is **not well studied**

[1] Thorpe et al. Dorylus: Affordable, Scalable, and Accurate GNN Training with Distributed CPU Servers and Serverless Threads. *OSDI'21*
[2] Wan et al. PipeGCN: Efficient Full-Graph Training of Graph Convolutional Networks with Pipelined Feature Communication. *ICLR'22*

BNS-GCN

- ✦ Identifying **drawbacks** of partition-based training
- ✦ Proposing a simple-yet-effective **solution**
- ✦ Providing theoretical and empirical **validation**

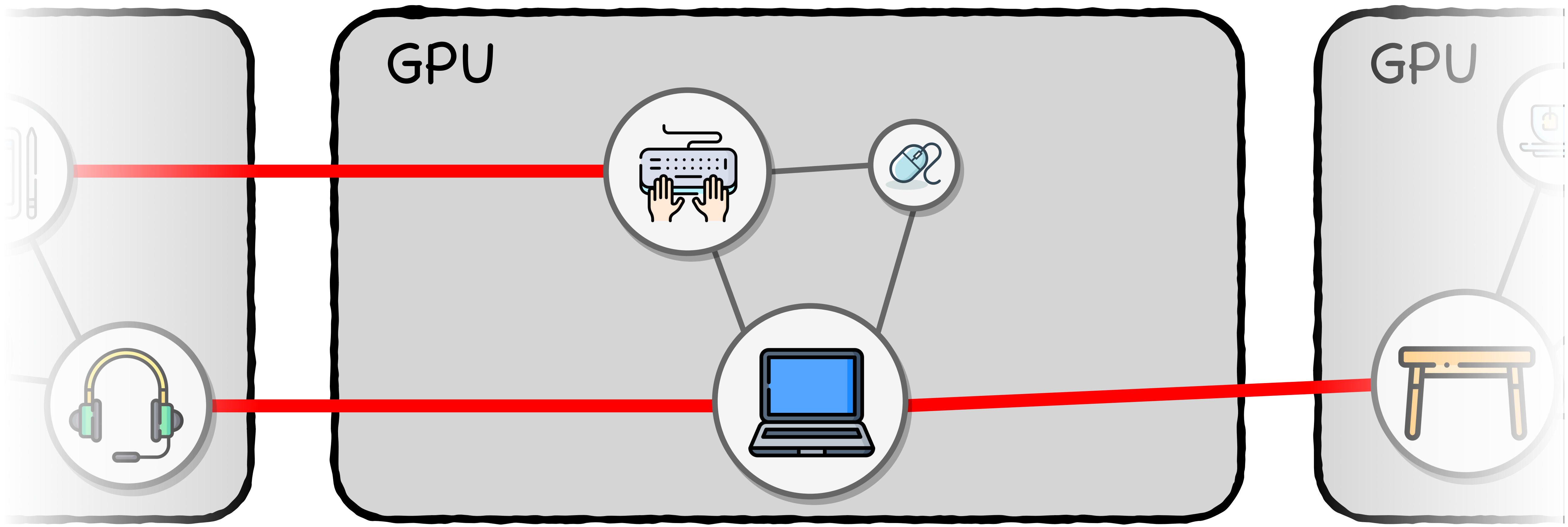
Understanding Partition-Based Methods



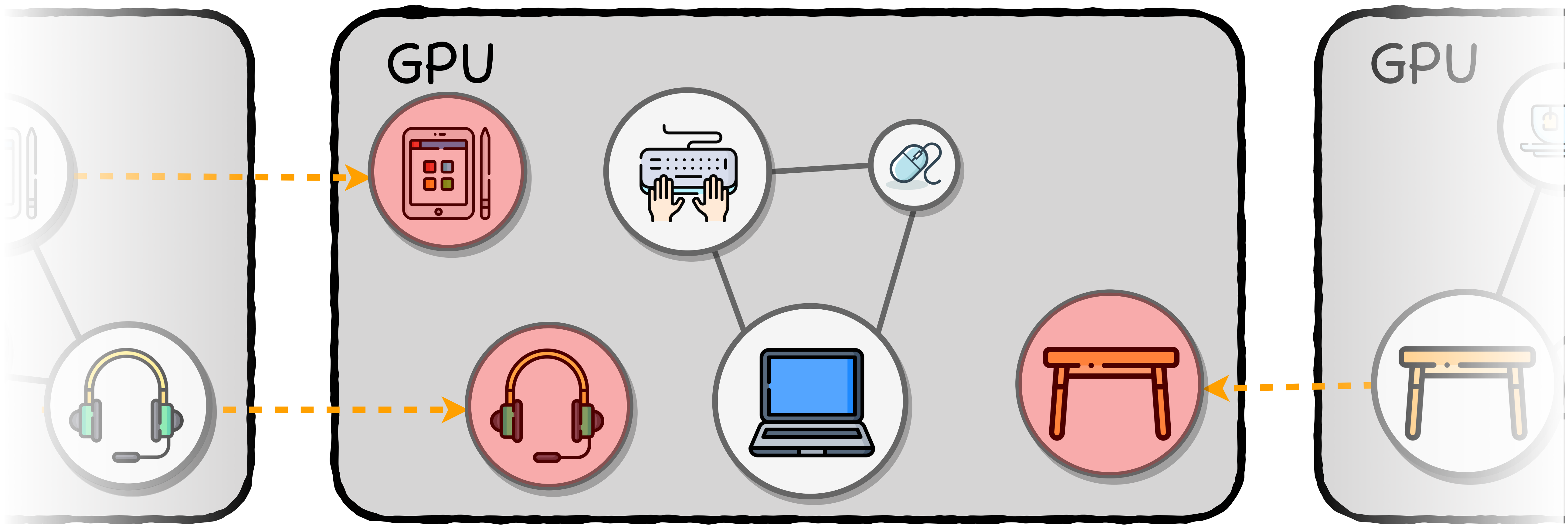
Similar to Data Parallelism

Difference: **Dependency** among Data

Understanding Partition-Based Methods

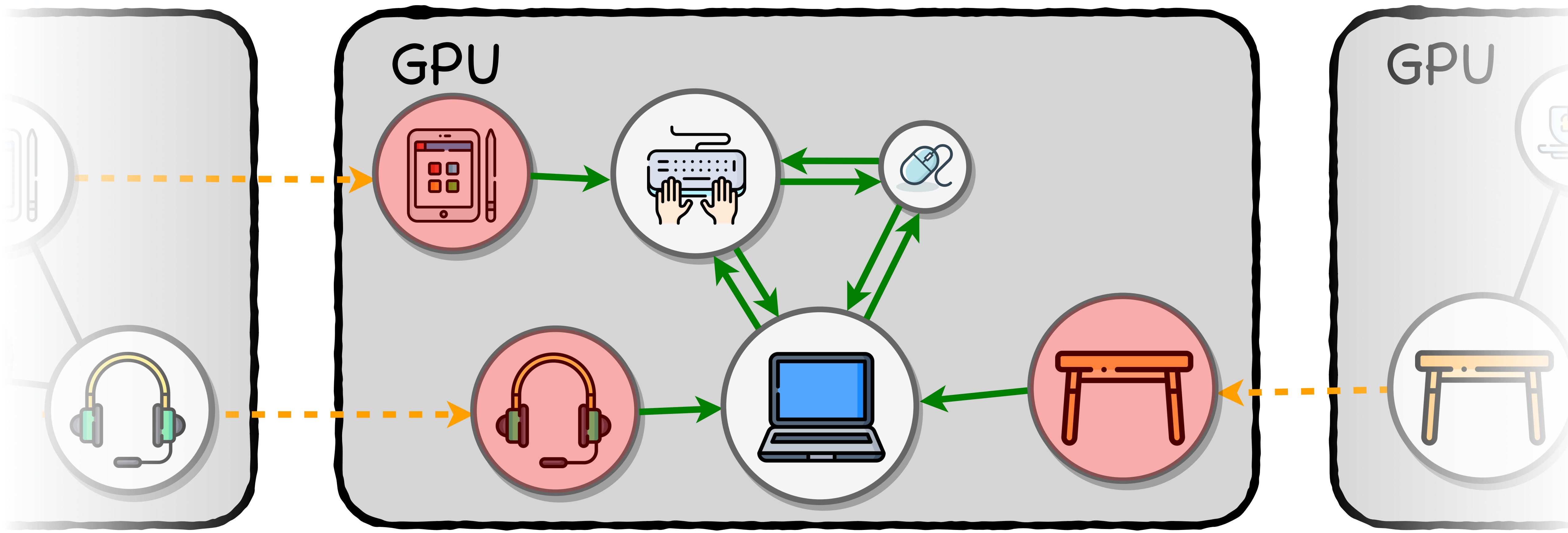


Understanding Partition-Based Methods



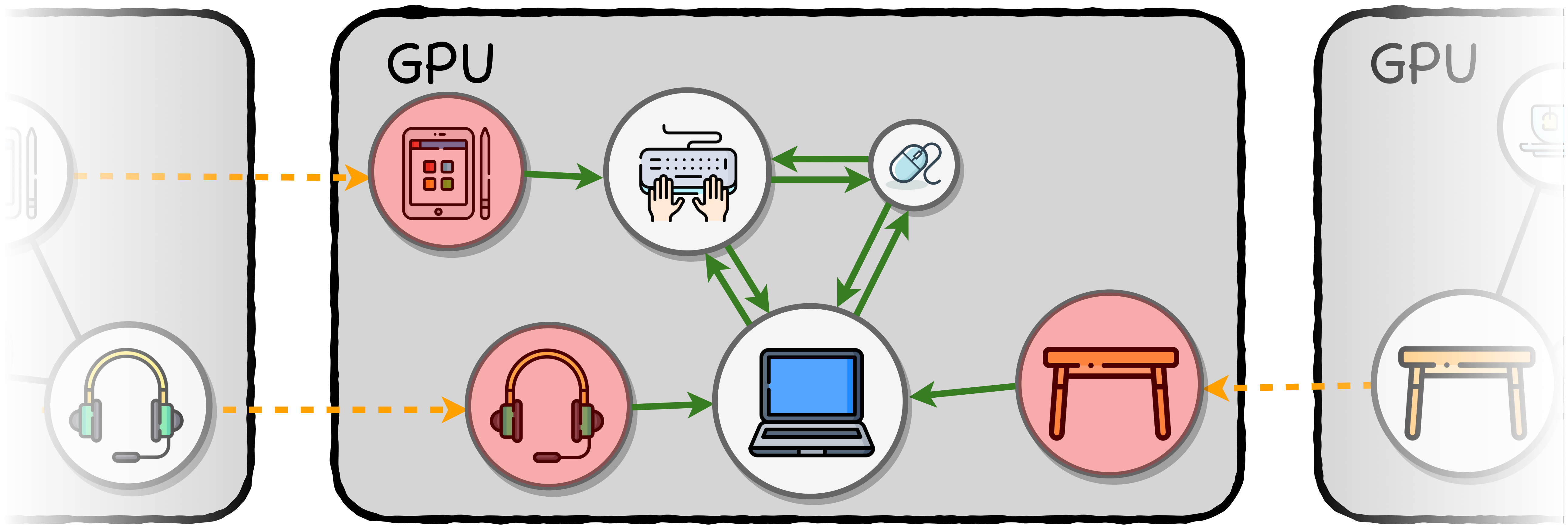
Communicating remote features

Understanding Partition-Based Methods



Computing local features

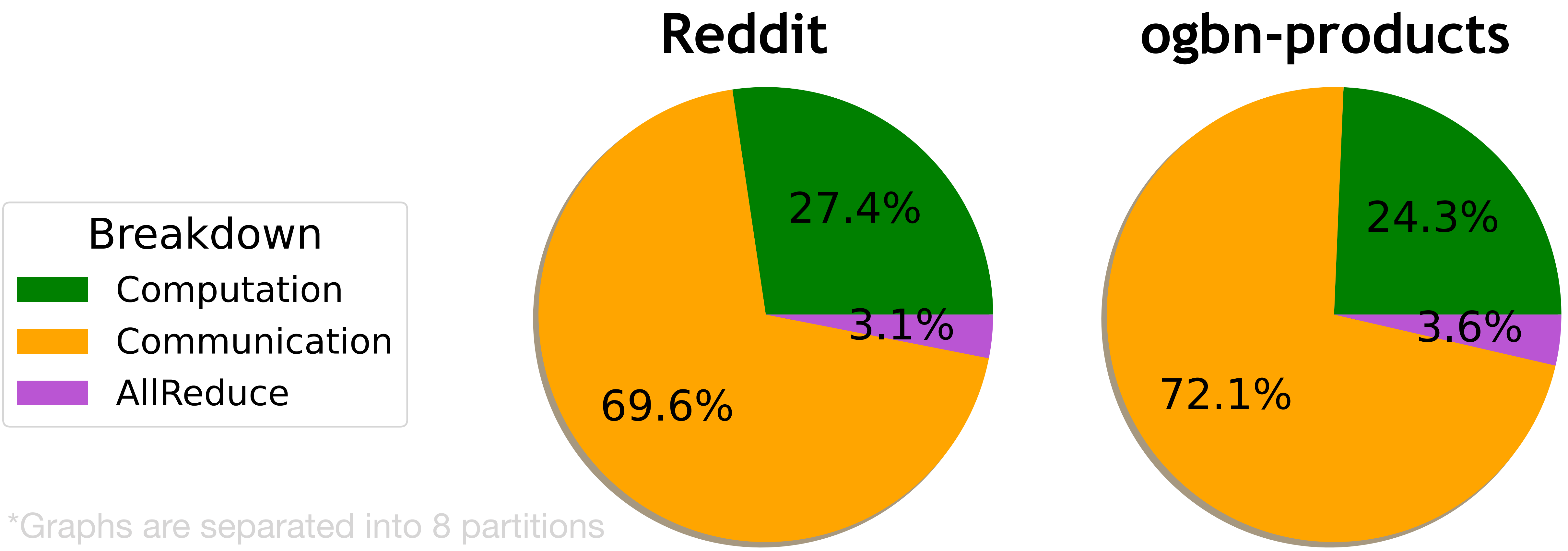
Understanding Partition-Based Methods



Inner Node   Boundary Node

Identifying Drawbacks

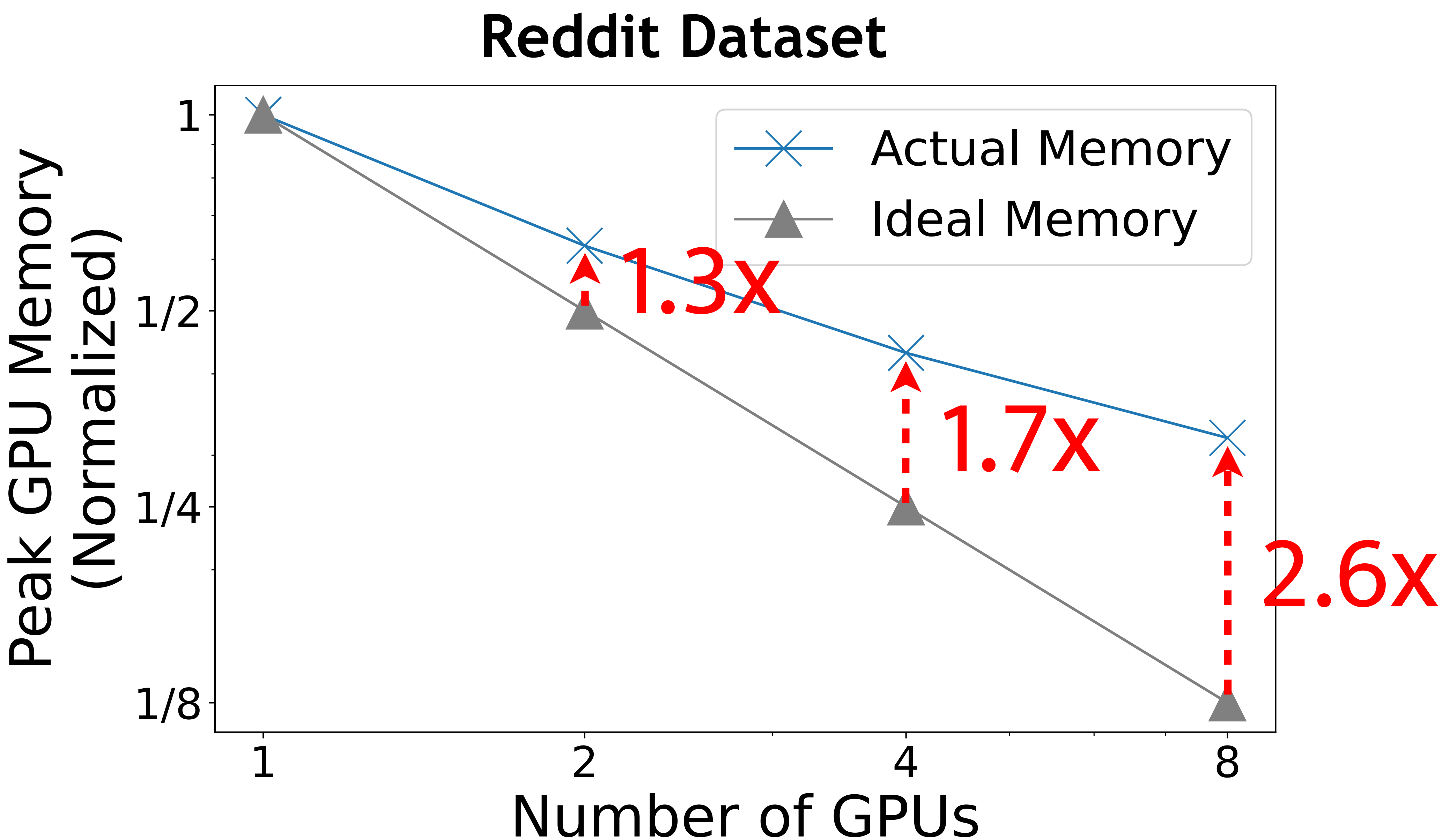
Training Time Breakdown



*Graphs are separated into 8 partitions

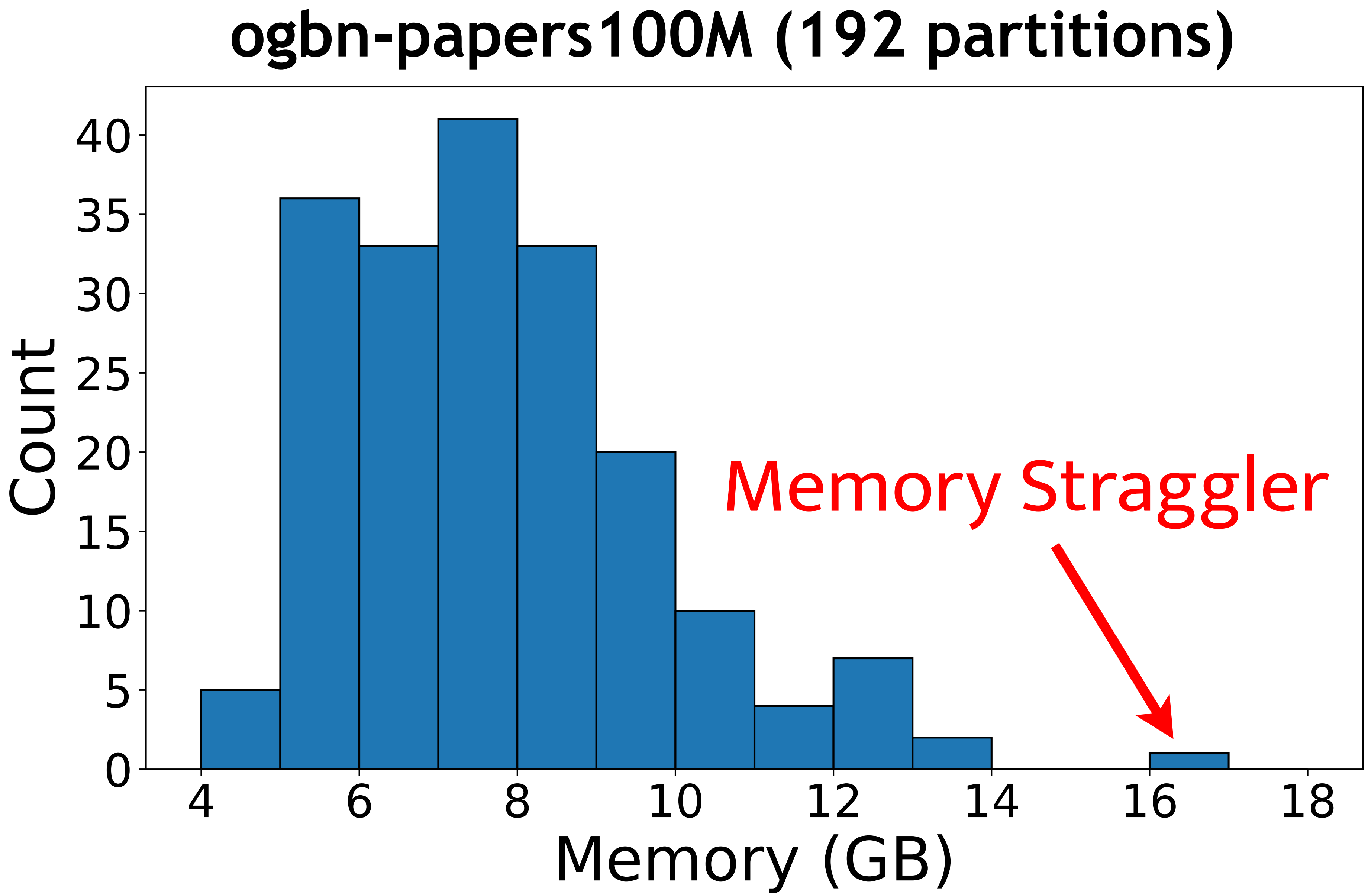
Drawback I: Significant Communication Overhead

Training Memory Requirement



Drawback II: Unscalable Memory Requirement

Per-GPU Memory Distribution

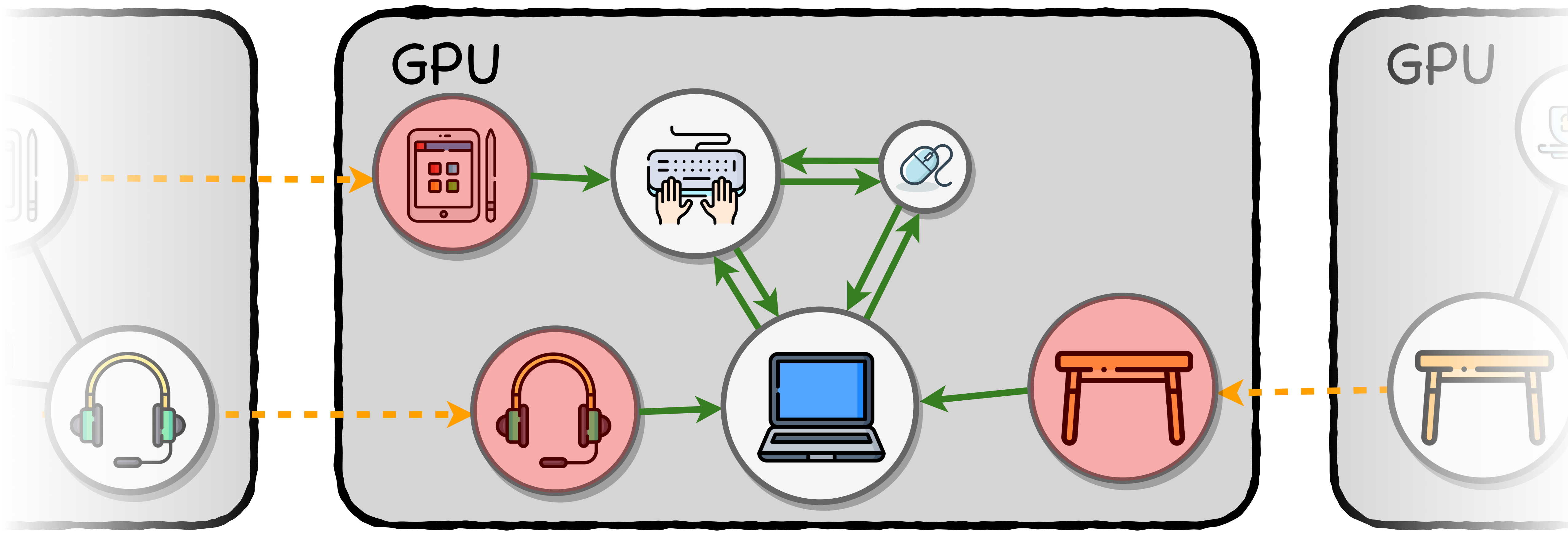


Drawback III: Imbalanced Memory across GPUs

What’s the underlying cause?

🤔

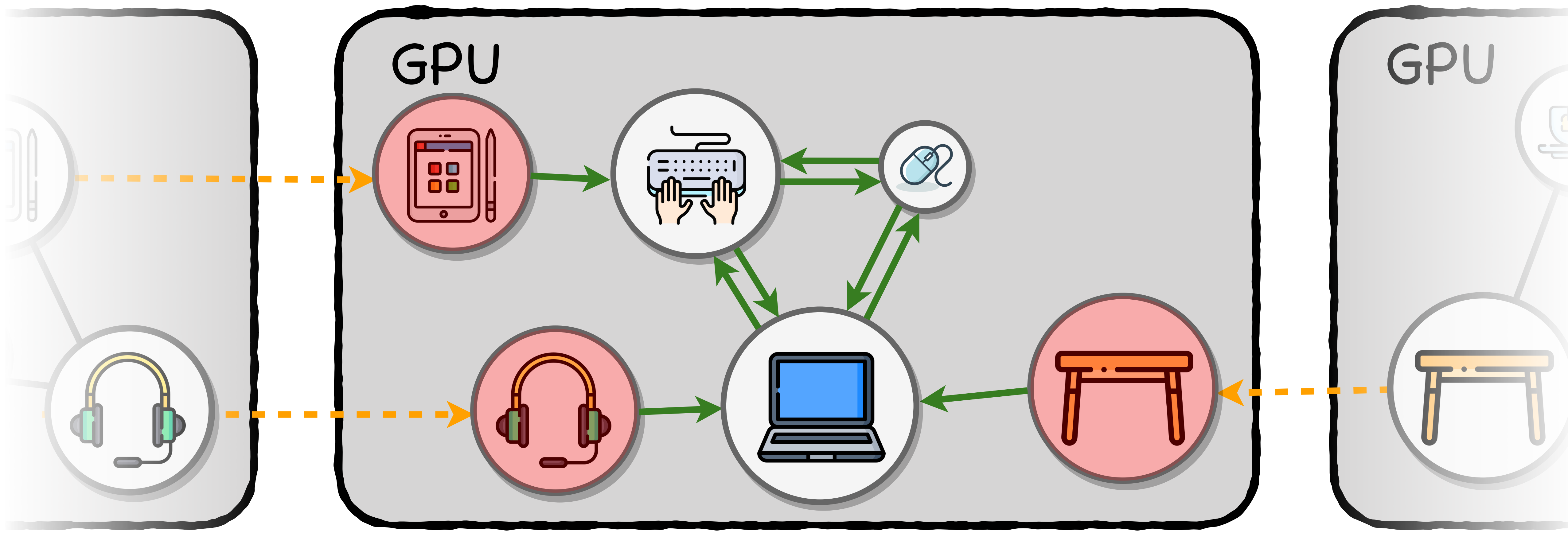
Understanding Communication Volume



Inner Node   Boundary Node

The i-th partition has $n_{in}^{(i)}$ inner nodes and $n_{bd}^{(i)}$ boundary nodes

Understanding Communication Volume

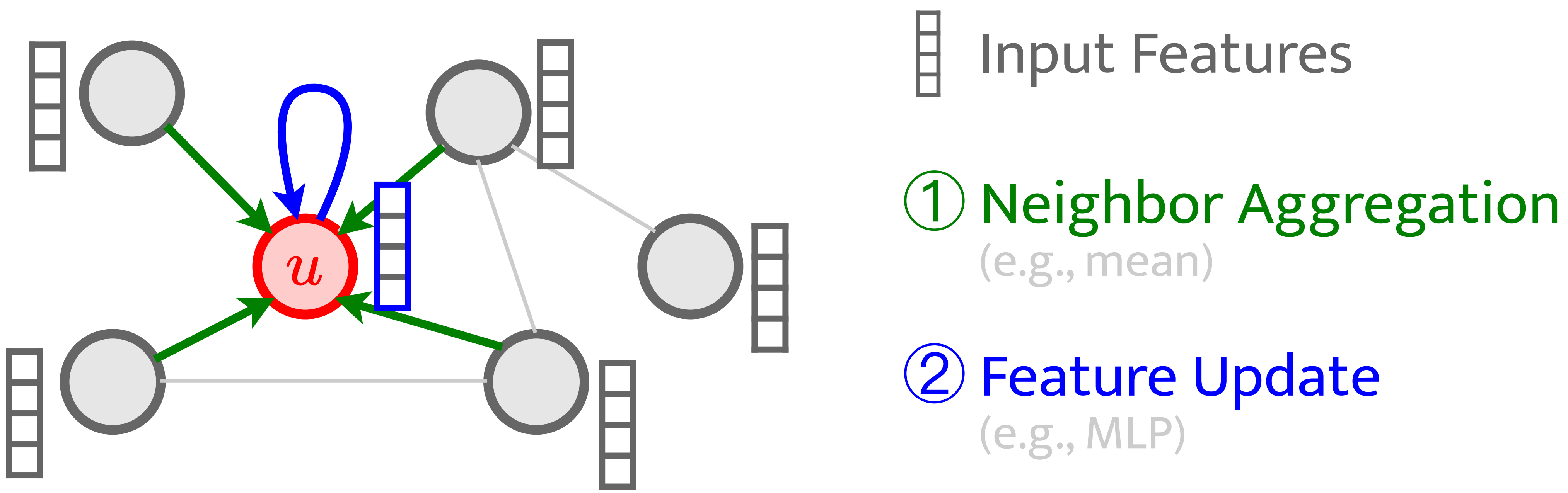


$$\mathrm{Vol}_{\mathrm{total}} = \sum_i \mathrm{Vol}(\mathcal{G}_i) = \sum_i n_{bd}^{(i)}$$

Comm. Volume ∝ # Boundary Nodes

! Min-Cut is not Optimal

Understanding Memory Requirement



$$\mathrm{Mem}(\mathcal{G}_i) \propto \underbrace{3n_{in}^{(i)} + n_{bd}^{(i)}}$$

Aggregation: $n_{in}^{(i)} + n_{bd}^{(i)}$

Linear + Activation: $2n_{in}^{(i)}$

Contribution I: Identify the Underlying Cause

I Significant Communication Overhead

II Unscalable Memory Requirement

III Imbalanced Memory across GPUs

What's the underlying cause?

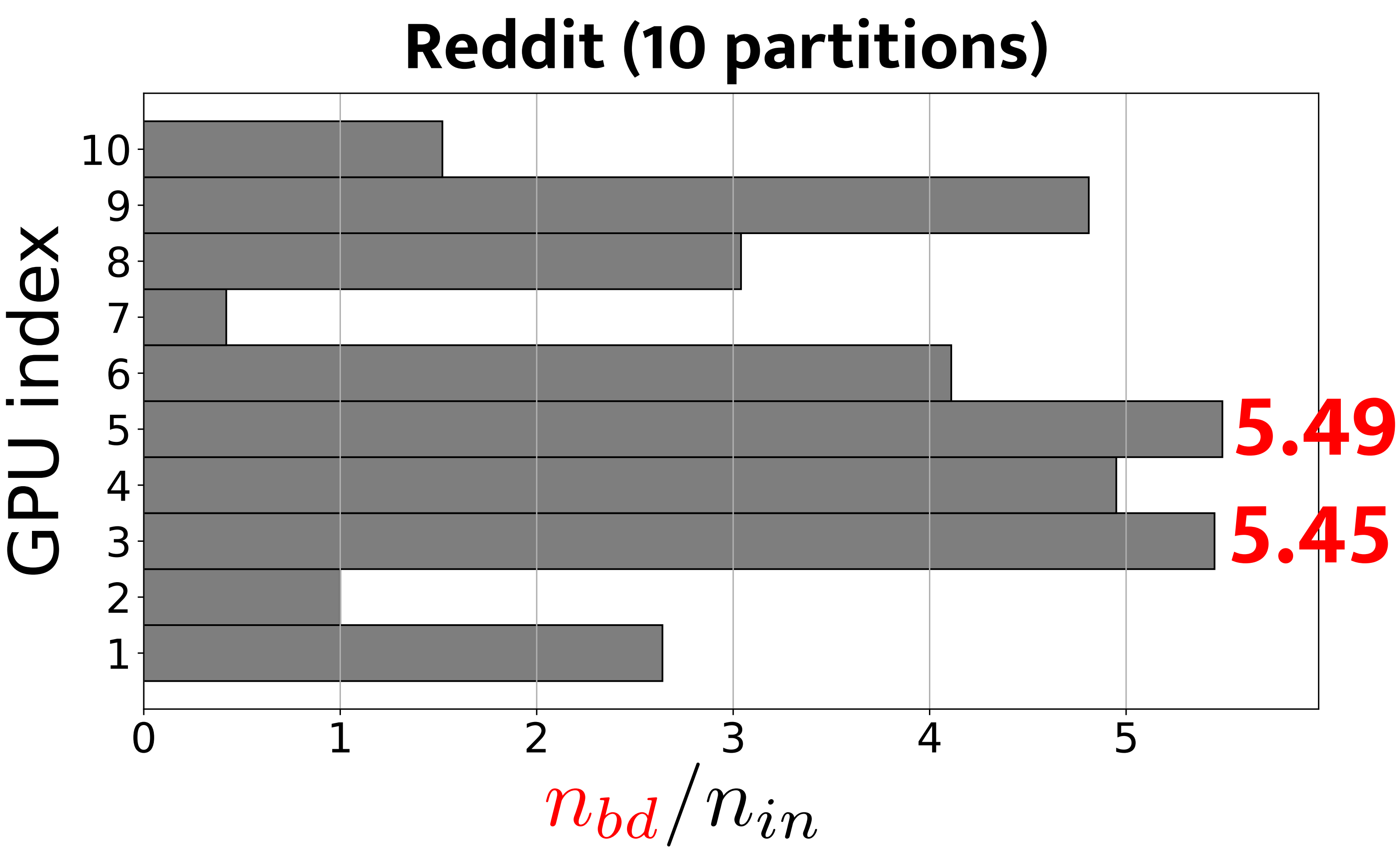
Contribution I: Identify the Underlying Cause

I Significant Communication Overhead — $\mathrm{Vol}_{\mathrm{total}} = \sum_i \mathrm{Vol}(\mathcal{G}_i) = \sum_i n_{bd}^{(i)}$

II Unscalable Memory Requirement

III Imbalanced Memory across GPUs

$\mathrm{Mem}(\mathcal{G}_i) \propto 3n_{in}^{(i)} + n_{bd}^{(i)}$

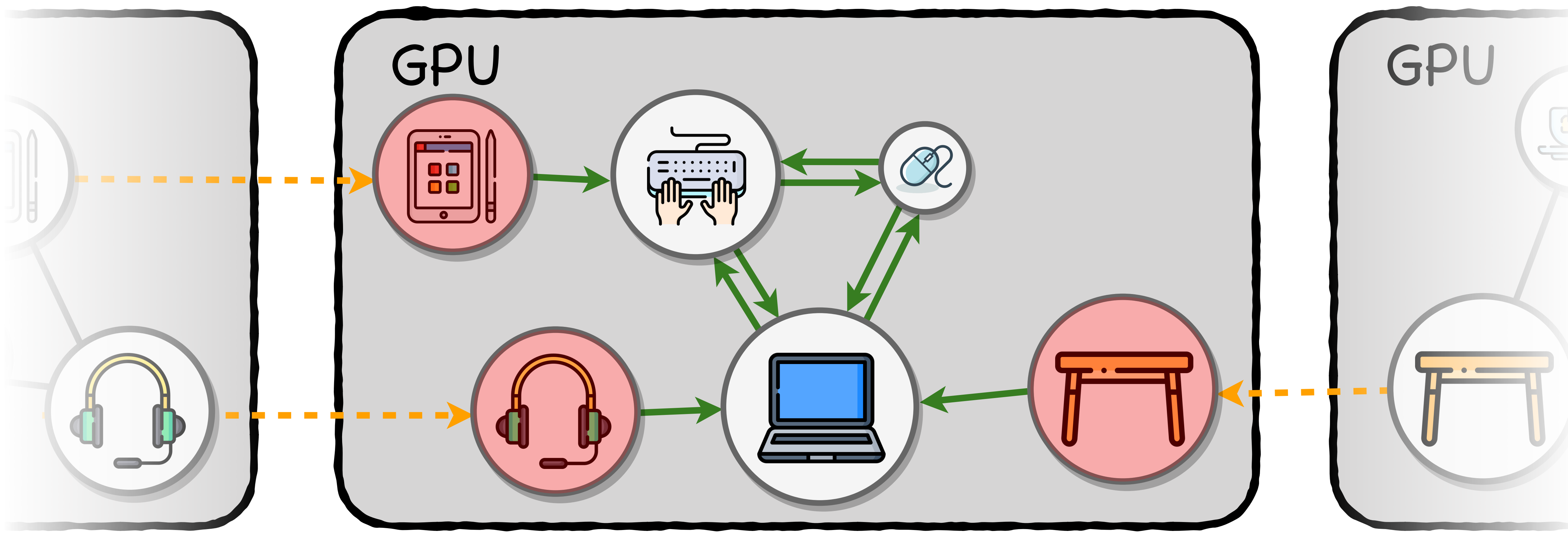


Boundary nodes are the cause 😣

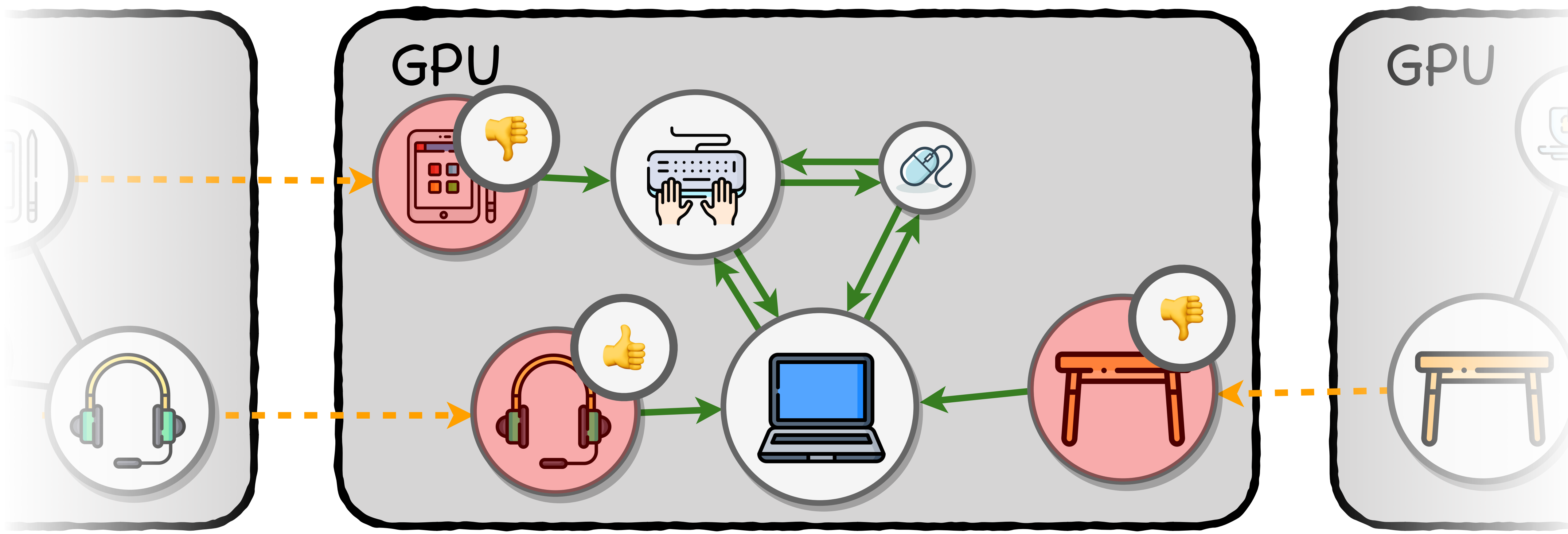
How to solve them? One stone three birds?

🤔

Contribution II: Propose Boundary Node Sampling

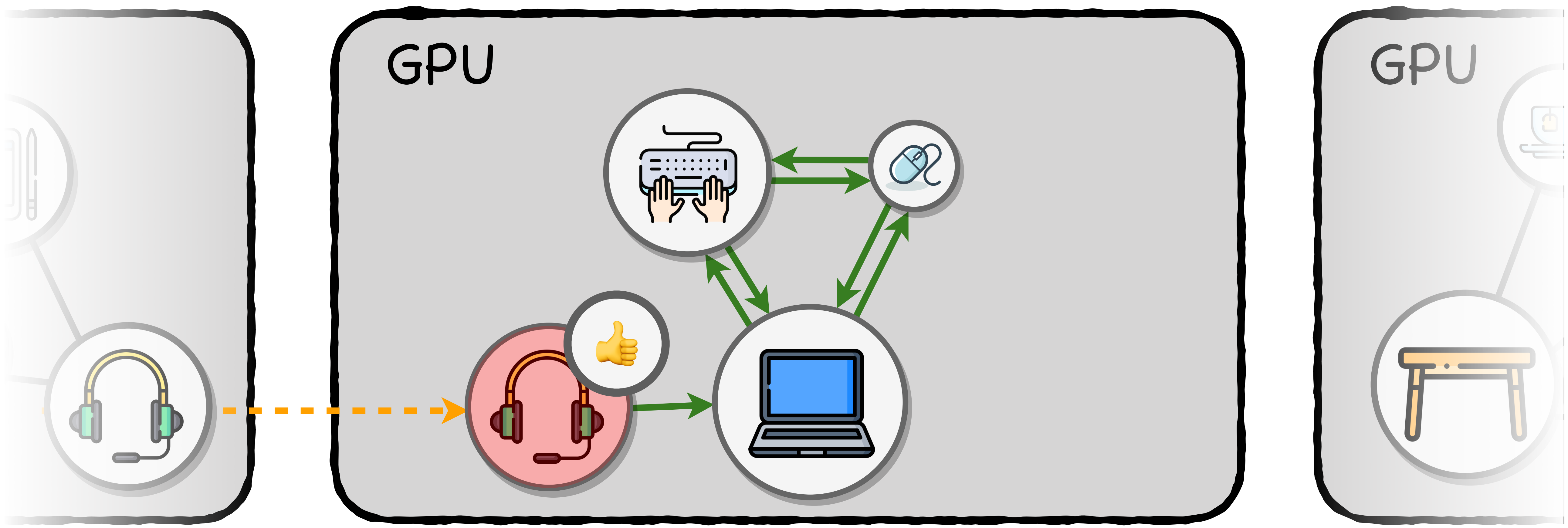


Contribution II: Propose Boundary Node Sampling



Step 1: Sampling each boundary node with probability p

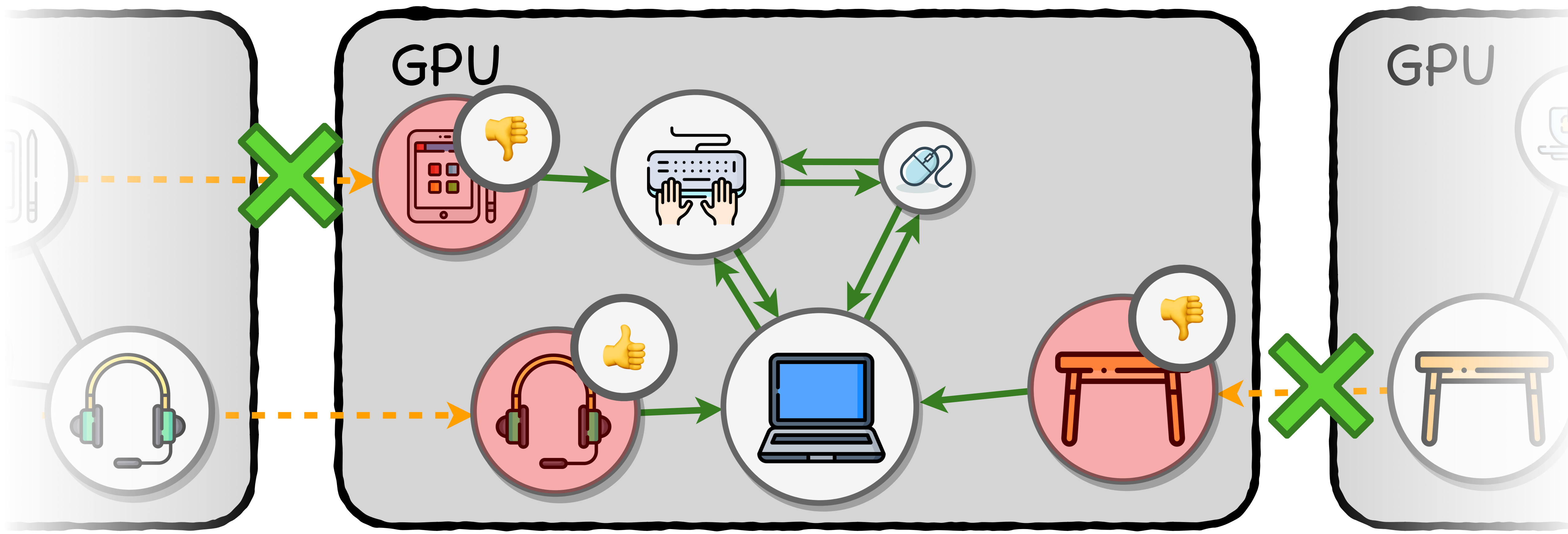
Contribution II: Propose Boundary Node Sampling



Step 1: Sampling each boundary node with probability p

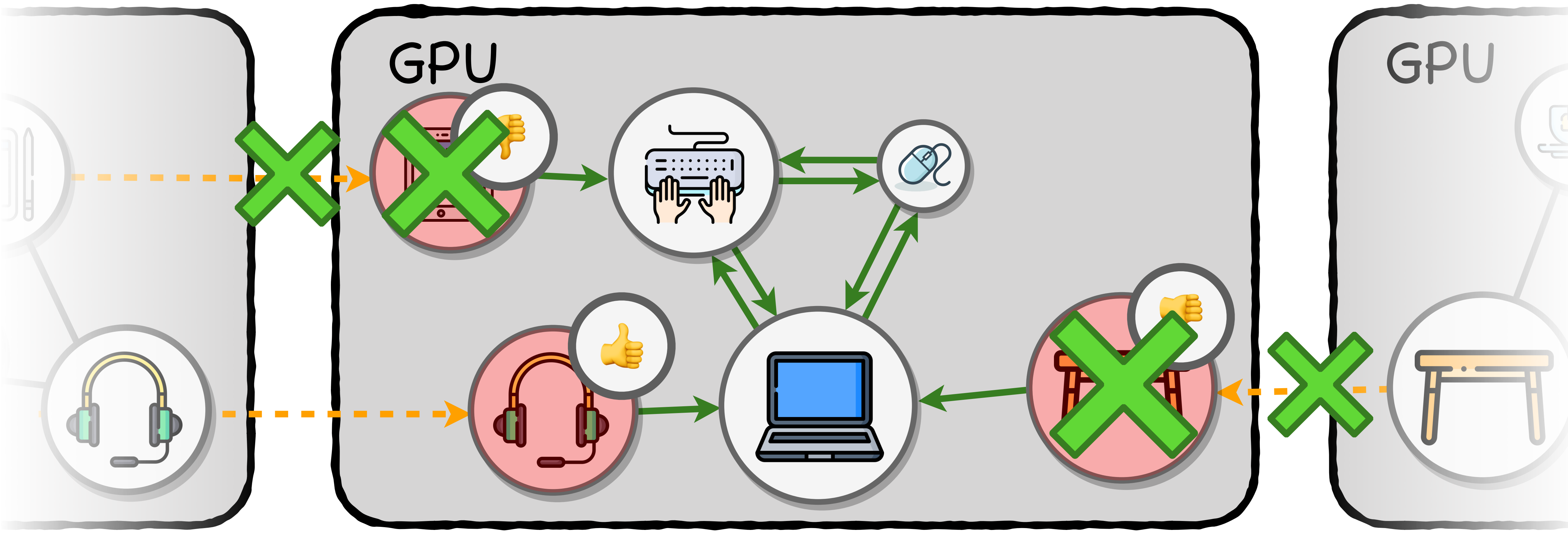
Step 2: Removing unsampled nodes

Contribution II: Propose Boundary Node Sampling



Reducing communication volume

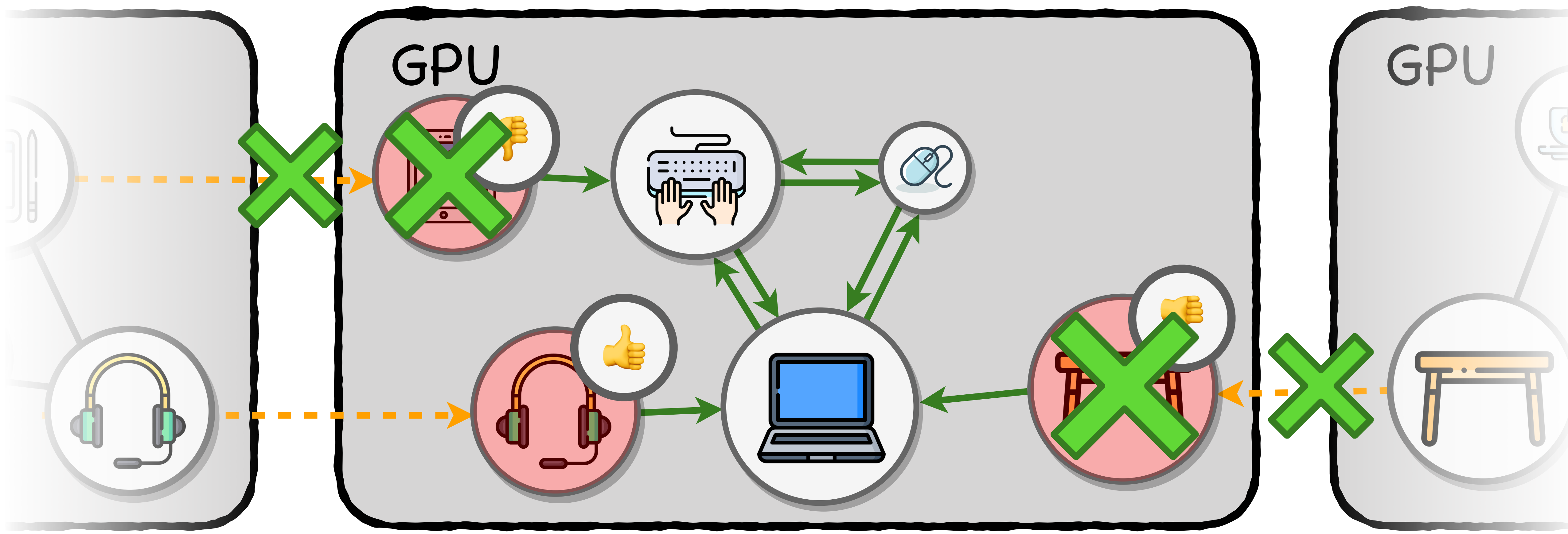
Contribution II: Propose Boundary Node Sampling



Reducing communication volume

Reducing memory requirement

Contribution II: Propose Boundary Node Sampling



Reducing communication volume

Reducing memory requirement

Balancing memory across GPUs

($n_{bd}^{(i)}$ becomes negligible)

Contribution III: Validate BNS-GCN in **Theory**

Method	Variance

We compare the **variance** of feature approximation

(lower is better)

Contribution III: Validate BNS-GCN in **Theory**

Method	**Variance**	
BNS-GCN	$\mathcal{O}(\lvert\mathcal{B}\rvert)$	boundary neighbor set
LADIES [NeurIPS'19]	$\mathcal{O}(\lvert\mathcal{N}\rvert)$	neighbor set
FastGCN [ICLR'18]	$\mathcal{O}(\lvert\mathcal{V}\rvert)$	global node set

*We fix output nodes and sampling size

$\mathcal{B} \subseteq \mathcal{N} \subseteq \mathcal{V}$ ⇨ BNS-GCN has the best feature approximation

Contribution III: Validate BNS-GCN in **Theory**

Method	**Variance**
BNS-GCN	$\mathcal{O}(\lvert\mathcal{B}\rvert\,\gamma^2)$
LADIES [NeurIPS'19]	$\mathcal{O}(\lvert\mathcal{N}\rvert\,\gamma^2)$
FastGCN [ICLR'18]	$\mathcal{O}(\lvert\mathcal{V}\rvert\,\gamma^2)$
VR-GCN [ICML'18]	$\mathcal{O}(D\Delta\gamma^2)$
GraphSAGE [NIPS'17]	$\mathcal{O}(D\gamma^2)$

*We fix output nodes and sampling size

More analysis is in our paper

Experiments

Experiment Setup

Considered Datasets

Reddit, ogbn-products, Yelp and ogbn-papers100M

Dataset Description

Name	# Nodes	# Edges	Environment
Reddit	233K	114M	10 RTX-2080Ti (11GB)
ogbn-products	2.4M	62M	
Yelp	716K	7.0M	
ogbn-papers100M	111M	1.6B	32 x (6 Tesla V100 (16GB))

Experiment Setup

Considered Datasets

Reddit, ogbn-products, Yelp and ogbn-papers100M

Benchmarked Baselines

ROC [MLSys'20] (swap-based) and CAGNET [SC'20] (slice-based)

Experiment Setup

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Reddit, ogbn-products, Yelp and ogbn-papers100M

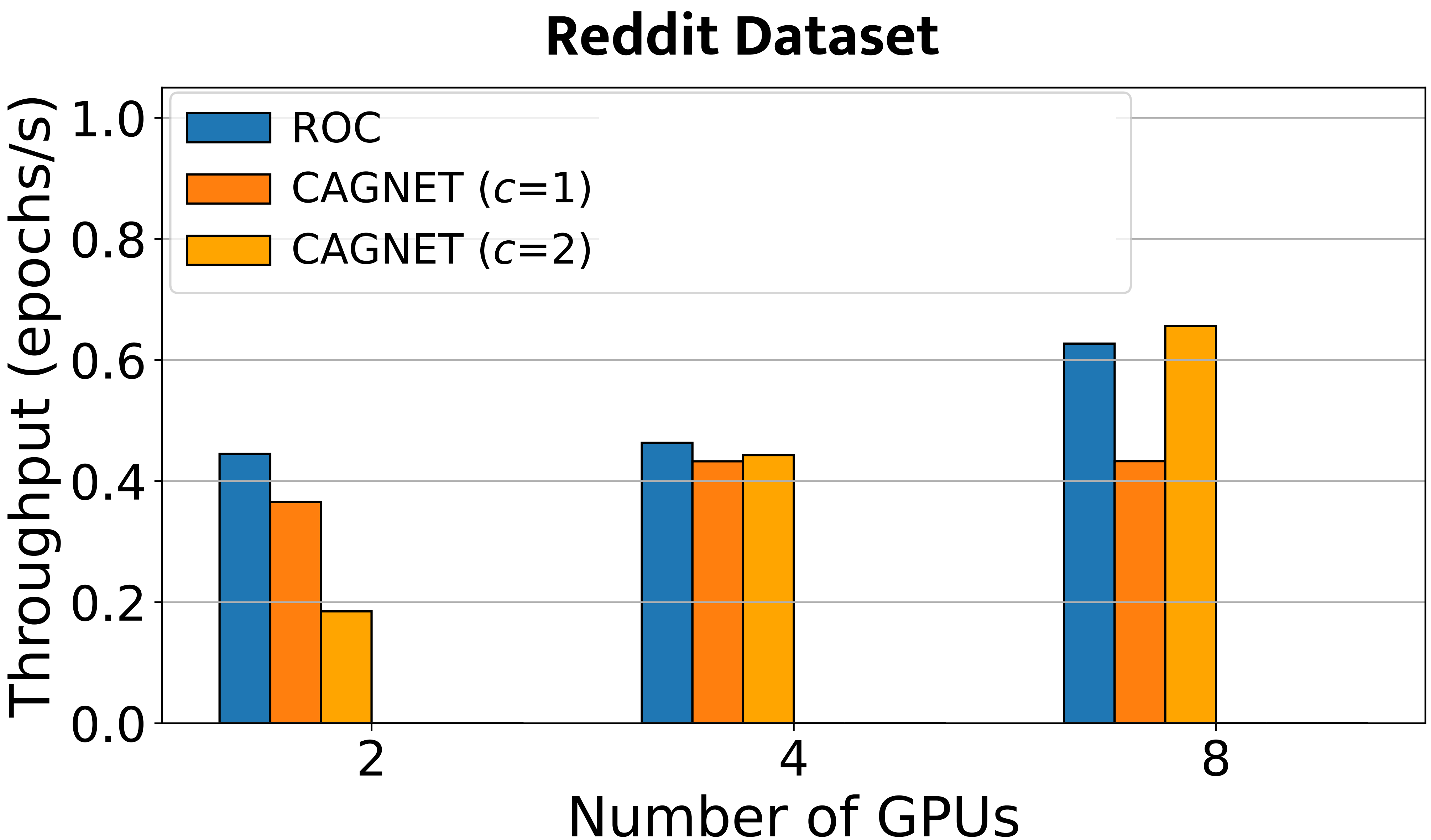
Benchmarked Baselines

ROC [MLSys'20] (swap-based) and CAGNET [SC'20] (slice-based)

Adopted Toolkits

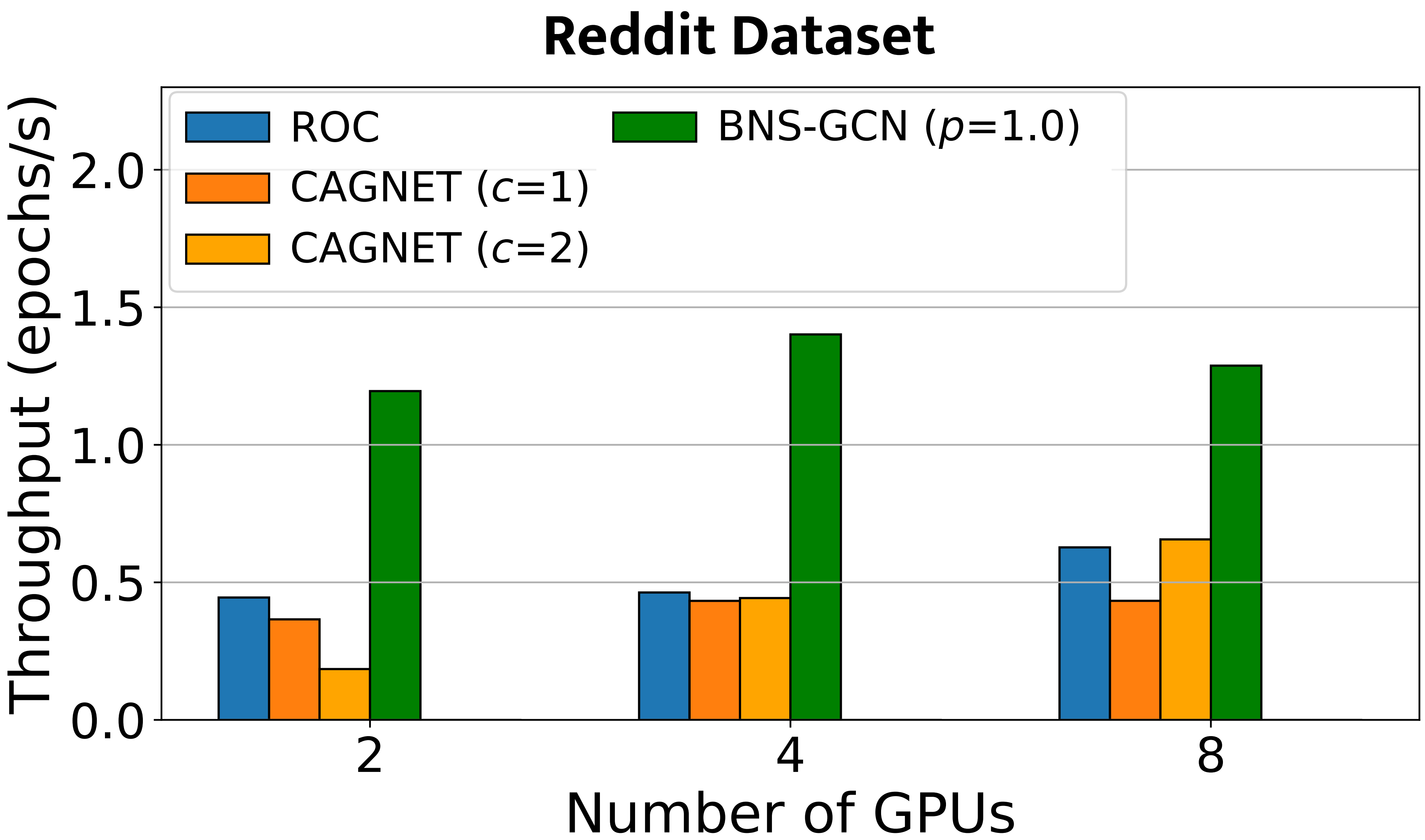
DGL 0.7.0 and PyTorch 1.9.1

Training Throughput Comparison



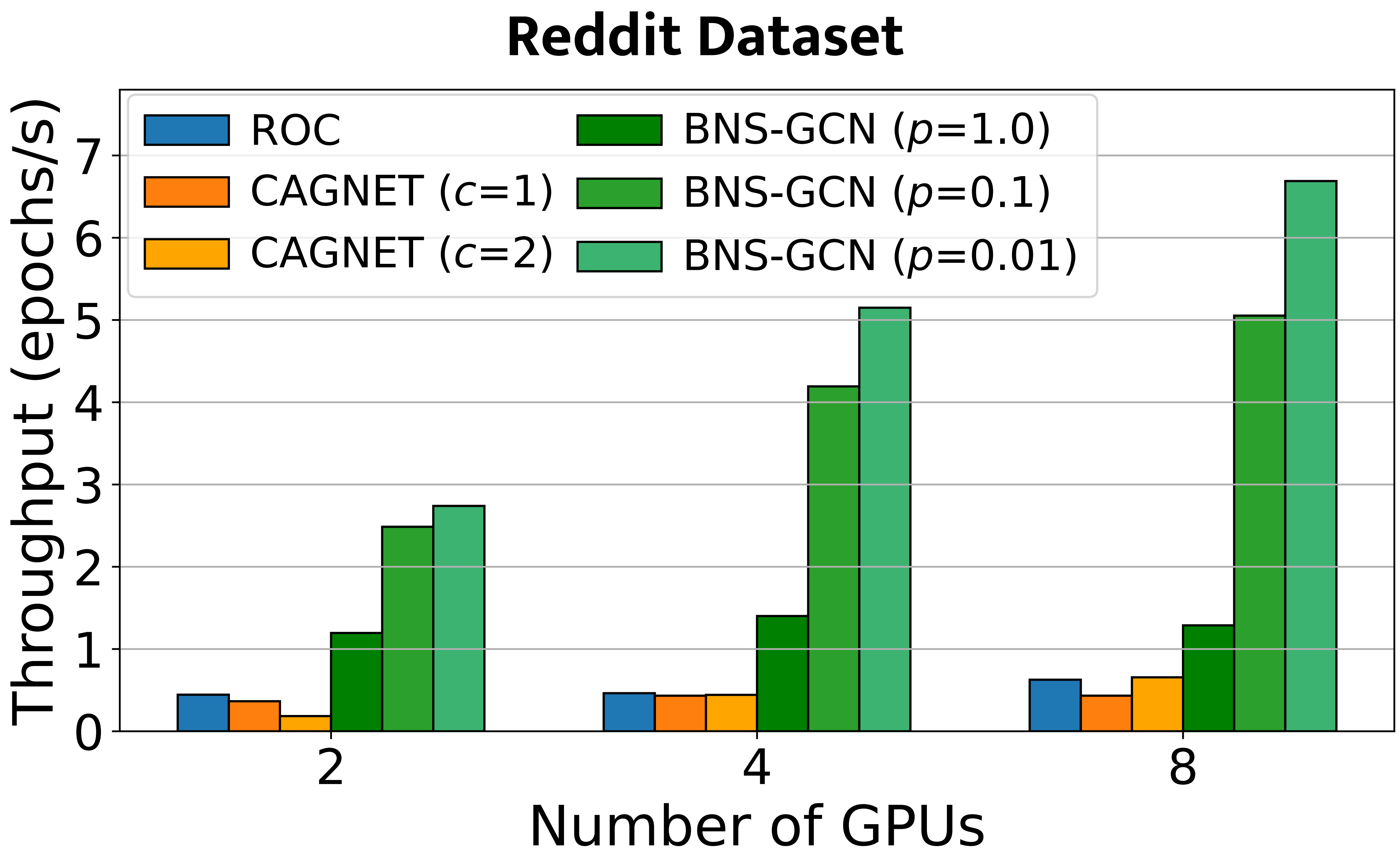
Baselines: throughput <0.7 epochs/s

Training Throughput Comparison



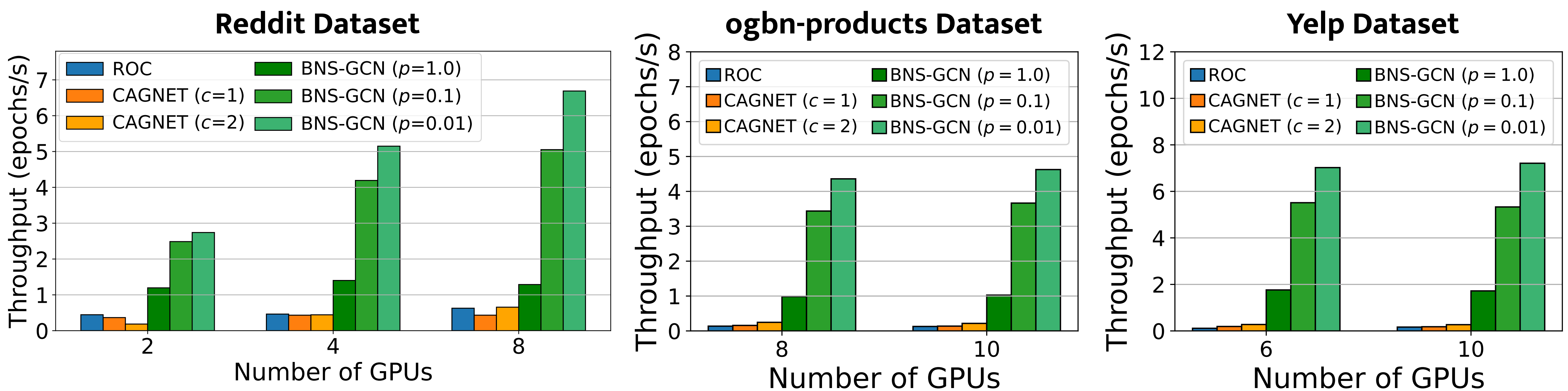
Partition-based training: throughput >1.2 epochs/s

Training Throughput Comparison



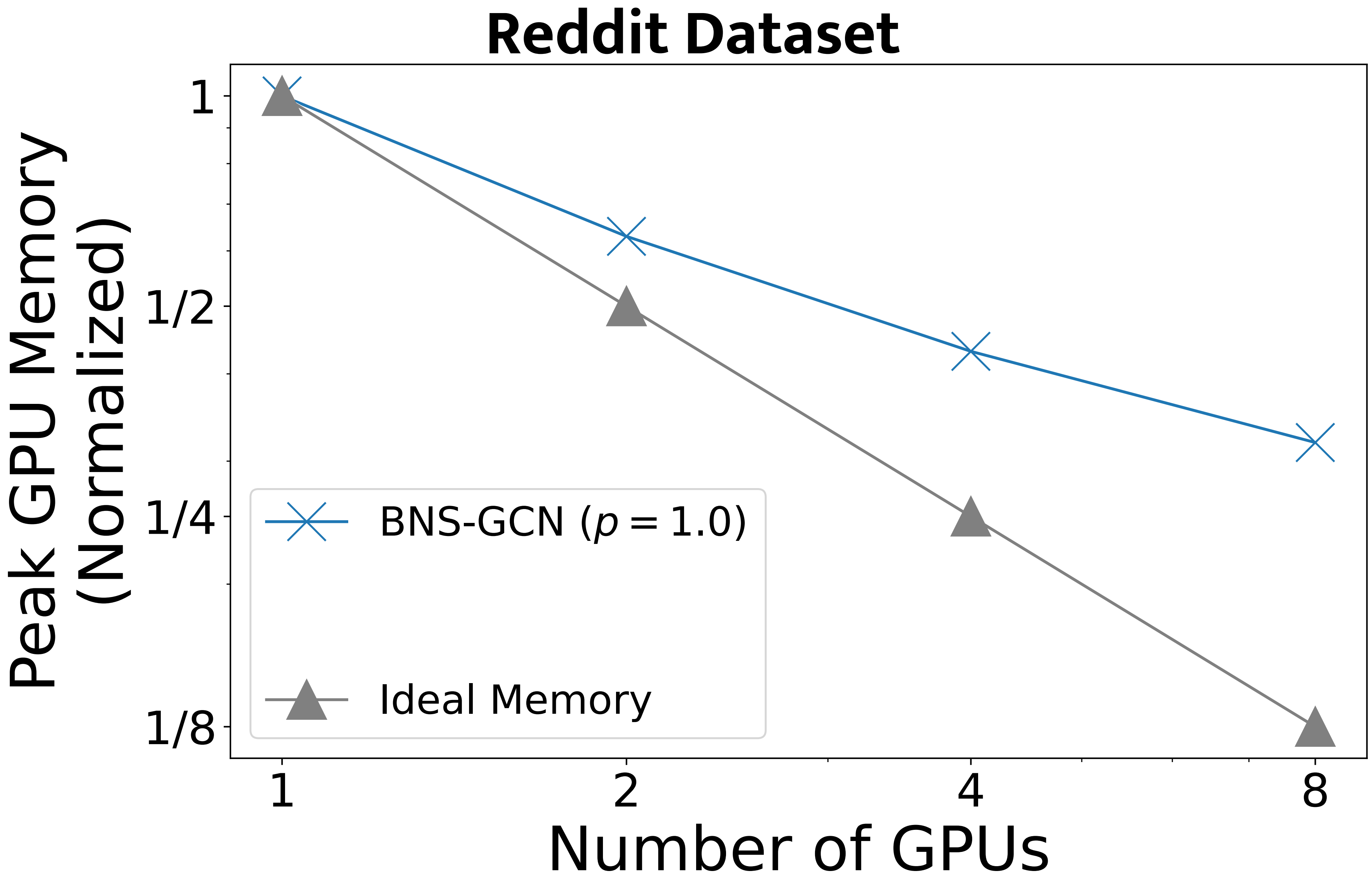
BNS-GCN: 8.9x~16.2x throughput improvement

Training Throughput Comparison

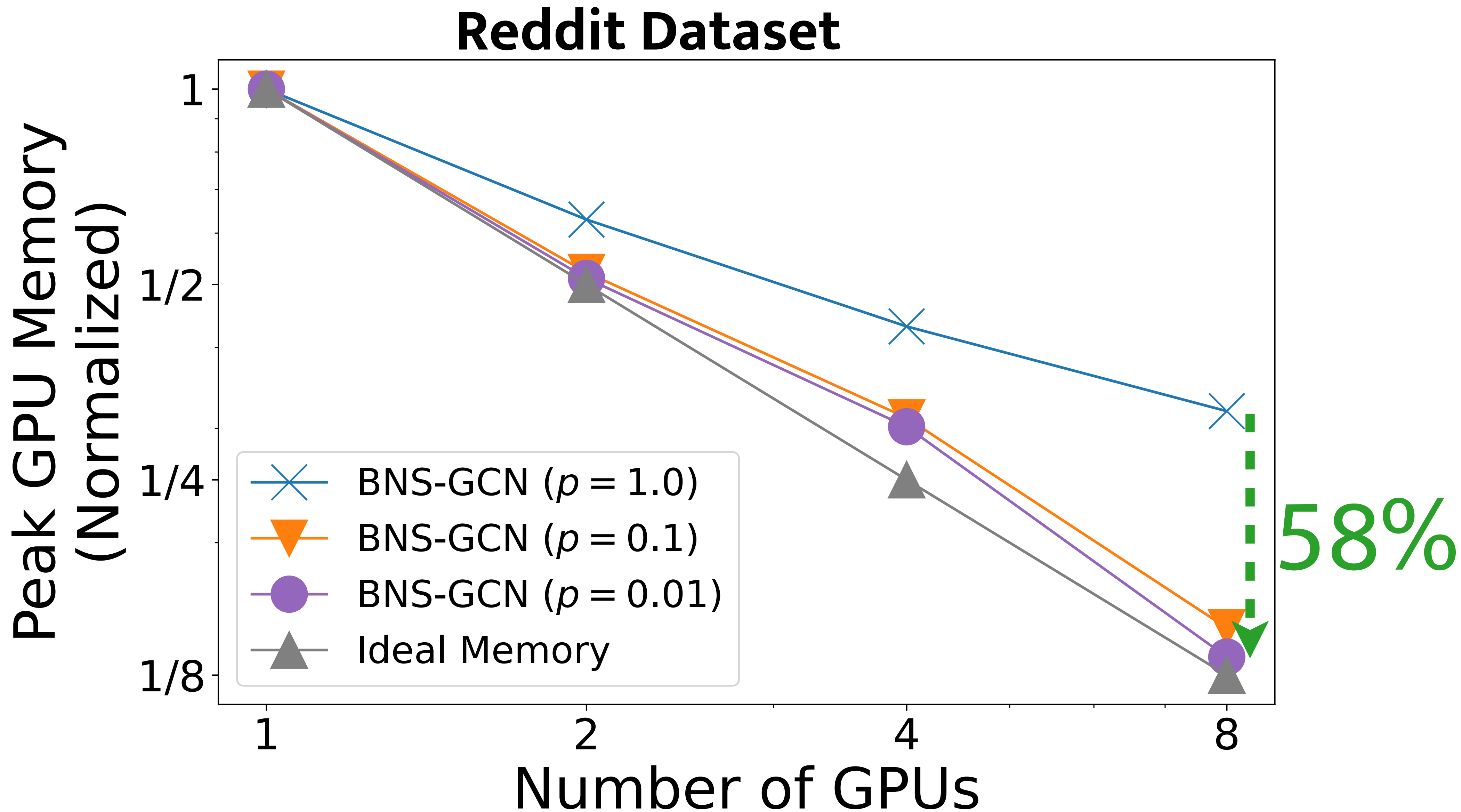


BNS-GCN is consistently faster

Memory Saving

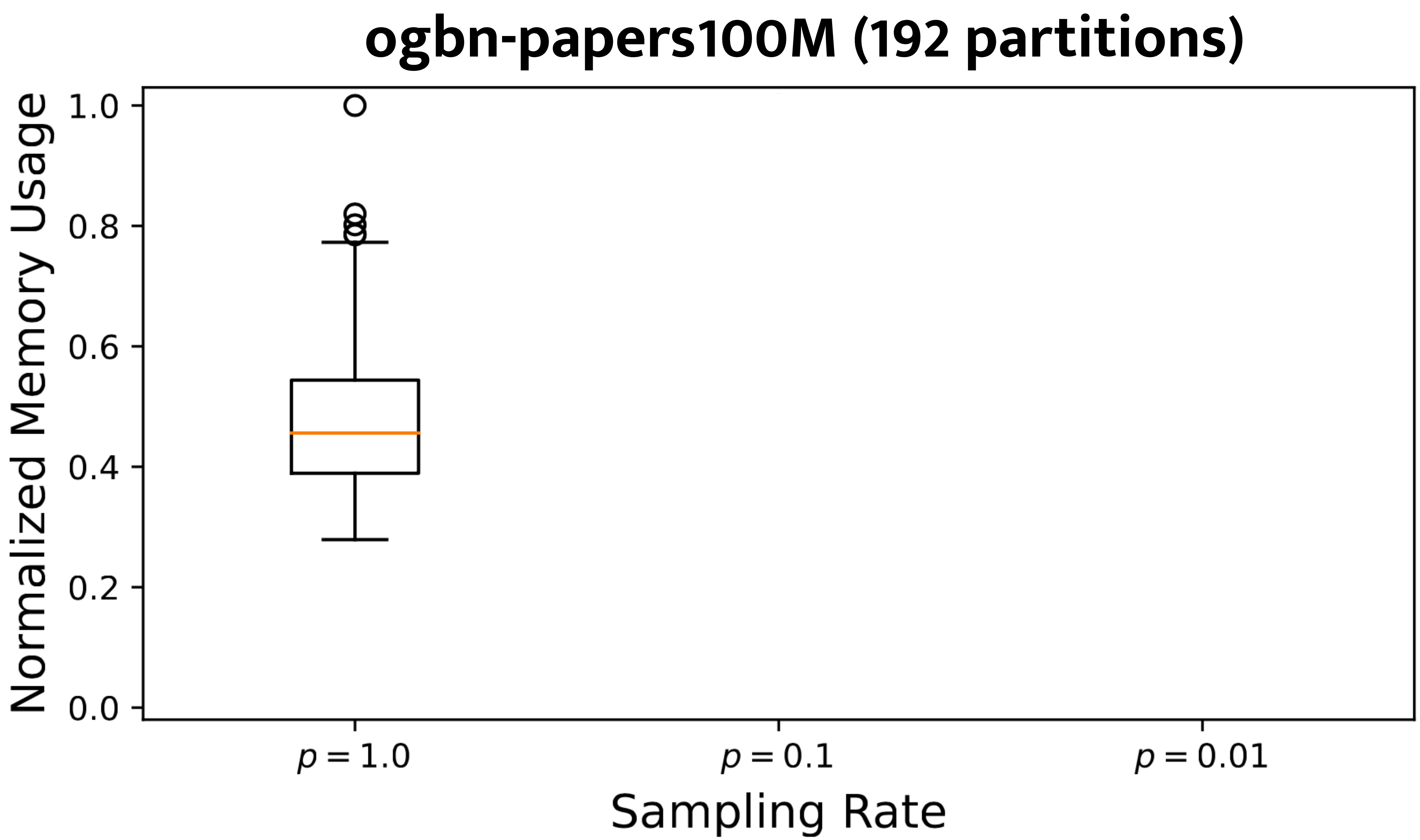


Memory Saving



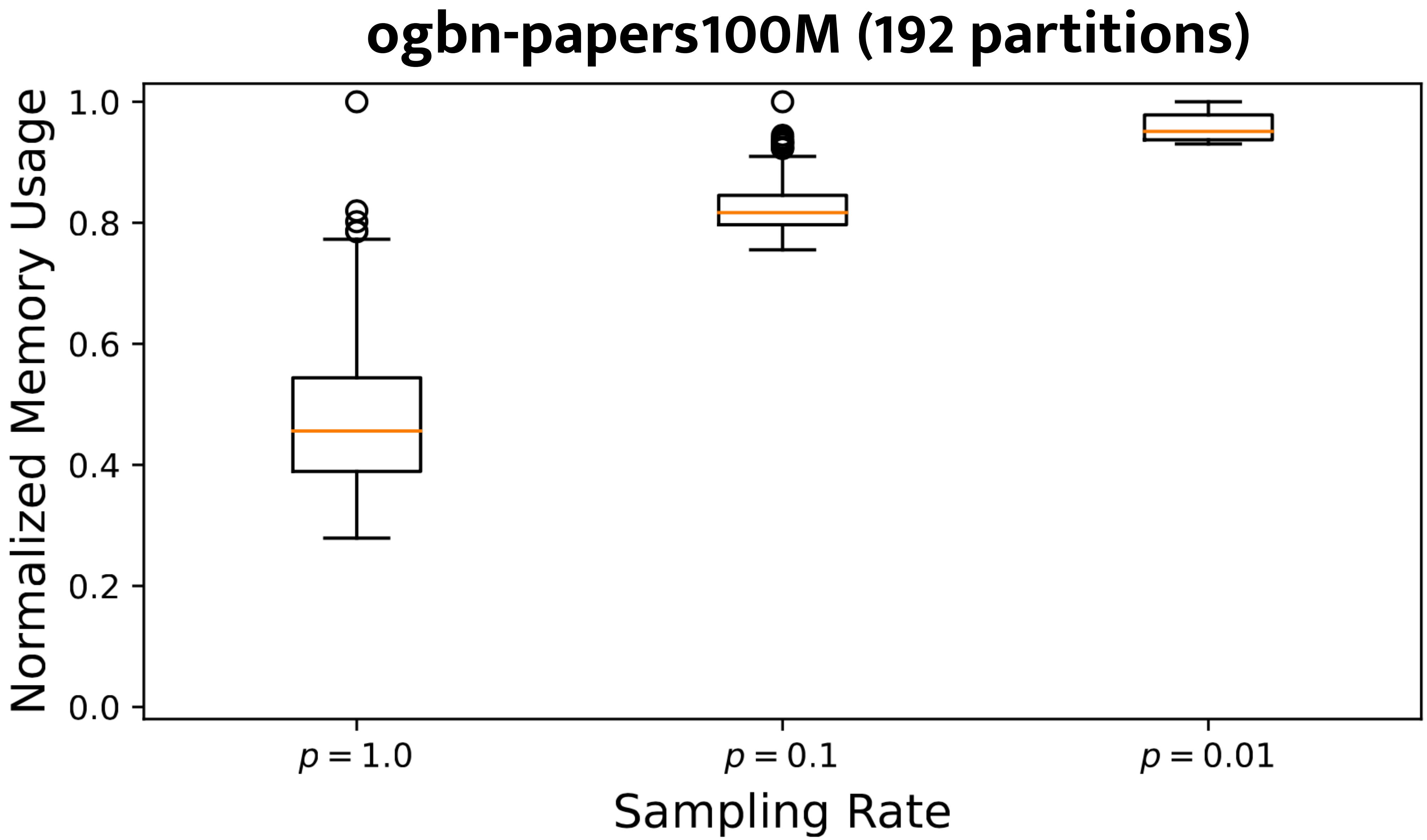
BNS-GCN saves the memory by up to 58%

Balancing Memory Requirement



Without BNS: >75% partitions utilize <60% memory

Balancing Memory Requirement



Without BNS: >75% partitions utilize <60% memory

With BNS: nearly all partitions utilize >80% memory

Training Accuracy Comparison

Dataset	**Reddit**			**ogbn-products**			**Yelp**		
# Partitions	2	4	8	5	8	10	3	6	10

Training Accuracy Comparison

Dataset	Reddit			ogbn-products			Yelp		
# Partitions	2	4	8	5	8	10	3	6	10
BNS-GCN (p=1.0)	97.11	97.11	97.11	79.14	79.14	79.14	65.26	65.26	65.26

BNS-GCN (p=1.0) is equivalent to vanilla training

Training Accuracy Comparison

Dataset	Reddit			ogbn-products			Yelp		
# Partitions	2	4	8	5	8	10	3	6	10
BNS-GCN (p=1.0)	97.11	97.11	97.11	79.14	79.14	79.14	65.26	65.26	65.26
BNS-GCN (p=0.1)	**97.15**	**97.14**	**97.18**	79.36	**79.48**	**79.30**	**65.32**	65.26	**65.34**
BNS-GCN (p=0.01)	97.09	97.03	96.91	**79.43**	79.28	79.21	65.27	**65.31**	65.29

BNS-GCN (p=1.0) is equivalent to vanilla training

Sampling boundary nodes maintains the accuracy

Training Accuracy Comparison

Dataset	Reddit			ogbn-products			Yelp		
# Partitions	2	4	8	5	8	10	3	6	10
BNS-GCN (p=1.0)	97.11	97.11	97.11	79.14	79.14	79.14	65.26	65.26	65.26
BNS-GCN (p=0.1)	**97.15**	**97.14**	**97.18**	79.36	**79.48**	**79.30**	**65.32**	65.26	**65.34**
BNS-GCN (p=0.01)	97.09	97.03	96.91	**79.43**	79.28	79.21	65.27	**65.31**	65.29
BNS-GCN (p=0.0)	97.03	96.87	96.81	78.65	78.83	78.79	65.28	65.27	65.23

BNS-GCN (p=1.0) is equivalent to vanilla training

Sampling boundary nodes maintains the accuracy

Dropping boundary nodes decreases the accuracy

Training Accuracy Comparison

Dataset	Reddit			ogbn-products			Yelp		
# Partitions	2	4	8	5	8	10	3	6	10
BNS-GCN (p=1.0)	97.11	97.11	97.11	79.14	79.14	79.14	65.26	65.26	65.26
BNS-GCN (p=0.1)	**97.15**	**97.14**	**97.18**	79.36	**79.48**	**79.30**	**65.32**	65.26	**65.34**
BNS-GCN (p=0.01)	97.09	97.03	96.91	**79.43**	79.28	79.21	65.27	**65.31**	65.29
BNS-GCN (p=0.0)	97.03	96.87	96.81	78.65	78.83	78.79	65.28	65.27	65.23
FastGCN [ICLR'18]	93.7			60.42			26.5		
GraphSAGE [NIPS'17]	95.4			78.70			63.4		
AS-GCN [NIPS'18]	96.3			OOM			OOM		
LADIES [NeurIPS'19]	94.3			77.46			60.2		
VR-GCN [ICML'18]	96.3			OOM			64.0		
ClusterGCN [KDD'19]	96.6			78.97			60.9		
GraphSAINT [ICLR'20]	96.6			79.08			65.3		

Full-graph training reaches higher accuracy than sampling-based methods

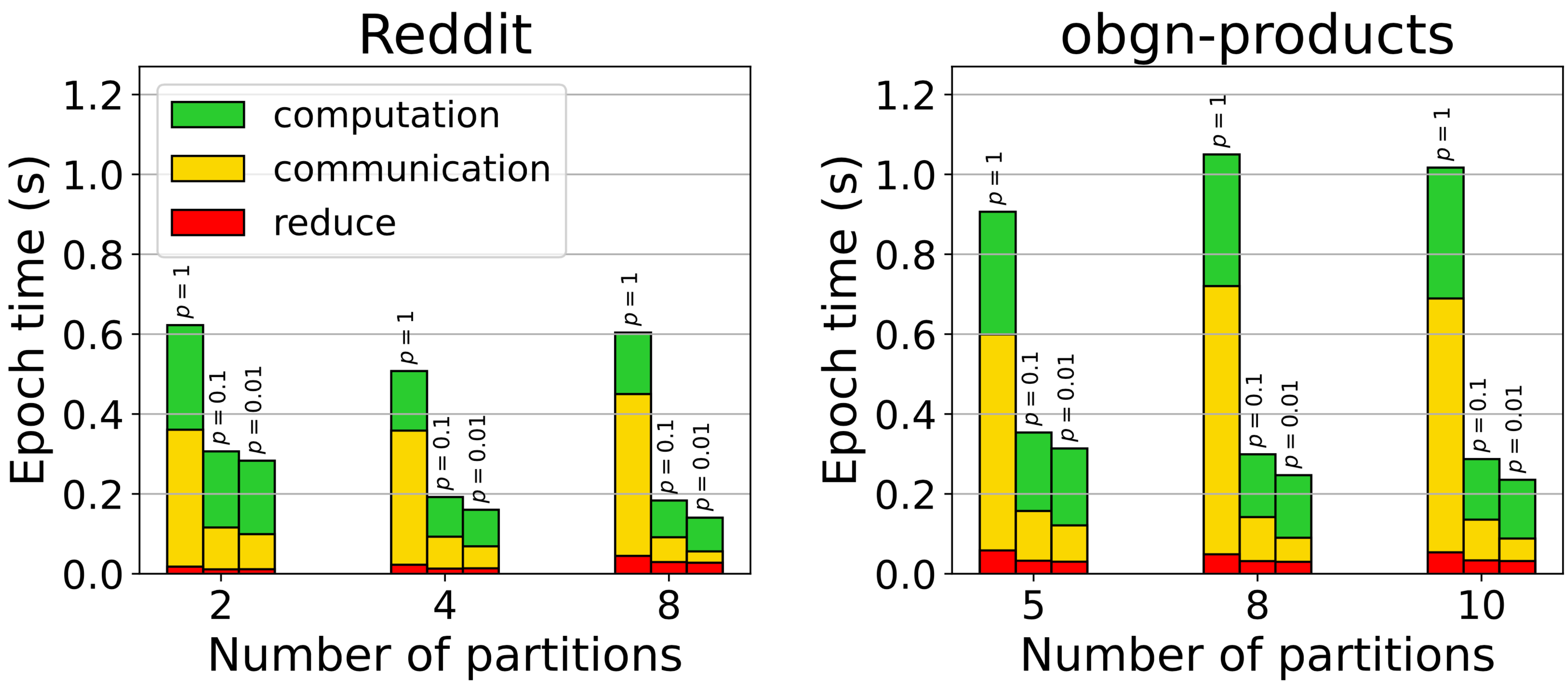
Conclusion

- ✦ Identified three key drawbacks in partition-based GCN training
    - Underlying cause: boundary nodes
- ✦ Proposed Boundary Node Sampling (BNS-GCN) to tackle the three drawbacks
- ✦ Validated BNS-GCN in both theory and experiments

https://github.com/RICE-EIC/BNS-GCN

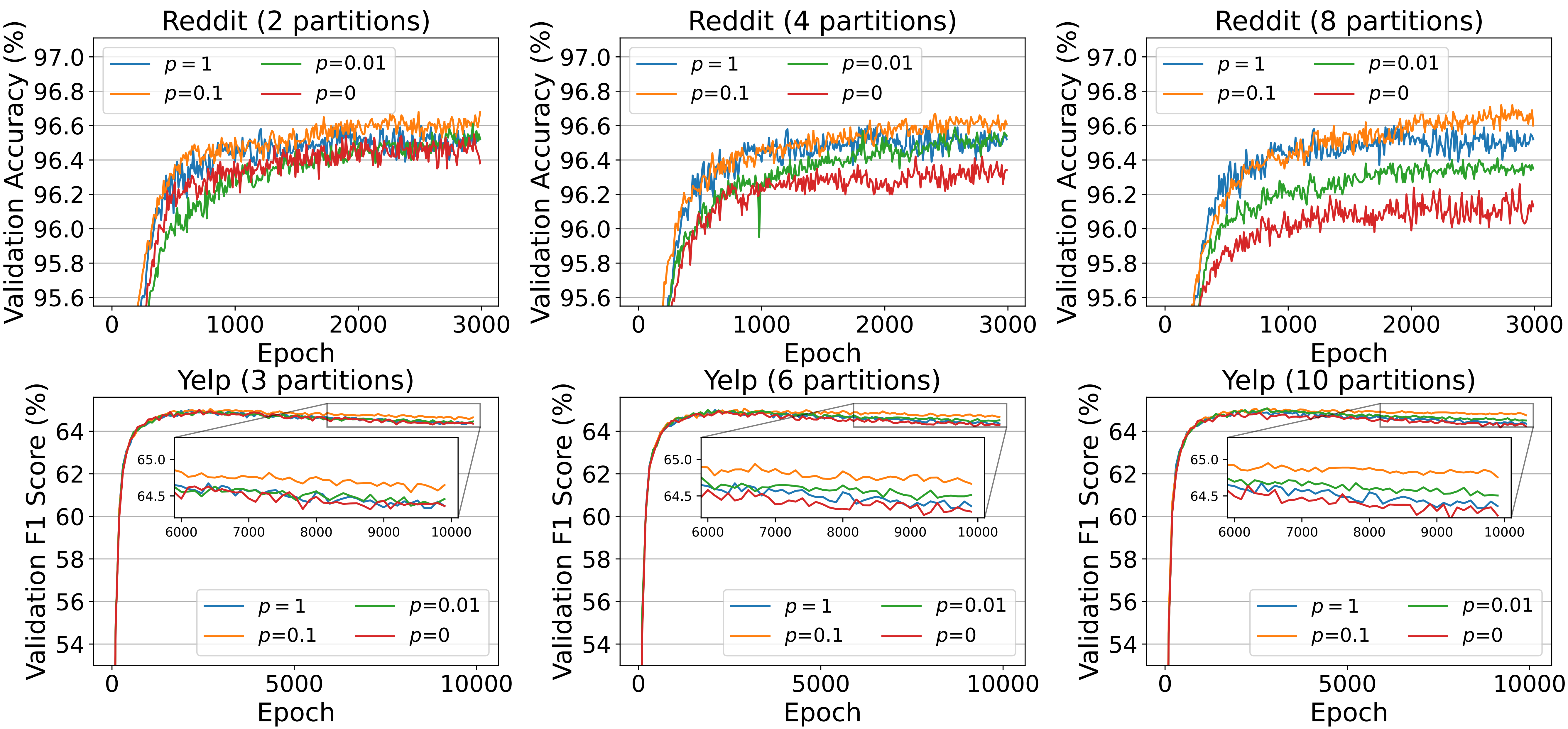
Backup Slides

Time Breakdown



Communication overhead is reduced by **74%~93%**

Training Convergence



On Reddit: p=0 has the worst convergence

On Yelp: p=0/1 suffers from overfitting

BNS-GCN with Random Partition

Table 7: Test score (%) of BNS-GCN on top of random partition, where +/- shows the accuracy difference from BNS-GCN on top of METIS in Table 4.

Method	Reddit (8 partitions)		ogbn-products (10 partitions)		Yelp (10 partitions)	
Random+BNS ($p = 1.0$)	97.11	+0.00	79.14	+0.00	65.26	+0.00
Random+BNS ($p = 0.1$)	96.95	-0.20	79.57	+0.27	65.18	-0.16
Random+BNS ($p = 0.0$)	93.37	-3.47	75.39	-3.40	64.92	-0.31

Table 8: Training efficiency improvement of BNS-GCN ($p = 0.1$) on top of different partition methods.

Dataset	Throughput		Memory		# Boundary Nodes	
	METIS	Random	METIS	Random	METIS	Random
Reddit (8 partitions)	3.1×	5.0×	0.47×	0.36×	460k	1,016k
ogbn-products (10 partitions)	3.4×	7.3×	0.75×	0.31×	1,848k	16,797k
Yelp (10 partitions)	3.1×	5.1×	0.83×	0.49×	649k	2,026k

BNS-GCN vs DropEdge vs BES

Table 9: Comparison between BNS-GCN and edge sampling methods, DropEdge and Boundary Edge Sampling (BES).

Dataset	Method	Epoch Comm (MB)	Epoch Time (sec)	Test Score (%)
Reddit (2 partitions)	DropEdge	301.3	0.613	97.12
	BES	207.9	0.484	97.16
	BNS-GCN	**30.4**	**0.319**	**97.17**
ogbn-products (5 partitions)	DropEdge	1364.0	0.938	**79.38**
	BES	521.1	0.551	79.31
	BNS-GCN	**138.7**	**0.388**	79.36
Yelp (3 partitions)	DropEdge	718.7	0.606	65.30
	BES	195.3	0.328	65.30
	BNS-GCN	**75.7**	**0.270**	**65.32**