Accelerating GNN Dataloading on Multi-GPU Systems: dgl.graphbolt

Muhammed Fatih Balın¹

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¹Computational Science and Engineering, Georgia Institute of Technology



Georgia

Motivation

Applications of GNNs



Source: https://pixabay.com/vectors/social-media-connections-networking-3846597/

Graph Neural Networks



Sampling strategies



- 1. Graph sampling
- 2. Feature loading
- 3. Forward-backward passes

Insights:

- ◎ All are memory-bound operations.
- Accelerators have fast memory.

- 1. Layer-Neighbor Sampling (NeurIPS'23)
- 2. Cooperative Minibatching (Under review)
- 3. Efficient GNN training system (dgl.graphbolt, WIP)

Background

Notation	Definition
$\mathcal{G}=(V,E)$	Graph \mathcal{G} consisting of vertices <i>V</i> and edges $E \subset V \times V$
$t \rightarrow s$	Edge from vertex t to seed vertex s
A_{ts}	Edge weight for edge $t \rightarrow s$
S	a set of vertices $S \subseteq V$
N(s)	1-hop neighborhood of s , $\{t (t \rightarrow s) \in E\}$
N(S)	1-hop neighborhood for S , $\cup_{s \in S} N(s)$
S^l	<i>l</i> -hop neighborhood of $S^0 = S$, $S^{(l+1)} = S^l \cup N(S^l)$
d_s	the degree of s , $ N(s) $

Notation	Definition
$H_t^{(l)}$	vertex embedding for t at layer l
$f^{(l)}$	GNN layer at layer <i>l</i>
$W^{(l)}$	trainable weight matrix at layer <i>l</i>
M_t	message from t , $M_t = H_t W$
M_{ts}	message over the edge $t \rightarrow s$, $M_{ts} = A_{ts}H_tW$

Notation	Definition
k	fan-out parameter or sampling budget per vertex
π_t	probability of sampling vertex <i>t</i>
π_{ts}	probability of sampling edge $t \rightarrow s$
Т	the sampled vertices in the next layer, $T \subseteq N(S)$

Common bandwidths and storage capacities of components in a modern PCIe-based multi-GPU computer system.

Component	Capacity			
1× NVMe SSD	4 TB			
System memory	2 TB			
GPU global memory	80 GB			
Connection	Bandwidth			
1× PCI-e 4.0 lane	2 GB/s			
NVMe SSD over $4 \times$ lanes	8 GB/s			
GPU over 16× lanes	32 GB/s			
CPU to system memory	400 GB/s			
GPU to GPU	300 GB/s			
GPU to GPU global memory	2 TB/s			

Example Interconnect Topology



Layer-Neighbor Sampling (LABOR)

Output States Unbiased sampling

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- Overlapping neighborhoods (LADIES)

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Solution:

◎ Poisson Sampling - flip biased coins: r ≤ π, r ∼ U(0, 1)

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- Poisson Sampling flip biased coins: *r* ≤ π, *r* ∼ *U*(0, 1)
- ◎ Combine NS & LADIES to get best-of-both-worlds LABOR.
- Generalizes to any unbiased sampling method.

• GCN equation: $H_s = \frac{1}{d_s} \sum_{t \to s} H_t W = \frac{1}{d_s} \sum_{t \to s} M_t$

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- Neighbor Sampling (NS):
 For given *s*, sample *k*-subset of $\{t \mid t \rightarrow s\}$
- ◎ Layer sampling: Given *S*, sample $T \subseteq \{t \mid t \to s \in S\}$, extract edges $\{t \to s \mid t \in T, s \in S\}$

◎ LABOR-0: given *s* and $r_t \sim U(0, 1)$, sample $t \rightarrow s$ if $r_t \leq \frac{k}{d_s}$.

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- Expected *k* sampled items, matching NS.

- ◎ LABOR-0: given *s* and $r_t \sim U(0, 1)$, sample $t \rightarrow s$ if $r_t \leq \frac{k}{d_s}$.
- ◎ Expected *k* sampled items, matching NS.
- Taking top-k r_t values makes # sampled items deterministic.













Algorithm LABOR-0 for uniform edge weights

- 1: Input: seed vertices S, fan-out k
- 2: Output: sampled edges E'
- 3: $T \leftarrow \{t \mid t \in N(S)\}$ 4: $r_t \sim U(0, 1), \forall t \in T$
- 5: $E' \leftarrow []$
- 6: for all $s \in S$ do
- 7: for all $t \in N(s)$ do 8: if $r_t \leq \frac{k}{d_s}$ then 9: E'.append $(t \rightarrow s)$

The loop corresponds to a 'copy_if' operation.

Experiments - Vertex efficiency



The validation F1-score and training loss curves.

Experiments - Edge efficiency



The validation F1-score and training loss curves.

Experiments - PLADIES and LABOR Evaluation

Dataset	Algo.	V ³	$ E^2 $	$ V^2 $	$ E^1 $	$ V^1 $	$ E^0 $	$ V^0 $	it/s	test F1-score
reddit	PLADIES	24	2390	14.1	927	6.0	33.2	1	1.7	96.21 ± 0.06
	LADIES	25	2270	14.5	852	6.0	32.5	1	1.8	96.20 ± 0.05
	LABOR-*	24	1070	13.7	435	6.0	26.9	1	4.1	96.23 ± 0.05
	LABOR-1	27	261	14.4	116	6.1	16.7	1	24.8	96.23 ± 0.06
	LABOR-0	36	177	17.8	67	6.8	9.6	1	37.6	96.25 ± 0.05
	NS	167	682	68.3	100	10.1	9.7	1	14.2	96.24 ± 0.05
products	PLADIES	160	2380	51.2	293	9.7	11.7	1	4.1	78.44 ± 0.24
	LADIES	165	2230	51.8	270	9.7	11.5	1	4.2	78.59 ± 0.22
	LABOR-*	166	1250	51.8	167	9.8	10.6	1	6.2	78.59 ± 0.34
	LABOR-1	178	799	53.4	136	9.8	10.5	1	21.3	78.47 ± 0.26
	LABOR-0	237	615	62.4	100	10.1	9.9	1	32.5	78.76 ± 0.26
	NS	513	944	95.4	106	10.6	9.9	1	24.6	78.48 ± 0.29
	PLADIES	100	1300	29.5	183	6.2	6.9	1	5.1	61.55 ± 0.87
	LADIES	102	1280	29.7	182	6.2	6.9	1	5-3	61.89 ± 0.66
yelp	LABOR-*	105	991	30.7	158	6.1	6.8	1	13.3	61.57 ± 0.67
	LABOR-1	109	447	31.0	96	6.2	6.8	1	27.3	61.71 ± 0.70
	LABOR-0	138	318	35.1	54	6.2	6.3	1	27.2	61.55 ± 0.85
	NS	188	392	42.5	55	6.3	6.3	1	23.0	61.50 ± 0.66
flickr	PLADIES	55	309	24.9	85	6.2	6.9	1	10.2	51.52 ± 0.26
	LADIES	56	308	25.1	85	6.2	6.9	1	10.5	50.79 ± 0.29
	LABOR-*	57	308	25.6	85	6.3	6.9	1	20.3	51.67 ± 0.27
	LABOR-1	58	242	25.9	73	6.3	6.9	1	32.7	51.66 ± 0.24
	LABOR-0	66	219	29.1	52	6.4	6.7	1	33-3	51.65 ± 0.26
	NS	73	244	32.8	52	6.4	6.7	1	31.7	51.70 ± 0.23
Cooperative Minibatching

- ◎ Full-batch training has no redundant computation.
- ◎ Minibatch training requires repetitive calculations.

- Work vs. batch size relationship
- Data & intra-layer parallelism: *Cooperative Minibatching*.
- ◎ Same idea in serial execution: *Dependent Minibatching*.

Cooperative Minibatching Background

- ◎ GNN equation: $H_s^{(l+1)} = f^{(l)}(H_s^{(l)}, \{H_t^{(l)} | t \in N(s)\})$
- ◎ Graph Sampling: $S^0 = S$, $S^{(l+1)} = S^l \cup N(S^l)$
- Work of an epoch with batch size $|S^0|$: $W(|S^0|) = \frac{|V|}{|S^0|} \sum_{l=1}^{L} E[|S^l|] \ge \frac{|V|}{|S^0|} \sum_{l=1}^{L} |S^0| = L|V|$

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- Redundant work for layer $l: W^{l}(|S^{0}|) \approx \frac{E[|S^{l}|]}{|S^{0}|}$

Independent Minibatching

- Each Processing Element (PE e.g., GPU) starts with its own S⁰.
- 2. Samples S^1, \ldots, S^L independently.
- 3. Loads input features and edge features for the sampled subgraphs independently.
- 4. Forward-backward independently with no communication.
- Problem: Redundant computations across PEs.

Independent Minibatching Example with 2 PEs



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Cooperative Minibatching



Green edges represent work savings.

Theorem

The work per epoch $\frac{E[|S^l|]}{|S^0|}$ required to train a GNN model using minibatch training is monotonically nonincreasing as the batch size $|S^0|$ increases.

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Theorem

The expected subgraph size $E[|S^{1}|]$ required to train a GNN model using minibatch training is a concave function of batch size, $|S^{0}|$.

Properties of the datasets used in experiments.

Dataset	V	E	$\frac{ E }{ V }$	# feats.	cache size	train - val - test (%)	# minibatches
flickr	89.2K	900K	10.09	500	70k	50.00 - 25.00 - 25.00	65
yelp	717K	14.0M	19.52	300	200k	75.00 - 10.00 - 15.00	595
products	2.45M	61.9M	25.26	100	400k	8.00 - 2.00 - 90.00	239
reddit	233K	115M	493.56	602	60k	66.00 - 10.00 - 24.00	172
papers100M	111M	3.2B	29.10	128	2M	1.09 - 0.11 - 0.19	1300
mag240M	244M	3.44B	14.16	768	2M	0.45 - 0.06 - 0.04	1215

Empirical results about theorems



Monotonicity of the work. x-axis shows the batch size, y-axis shows $\frac{E[|S^3|]}{|S^0|}$ (work per epoch) for node prediction (top row) and $E[|S^3|]$ (expected subgraph size) for edge prediction (bottom row).

Pseudocode

Algorithm Cooperative minibatching

```
1: Input: seed vertices S_p^0 for each PE p \in P, # layers L
 2: for all l \in \{0, ..., L - 1\} do {Sampling}
      for all p \in P do in parallel
 3:
         Sample next layer vertices \tilde{S}_{v}^{l+1} and edges E_{v}^{l} for S_{v}^{l}
 4:
          all-to-all to redistribute vertex ids for \tilde{S}_n^{l+1} to get S_n^{l+1}
 5:
 6: for all p \in P do in parallel {Feature Loading}
       Load input features H_p^L from Storage for vertices S_p^L
 7:
       all-to-all to redistribute H_n^L to get \tilde{H}_n^L
 8:
 9: for all l \in \{L - 1, \dots, 0\} do {Forward Pass}
      for all p \in P do in parallel
10:
      if l + 1 < L then
11:
            all-to-all to redistribute H_p^{l+1} to get \tilde{H}_p^{l+1}
12:
         Forward pass on bipartite graph \tilde{S}_p^{l+1} \rightarrow S_p^l with edges
13:
         E_{v}^{l} with input \tilde{H}_{p}^{l+1} and output H_{p}^{l}
14: for all p \in P do in parallel
       Compute the loss and initialize gradients G_n^0
15:
16: for all l \in \{0, \dots, L-1\} do {Backward Pass}
      for all p \in P do in parallel
17:
         Backward pass on bipartite graph S_p^l \rightarrow \tilde{S}_p^{(l+1)} with
18:
         edges E_n^l with input G_n^l and output \tilde{G}_n^{l+1}
         if l + 1 < L then
19:
             all-to-all to redistribute \tilde{G}_n^{l+1} to get G_n^{l+1}
20:
```

Any parallel algorithm can be executed sequentially.

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- 1. Sample a mega-batch of size $\kappa\beta$.
- 2. Extract κ minibatches of size β from it.
- 3. Static sampled neighborhoods for κ consecutive minibatches.

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 $(t \rightarrow s)$ is sampled if $r_t \leq \frac{k}{d_s}$, $r_t \sim U(0, 1)$.

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- ◎ LABOR-0 recap:

 $(t \rightarrow s)$ is sampled if $r_t \leq \frac{k}{d_s}$, $r_t \sim U(0, 1)$.

 \odot r_t evolves κ times slower.

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- ◎ LABOR-0 recap:

 $(t \rightarrow s)$ is sampled if $r_t \leq \frac{k}{d_s}$, $r_t \sim U(0, 1)$.

- \odot r_t evolves κ times slower.
- Result: Increased temporal access locality.

Dependent Minibatching example for LABOR-0 with $\kappa = 2$

Blue: seed vertices, green: sampled, gray: not sampled



Two completely independent minibatches.

Dependent Minibatching example for LABOR-0 with $\kappa = 2$

Blue: seed vertices, green: sampled, gray: not sampled



Middle minibatch is an interpolated between 2 independent minibatches.

Experimental Results - Dependent Minibatching



The validation F1-score for LABOR-0 varying κ .



Cache miss rates varying κ .

Cooperative Minibatching Runtime Results

# PEs, γ $\alpha, \beta, S^0 $	Dataset & Model	Sampler	I/C	Samp.	-	Feature Co Cache	opy Cache, κ	F/B	Total
$\begin{array}{c} 4 \text{ A100} \\ \gamma = 2\text{TB/s} \\ \alpha = 600\text{GB/s} \\ \beta = 64\text{GB/s} \\ S^0 = 2^{12} \end{array}$	papers100M GCN	LABOR-0	Indep	21.7	18.4	16.8	11.2	8.9	41.8
			Coop	17.7	14.0	10.1	5.8	13.0	36.5
		NS	Indep	16.1	26.5	22.1	-	10.1	48.3
			Coop	11.9	21.3	12.9	-	15.0	39.8
	mag240M R-GCN	LABOR-0	Indep	26.0	57.9	56.0	41.0	199.9	266.9
			Coop	20.0	51.1	36.9	23.4	183.3	226.7
		NS	Indep	14.4	78.0	71.2	-	223.0	308.6
			Coop	12.3	73.9	47.5	-	215.6	275.4
$\begin{array}{l} 8 \text{ A100} \\ \gamma = 2\text{TB/s} \\ \alpha = 600\text{GB/s} \\ \beta = 64\text{GB/s} \\ S^0 = 2^{13} \end{array}$	papers100M GCN	LABOR-0	Indep	21.3	21.1	18.7	12.0	9.3	42.6
			Coop	16.5	12.4	7.1	4.0	13.5	34.0
		NS	Indep	15.8	31.0	24.5	-	10.3	50.6
			Coop	12.5	19.4	9.0	-	15.6	37.1
	mag240M R-GCN	LABOR-0	Indep	30.6	70.1	66.2	46.8	202.1	279.5
			Coop	21.6	50.6	29.0	19.3	172.2	213.1
		NS	Indep	15.0	94.9	80.9	-	224.8	320.7
			Coop	14.9	71.6	39.6	-	209.0	263.5
	papers100M GCN	LABOR-0	Indep	39.1	44.5	40.2	29.4	15.1	83.6
$\begin{array}{l} 16 \ \mathrm{V100} \\ \gamma = 0.9 \mathrm{TB/s} \\ \alpha = 300 \mathrm{GB/s} \\ \beta = 32 \mathrm{GB/s} \\ S^0 = 2^{13} \end{array}$			Coop	26.9	22.7	10.4	4.9	19.1	50.9
		NS	Indep	18.0	61.3	52.0	-	16.2	86.2
			Coop	19.2	34.9	13.0	-	21.3	53-5
	mag240M R-GCN	LABOR-0	Indep	50.8	128.8	121.3	96.2	156.1	303.1
			Coop	29.2	78.1	42.8	23.5	133.3	186.0
		NS	Indep	19.3	167.3	152.6	-	170.9	342.8
			Coop	19.3	116.1	53.1	-	160.4	232.8

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Speedup with changing # PEs

Improvements of cooperative batching over independent batching for 4, 8 and 16 PEs compiled from the **Total** column.

Dataset & Model	Sampler	Speedup - 4	Speedup - 8	Speedup - 16
papers100M	LABOR-0	14.5%	25.3%	64.2%
GCN	NS	21.4%	36.4%	61.1%
mag240M	LABOR-0	17.7%	31.2%	63.0%
R-GCN	NS	12.1%	21.7%	47·3%



4 cooperating PEs were used, κ is varied (1, 4, ...).

- Work reduction with Cooperative Minibatching
- O Communication negligible in expensive GNN models
- PEs need fast all-to-all communication
- ◎ Less work = faster runtimes as expected.

dgl.graphbolt

- Graph sampling (Graph caching on the accelerator)
- Feature loading (Feature caching on accelerator and system memory)
- Sorward-backward on the accelerator

Algorithm Optimized Cooperative Minibatching

- 1: **Input:** seed vertices S_p^0 for each PE $p \in P$, # layers L
- 2: for all $l \in \{0, ..., L 1\}$ do {Sampling}
- 3: for all $p \in P$ do in parallel
- 4: Query GPU graph cache and fetch vertex neighborhoods
- 5: co_await Load missing vertex neighborhoods from Storage
- 6: Sample next layer vertices \tilde{S}_p^{l+1} and edges E_p^l for S_p^l
- 7: co_await all-to-all to redistribute vertex ids for \tilde{S}_p^{l+1} to get S_p^{l+1}
- 8: for all $p \in P$ do in parallel {Feature Loading}
- 9: Query GPU feature cache and fetch existing input features
- 10: co_await Load missing features H_p^L from Storage for vertices S_p^L
- 11: co_await all-to-all to redistribute H_p^L to get \tilde{H}_p^L

dgl.graphbolt - Constructing a dataloader

2

1 # We use torch datapipes below, it describes what the operations are, does not run the operations.

```
def create_dataloader(graph, features, itemset,
3
      batch_size , fanout , device):
      datapipe = gb.ItemSampler(
4
          itemset, batch_size=batch_size, shuffle=True
6
      datapipe = datapipe.copy_to(device=device,
      extra_attrs = ["seed_nodes"])
      datapipe = datapipe.sample_layer_neighbor(graph,
8
      fanout)
      datapipe = datapipe.fetch_feature(features,
9
      node_feature_keys=["feat"])
      return gb.DataLoader(datapipe)
10
```

Pipeline



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- Ocompute: 'features[index].to(device)'
- First, 'features[index]' is executed on CPU, then '.to(device)' is performed.
- This requires multiple touches to the same data, can we do better?

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- ◎ CUDAStreams are queues to schedule work to the GPU.
- If the work launched in a stream does not occupy all the SMs, the work from another stream can run concurrently.

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```
torch.ops.graphbolt.set_max_uva_threads(max_uva_threads)
  feature_fetchers = dp_utils.find_dps(
2
      datapipe_graph,
3
      FeatureFetcher,
4
  for feature_fetcher in feature_fetchers:
      feature_fetcher.stream = _get_uva_stream()
7
      datapipe_graph = dp_utils.replace_dp(
8
          datapipe_graph,
9
          feature_fetcher,
10
          feature_fetcher.buffer(1).wait(),
```

Transformed Pipeline



```
torch.ops.graphbolt.set_max_uva_threads(max_uva_threads)
 samplers = dp_utils.find_dps(
2
      datapipe_graph,
3
      SamplePerLayer,
4
  executor = ThreadPoolExecutor(max_workers=1)
6
  for sampler in samplers:
      datapipe_graph = dp_utils.replace_dp(
8
          datapipe_graph,
9
          sampler,
10
          sampler.fetch_and_sample(_get_uva_stream(),
      executor, 1),
      )
```

Pipelining optimizations in gb.DataLoader - Graph Fetch

```
@functional_datapipe("fetch_and_sample")
```

3

4

```
<sup>2</sup> class FetcherAndSampler(MiniBatchTransformer):
```

```
"""Overlapped graph sampling operation replacement.
```

```
def __init__(self, sampler, stream, executor,
     buffer size):
          datapipe = sampler.datapipe.
6
     fetch_insubgraph_data(
              sampler, stream, executor
8
          datapipe = datapipe.buffer(buffer_size).
9
     wait_future().wait()
          datapipe = datapipe.
     sample_per_layer_from_fetched_subgraph(sampler)
         super().__init__(datapipe)
```

Transformed Pipeline



DGL 2.1 Node Classification Speedups on ogbn-products



DGL 2.1 Link Prediction Speedups on ogbl-citation2



Multi-GPU Speedups on ogbn-papers100M



Single-GPU Speedups with PyG on ogbn-products



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- Overlap communication

- Given a chain of datapipes, we want to enable Cooperative Minibatching seamlessly.
- Insert all-to-all operations in-between, similar to the graph and feature fetch optimizations.
- Overlap communication
- Simple online graph partitioning can reduce the amount of needed communication between GPUs.

Thanks!

o For more information

- Email: balin@gatech.edu
- Visit: mfbal.in
- Visit: tda.gatech.edu
- Acknowledgement of Support:







THANK YOU

Variance formula derivation

$$H'_{s} = \frac{1}{d_{s}} \sum_{t \to s} \frac{M_{t}}{\pi_{t}} \mathbb{1}[r_{t} \le \pi_{t}]$$

$$Var(H'_{s}) = Var\left(\frac{1}{d_{s}} \sum_{t \to s} \frac{M_{t}}{\pi_{t}} \mathbb{1}[r_{t} \le \pi_{t}]\right)$$

$$= \frac{1}{d_{s}^{2}} \sum_{t \to s} \frac{Var(M_{t})}{\pi_{t}^{2}} Var(\mathbb{1}[r_{t} \le \pi_{t}])$$

$$= \frac{1}{d_{s}^{2}} \sum_{t \to s} \frac{Var(M_{t})}{\pi_{t}^{2}} \pi_{t}(1 - \pi_{t})$$

$$= \frac{1}{d_{s}^{2}} \sum_{t \to s} \frac{Var(M_{t})}{\pi_{t}} (1 - \pi_{t}) = \frac{1}{d_{s}^{2}} \sum_{t \to s} \frac{1}{\pi_{t}} (1 - \pi_{t})$$

$$= \frac{1}{d_{s}^{2}} \sum_{t \to s} (\frac{1}{\pi_{t}} - 1) = \frac{1}{d_{s}^{2}} \sum_{t \to s} \frac{1}{\pi_{t}} - \frac{1}{d_{s}}$$
(1)

Smoothed Dependent Minibatching (cont.)

• $r_t = PRNG(z, t)$, where z is the random seed, t is the vertex id.

◎
$$r_t(c) = PRNG(z_1, z_2, c, t), \forall c \in [0, 1],$$

 $PRNG(z_1, z_2, 0, t) = PRNG(z_1, t),$
 $PRNG(z_1, z_2, 1, t) = PRNG(z_2, t).$

- $ontial n_t(c) = \cos(\frac{c\pi}{2})n_t^1(z_1) + \sin(\frac{c\pi}{2})n_t^2(z_2)$
- $\odot r_t(c) = \Phi(n_t(c)) \sim U(0,1)$
- ◎ For *i*th minibatch, $c = \frac{i}{\kappa}$. When $i = \kappa$, we set $z_1 \leftarrow z_2, z_2$ becomes a new random seed.

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