Unifying Parallelization Schemes to Train Deep Nets

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Introduction

There are several strategies to train large neural networks over multiple GPUs. The best practice today is to employ a mix Data Parallelism, Pipeline Parallelism, and Tensor Parallelism simultaneously. This document describes a master schedule that unifies all these schemes under one code base. From this unified view , we derive a new distributed schedule that can mix and match the tradeoffs between these schemes, obviating the need to deploy all three schemes simultaneously.

There are two main reasons to use multiple GPUs when training large models: First, it speeds up training by making more FLOPS available. Second, it supplies the memory needed to store the weights, activations, and the optimizer state to train a large model. In Distributed Data Parallelism (DDP), each worker is assigned to a subset of the training batch called a micro-batch. Each worker computes the gradient on its micro-batch using backpropagation. The main advantage of this scheme is that all workers operate independently of each other, so they are almost fully utilized during backpropagation. One down side of this method is that each worker must retain the activations of all the layers of the network, which is infeasible for large models. Another down side of this scheme is that the number of workers must exactly match the number of micro-batches. Large batch sizes improve compute utilization, but they also cause each epoch of training to make less progress on the training loss than with smaller batches (see Section 2.1 of this folk wisdom paper and Theorem 5.8 of this more theoretical paper). In other words, the training loss drops more slowly per training datum as the number of micro-batches in a batch grows, and therefore as the number of workers increases. Yet another disadvantage of this method is that each worker must store the weights for all the layers, which is again infeasible for large models. Fully Sharded Data Parallelism (FSDP) addresses this latter issue by having each worker hold the weights for only one stage, and page in the weights for other states from other workers as needed. Pipeline Parallelism (PP) addresses some of these problems by assigning to each worker a subset of the stages. Each worker still processes all micro-batches in the batch, but only for the stage assigned to the worker. A micro-batch works its way through the stages by passing from one worker to the next. An advantage of this method is that each worker need only store the weights for the stages assigned to it. Another advantage is that it accommodates more workers than there are micro-batches, offering a way to add more workers to the task A problem this it is that it has higher latency than DDP: Some workers remain idle until the first mini-batch has made it through the final stage, and then some workers become idle again as the last micro-batch winds its way through the stages. Surprisingly, the amount of activations each worker stores still scales with the number of micro-batches because each worker most store the activations of all the batches that traverse it (though see the table below for a cap on this number). To address these issues, Looped Pipeline Parallelism (LPP) operates several Pipeline Parallel processes in independent groups, and distributes the micro-batches evenly across these groups. This makes LPP run almost as fast as DDP when the number of groups is large. Fully Sharded Looped Pipeline Parallelism (FSLPP) is a variant of LPP where each worker stores the weights of only one stage, and pages in the weights of the other stages it must process from other workers as needed.

The table below summarizes the performance tradeoff between these schemes. To keep the table simple, we assume the stages of the pipeline are identical in the amount of computation they perform and in the shapes of their inputs and outputs.

Scheme	Constraints	Latency	Activation Xmit per Worker	Weight Xmit per Worker	Activation Storage per Worker	Weight Storage per Worker
Distributed Data Parallel (DDP)	$W = B$	S	0	0	S	S
Fully Sharded DDP (FSDP)	$W = B$	S	0	$S - 1$	S	1
Pipeline Parallel (PP)	$W = S$	$B + S - 1$	B	0	$\min(S, B)$	1
Looped PP (LPP)	$W = GR$	$S + \frac{B}{G} - 1$	B	0	$\frac{S}{R} \min\left(S, \frac{B}{G}\right)$	$\frac{S}{R}$
Fully Sharded LPP (FSLPP)	$W = GR$	$S + \frac{B}{G} - 1$	B	$S - 1$	$\frac{S}{R} \min\left(S, \frac{B}{G}\right)$	1

Table 1: *Latency, network, and memory usage for the schedules unified in this document. W is the number of workers, S is the depth of the network being trained, and B is the number of microbatches. Looped models break W into G groups of R workers. The formulas assume computing a forward and backward step on any stage takes a unit of time, weights for all stages take a unit of weight storage and a unit of transmit, and activations for all stages take a different kind of unit of activation storage and transmit. To keep the latency computation simple, we assume that transmission latencies can be hidden by overlapping them with compute.*

Some useful patterns emerge from the table above. LPP's performance smoothly interpolates between that of PP and DPP as G, the number of worker groups, and R, the number of workers in each group are varied: When $G = 1$ and $R = S$, LPP is identical to PP. When $G = B$ and $R = 1$, LPP is identical to DDP. We'll take advantage of this observation to unify these algorithms under one implementation. The activation storage for each worker under LPP can be reduced by either increasing either R or G. An attractive regime is when the number of workers scales far beyond the number of batches and stages, with $W = \epsilon SB$ for some fixed $\epsilon \in (0, 1)$. Setting the number of groups $G = \epsilon B$ and the number of workers in each group to $R = S$ causes the latency to be $S + \frac{1}{\epsilon} - 1$, the activation storage for each worker to be $\frac{1}{\epsilon}$, and have each worker store just one set of weights. Concretely, with $\epsilon = \frac{1}{2}$, the latency of LPP becomes $S + 1$, almost as low as that of DDP, yet each worker need store at most two sets of activations and just one set of weights at any time. We show below that this configuration almost achieves the best possible utilization for the workers given the activation memory constraints.

On the surface, these forms of parallelism appear so different that they're traditionally implemented with different code bases. For example, PyTorch implements Data Parallism under `torch.nn.parallel.DistributedDataParallel`, Fully Sharded Data Parallism under `torch.distributed.FSDP` avariants of Pipeline Parallelism under `torch.distributed.pipelining`, and Tensor Parallelism under `torch.distributed.tensor.parallel`. Large models training code bases rely on all these packages simultaneously. But all these schemes turn out to be instances of the same master schedule. This master schedule takes as input two functions: A function that maps a work unit to a compute worker, and a second function that maps each stage of the pipeline to a worker that stores the source of truth for that stage's weights. Together, these two functions specify the schedule of computation and the implied transfer of weight and activation data. Changing these two functions produces the entire spectrum of distributed trainig algorithms. With the master scheduler offered in this document, all these different schedules and their hybrids can be implemented with just one compute and one weight storage function. The resulting training recipe would be easier to debug and maintain, and will make it easier to explore the larger space of possible schedules.

In summary, this document offers the following contributions:

- A way to implement several distributed training schemes in a unified code base. Under this abstract, a parallel training scheme is defined by a compute function and a weight storage function. This in turn simplifies the client code by obviating the need to import different APIs for each distribution scheme. The client code can instead supply the the compute and weight storage function that describes a mix of parallel schemes.
- A variant of Pipeline Parallelism, called Fully Sharded Looped Pipeline Parallelism (FSLPP), whose behavior smoothly interpolates between FSDP, and PP, allowing it to enjoy the best all worlds these methods. Along the way, we also modify Looped Pipeline Parallelism to interpolate between DDP and PP.
- Guidlelines to set the parameters of LPP. We show that scaling the number groups in LPP to be proportional to the number of micro-batches and setting the number of workers in each group to limit the amount of activation memory required from each worker causes LPP to nearly attain the optimal throughput achievable by any distributed training scheme. This implies that under the assumptions of this doc, not much improvement is possible over the LPP family of schedules.

Distributing back-propagation

Our job is to compute, with the help of W workers, the following set of operations:

$$\begin{aligned} x_{s+1}^b &= F_s \; x_s^b \\ z_s^b &= B_s(x_s^b) \; z_{s+1}^b \\ s &\in [0, S), \; b \in [0, B), \end{aligned}$$

Here, S is the number of layers of the neural network (which we refer to as stages of the pipeline), B is the number of mini-batches, x_s^b is the output of stage s on mini-batch b, and z_s^b is the corresponding backward iterate. F_s and B_s are the forward and backward operators for stage s. See the appendix for formal definitions of these quantities.

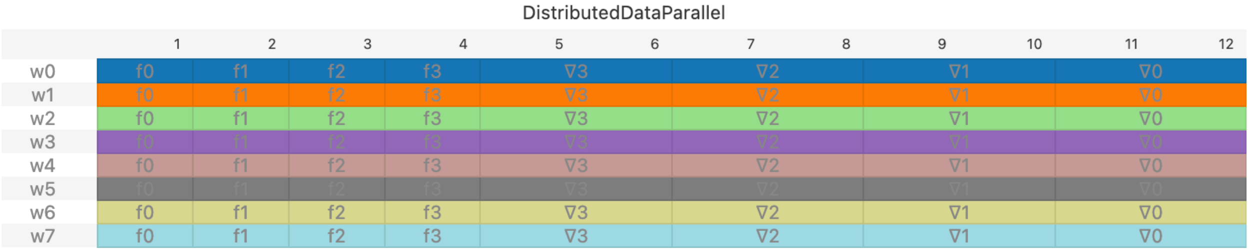
Formal definitions of distributed schedules

To specify which worker should compute which stage, define a function $w_{\text{compute}}(s, b, d) : [S] \times [B] \times \{\text{Forward}, \text{Backward}\} \rightarrow [W]$. This function maps a stage and mini-batch's compute to a worker. To specify which worker stores the source of truth for a stage's parameters, define a function $w_{\text{weights}}(s) : [S] \times [B] \times \{\text{Forward}, \text{Backward}\} \rightarrow [W]$. This pair of functions explicitly specifies where the compute and storage happens. It also implicity specifies what data will be transmitted between workers. It's understood that whenever $w_{\text{compute}}(s, b, d) \neq w_{\text{weights}}(s, b, d)$, worker $w_{\text{compute}}(s, b, d)$ will fetch the weights for stage s from worker $w_{\text{weights}}(s, b, d)$. Furthermore, worker $w_{\text{compute}}(s, b, \text{Forward})$ will fetch the activations from worker $w_{\text{compute}}(s-1, b, \text{Forward})$, and worker $w_{\text{compute}}(s, b, \text{Backward})$ will fetch the gradients from worker $w_{\text{compute}}(s+1, b, \text{Backward})$. We'll combine these two functions into a single function $w(s, b, d)$ that returns the tuple

$$w(s, b, d) \equiv (w_{\text{weights}}(s, b, d), \; w_{\text{compute}}(s, b, d)).$$

This formulation assumes that the smallest unit of work that can be assigned is a mini-batch at a particular stage. But finer-grained units of work are possible and in common use. One could, for example, split each F_s into pieces that execute on a different worker, as is done in tensor parallelism. Or one could split B_s into two pieces, one for the recursive step and one to compute the gradient of the weights, as is done in Zero Bubble. Both of these cases amounts to adding additional parameters to the function $w(s, b, d)$, corresponding to additional axes of parallelism. To keep the notation simple, we'll proceed with mini-batch and stage-wise granularity. This formulation accommodates F_s and B_s for the same mini-batch to execute on different workers, an idea we explored in the companion notebook..

We'll illustrate the various training schedules with pipeline diagrams. In these diagrams, the columns are time indices, and each row corresponds to a worker. The cells in the diagram describe the activity of the worker during the corresponing time. The color of each cell indicates the id of the batch being processed. The cell value indicates whether the work is for the forward or backward pass, and the pipeline stage being processed. For example, here is the pipeline diagram for Distributed Data Parallelism, when there are 8 workers, 8 batches, and 4 stages:



DistributedDataParallel

	1	2	3	4	5	6	7	8	9	10	11	12
w0	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w1	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w2	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w3	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w4	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w5	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w6	f0	f1	f2	f3	∇3		∇2		∇1		∇0	
w7	f0	f1	f2	f3	∇3		∇2		∇1		∇0	

In Distributed Data Parallelism, there is a one-to-one correspondence between workers and batches. Each worker processes every stage of the batch assigned to it in sequence. Distributed Data Parallelism (DDP) can be formally defined as:

$$w_{\text{DDP}}(s, b, d) = (b, b).$$

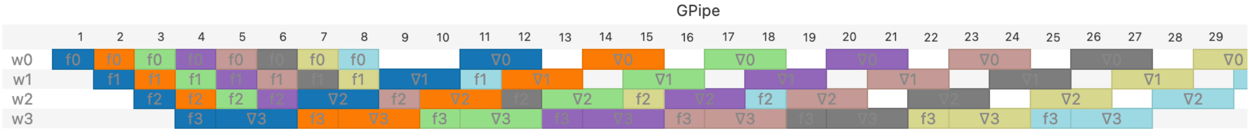
The mini-batch index dictates where compute happens and where the parameters are stored, so w is only a function of b, and $W = B$. Because the two components of w are always equal, the weights are always on the worker that performs the compute, so weights don't need to be transferred. Further, because $w_{\text{DDP}}(s, b, d) = w_{\text{DDP}}(s-1, b, d)$, no activations need be transferred either. In return, every worker must store all weights and activations for every stage, which makes DDP thrash from memory to slower storage for large models, or recompute the activations during backward pass. Another shortcoming of DDP is that the degree of parallism must scale with B, which forces us to use large batch sizes.

Fully Sharded Data Parallelism (FSDP) overcomes some of these difficulties by sharding model parameters and the optimizer state across workers. The pipeline diagram for FSDP looks identical to that of plain DDP. Formally, FSDP is:

$$w_{\text{FSDP}}(s, b, d) = (s, b).$$

Like DDP, the choice of compute worker only depends on b, but unlike DDP, each compute worker must fetch the weights from worker s. When $s = b$, the weights for the stage are resident on the worker, so no transfer is needed. Each worker must still store all the activations for every stage, which again introduces thrashing.

In Pipeline Parallelism, aka GPipe, there is a one-to-one correspondence between workers and stages. Each worker processes every batch, but only at the stage assigned to the worker:

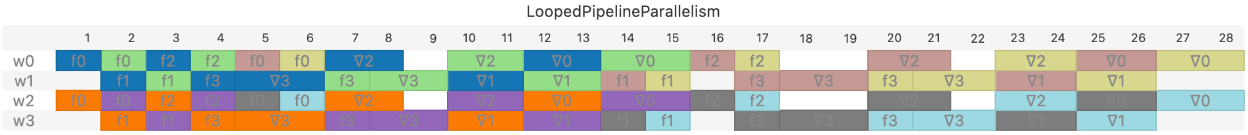

GPipe
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
w0 f0 f0 f0 f0 f0 f0 f0 f0 ∇0 ∇0 ∇0 ∇0 ∇0 ∇0 ∇0 ∇0
w1 f1 f1 f1 f1 f1 f1 f1 ∇1 f1 ∇1 ∇1 ∇1 ∇1 ∇1 ∇1 ∇1
w2 f2 f2 f2 f2 ∇2 f2 ∇2 f2 ∇2 f2 ∇2 f2 ∇2 ∇2 ∇2 ∇2
w3 f3 ∇3 f3 ∇3 f3 ∇3 f3 ∇3 f3 ∇3 f3 ∇3 f3 ∇3 f3 ∇3

GPipe is specified by

$$w_{\text{GPipe}}(s, b, d) = (s, s).$$

In GPipe, each stage s has its own compute worker, so $W = S$. The weights for stage s are also stored on worker s, so no weight need to be transferred. But unlike DDP, $w_{\text{GPipe}}(s, b, d) \neq w_{\text{GPipe}}(s-1, b, d)$, so activations must be tarnsferred between adjacent stages. More importantly, because s determines the worker, no two mini-batches can simultaneously be in the same stage. This introduces pipeline bubbles that increase the latency of the pipeline.

An improvement on GPipe is Looping Pipeline Parallelism (LPP). In LPP, each worker can process more than one stage of the pipeline. It does this by organizing the W workers into G groups of R workers, so $W = RG$. Each worker stores parameters for S/R stages, so each group is capable of processing all S stages of the pipeline. Here is a pipeline diagram when there are $G = 2$ groups:



LPP is specified by

$$w_{\text{LPP}}(s, b, d) = (h(s, b),\ h(s, b))$$
$$h(s, b) = (Rb \bmod W) + (s \bmod R)\,.$$

The first term of h can be rewritten as $R(b \bmod G)$. It maps b to one $0, R, 2R, \ldots, W - R$. The second term maps s to the range $[0, R)$, filling in the gaps generated by the first term. The hash h isn't the only viable mapping for LPP. Any other function that distributes (s, b) uniformly over the workers and maps an increment in s to an increment in the worker id modulo R would also be adequate. But h has additional properties that make it appealing: When $W = S$ and there is just one group, $G = 1$, $R = W$, and we get $h(s, b) = s$, so LPP becomes GPipe. When $W = B$ and each worker is in its own group, $G = W$, $R = 1$, and we get $h(s, b) = b$, so LPP becomes DDP. This way of representing LPP therefore lets us interpolate from DDP to GPipe by just varying R.

In LPP, workers store the weights of all the stages they process because we forced $w_{\text{compute}} = w_{\text{weight}}$. We can relax this restriction and make LPP behave more like FSDP. We call this hybrid idea Fully Sharded Looped Pipeline Parallelism (FSLPP):

$$w_{\text{FSLPP}}(s, b, d) = (h(s, b),\ h(s, s)).$$

The hash function h is identical to LPP, but w_{weights} replaces the batch id with the stage id. Consider the simpler situation when $G = R$, so that there are $W = R^2 = G^2$ workers. First, no worker stores weights for more than one stage. Second, the weights are stored evenly across groups. Indeed, the first group of workers are $0 \ldots R - 1$, the second group are are $R \ldots 2R - 1$, and so on, and $h(s, s)$ maps $s \in [0, S)$ to $0, R + 1, 2R + 1, \ldots W - 1$. Each of these lands in a different group, and they are evenly distributed across the groups.

One code to schedule them all

The appendix shows how one scheduler can implement the full variety of schedules described above by just specifying their corresponding $w(s, b, d)$. This subroutine implements the nuances between DDP, FSDP, PP, LPP, and the hybrid techniques mentioned aboved. It can also accommodates depth first and a breadth first schedules, and the various latency hiding techniques used in them. In this implementation, there are two worker threads per worker. The first thread peeks at the set of (s, b, d) triplets that are ready to execute, and greedily executes whichever one it can execute as soon as it appears in a global work queue. The second thread peeks at the work queue and prefetches the weights and activations for the next job the worker will need to execute.

Backpropagation on a pipeline requires lower stages to be computed before higher stages, and the entire forward pass to be computed before the backward pass on the same batch. We'll formalize the dependencies between these operations with a predictate $\text{pred}(s, b, d)$, which returns the set of triples (s', b', d') that must be computed to compute (s, b, d). When pred defines a tree structure, we'll also rely on succ, the inverse of pred. If a node does not have a predecessor (for example because it is the leaf of a tree) pred returns $\perp$. If a node does not have a successor (for example, because it is the root of a tree), succ returns $\top$. For all $s \geq 0$, backprop requires

$$\begin{aligned}
\text{pred}(s, b, \text{Forward}) &= \{(s-1, b, \text{Forward})\} \\
\text{pred}(S-1, b, \text{Backward}) &= \{(S-1, b, \text{Forward})\} \\
\text{pred}(s, b, \text{Backward}) &= \{(s+1, b, \text{Backward})\}
\end{aligned}$$

The first condition says that stage $s-1$ must be computed before stage s. The second condition says that the backward pass can only run after the final stage of the forward pass has run. The third conditions says that the backward pass progresses in the reverse direction of the forward pass.

This formalism simplifies the code, and will be particularly handy when when we upgrade the model from a pipeline structure to a tree or DAG structure, as is the case in models with multiple encoder legs.

Some schedules differ in how worker break ties when the preconditions for more than two jobs (s, b, d) are satisfied. For example, in the 1F1B schedule, a worker processes the backward pass preferentially over the forward pass. In the so called "depth first" schedule, a worker processes whichever job has been pending the longest. We'll define the function $n(s, b, d)$, which maps each job to a unique integer, thereby providing a total order on the set of jobs. defining the order of operations. The higher priorty the job has, the smaller the number. The schedules only consult this function only to break ties not otherwise resolved by the pred function.

Looped Pipeline Parallelism has nearly optimal latency subject to activation storage constraints

Under the foregoing model, DDP and FSDP make optimal use of the workers: They are occupied at all time, performing useful computations. But when activation memory is constrainted, the DDP family of models can't be applied. It turns out that for any bound on the activation memory, there is a configuration of LPP that also nearly optimally occupies the workers, which makes the LPP family of schedules more versatile than the DDP family. The implication is that any improvements on the LPP family of models is due to affects not modeled in Table 1 above (for example, the stages are not identical, or because not all communication latencies can be hidden). To formalize this claim, we'll need the following definition and upper bound:

Definition: The throughput per worker ρ is the number of jobs the average worker finishes per unit time under a schedule. We denote this by $\rho \equiv \frac{SB}{LW}$, where L is the latency of the schedule.

Definition: The peak activation storage, M, for a worker is the maximum number of activations the worker must maintain at any time during the schedule.

For example, for DDP, $\rho = \frac{SB}{SB} = 1$, the highest one could hope for, and the peak activation storage for a worker is $M = S$ since each worker must maintain the activations for all stages.

The peak activation imposes an upper bound on the throughput per worker:

Theorem: Any schedule whose communications latencies can be hidden on a pipeline with identical stages must satisfy $\rho \leq \frac{M}{S}$.

The proof appears in the appendix. Since with DDP, $M = S$, DDP attains the upper bound $\rho \leq 1$. But this required M to be large.

Remarkably, LPP offers more freedom in setting M, yet its throughput per worker also nearly saturates this bound. For any desired M, set the number of groups to $G = B/2$ and the number of workers in each group to $R = \frac{2S}{M}$. Assuming $S > 2$, the peak memory consumption per worker under this configuration indeed satisfies $M = \frac{S}{R} \min\left(S, \frac{B}{G}\right)$. The latency of LPP in this configuration is $S+1$, so its throughput per worker is $\rho = \frac{SB}{(S+1)RG} = \frac{M}{S+1}$. This nearly matches the upper bound $\rho \leq \frac{M}{S}$.

Latency, network, and memory usage from $w(s, b, d)$

The quantities in Table 1 were computed manually for each strategy. All of these strategies have a setup phase, where the workers gradually fill up with work, a steady state phase during which all workers are busy, and a drainage phase where the pipeline gradually gets lets busy. DDP and FSDP enter the steady state phase immediately. For GPipe, the setup phase takes S steps, and for LPP, it takes S/G steps. Not all schedules need to adhere to this pattern.

But we can compute these metrics mechanically for arbitrary strategies by inspecting $w(s, b, d)$ and $n(s, b, d)$. To keep the analysis simple, we'll assume all transmission latencies can be hidden with prefetching. The multi-threaded process described above can be simulated with a recursive set of equations. We'll use the following variables to model the system:

- j: A job (s, b, d). We'll use $w_{\text{compute}}(j)$ as a short-hand for
- J: The set of jobs that have executed so far. We'll define the "frontier" to be the set of jobs that have successors that have not yet been executed. Formally, we say $j \in J$ is in the frontier if $\text{succ}(j) \notin J$. $w_{\text{compute}}(s, b, d)$.
- $t(j)$: When the job j will finish, expressed in units of time. Only valid for jobs in J.
- $t(w)$: The when worker w finishes its latest job in J. This is a shorthand for $\max_{j \in J : w(j) = w} t(j)$.

The following operation identifies a job j^* on the frontier whose successor can be executed soonest:

$$\begin{aligned} j^* = \arg\min_{j \in J} \quad & \max\left[t(w_{\text{compute}}(\text{succ}(j))),\ t(j)\right] \\ \text{s.t.}\ \ & \text{succ}(j) \notin J. \end{aligned}$$

It does this by examining every job j on the frontier. The constraints just ensure j is on the frontier. $t(j)$ is when the job on the frontier will finish. Its successor cannot start until then. $t(w_{\text{compute}}(\text{succ}(j)))$ is the first available slot for its successor's worker, so $\max\left[t(w_{\text{compute}}(\text{succ}(j))),\ t(j)\right]$ is when the successor job can first be executed. Once the frontier job j^* has been identified, we update

$$\begin{aligned} t(j^*) &= \text{duration}(\text{succ}(j^*)) + \max\left[t(w_{\text{compute}}(\text{succ}(j))) + t(j^*)\right] \\ J &\leftarrow J \cup \{\text{succ}(j^*)\} \end{aligned}$$

This process mimicks almost exactly the greedy schedule followed by the multi-threaded code snippet in the appendix. The difference is that we have not modeled the tie breaking logic that uses $n(s, b, d)$. To accommodate this order, it suffices to add a term $\epsilon \cdot n(s, b, d)$ to the objective of the $\arg\min$. For sufficiently small $\epsilon > 0$, this nudges the minimizer toward job preferred by $n(s, b, d)$.

After $2 \times S \times B$ iterations, J will contain all jobs. The latency of the pipeline can be read from $t(j)$:

$$\text{latency of the pipeline} = \max_j t(j).$$

Some statistics of the schedule can be computed more directly from $w(s, b, d)$, and don't need the full weight of the simulator. The number of times worker w must fetch input activations from another worker is

$$\text{number of times worker } w \text{ receives activations over the network} = \sum_{s,b\,:\,w_{\text{compute}}(s,b)=w} 1\left[w_{\text{compute}}(s-1, b) \neq w\right].$$

This is the number of times the worker has to process a work item (s, b) whose predecessor was computed by another worker.

The number of times worker w must fetch weights from another worker is

$$\text{number of times worker } w \text{ receives weights over the network} = \sum_{s,b\,:\,w_{\text{compute}}(s,b)=w} 1\left[w_{\text{weights}}(s, b) \neq w\right].$$

This is the number of times the host has to process work for which it doesn't host the weights.

The amount of activation storage required by a particular worker depends on both $w(s, b, d)$ and $n(s, b, d)$. We don't have a tidy formula to report this quantity, but we do have an upper bound:

$$\text{peak activation storage for worker } w \leq \sum_{s,b} 1\left[w_{\text{compute}}(s, b) = w\right].$$

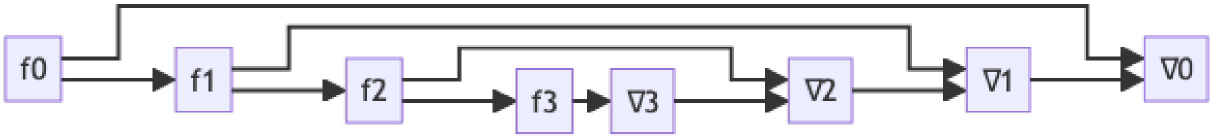
This is just the total number of items the worker processes.

Appendices

Appendix: Proof of the throughput lower bound

The proof relies on the concept of memory-time for a variable. This is the number of time steps during which a variable must stay live during a computation. The memory-time of a computation is the sum of memory-times of all the variables it computes. A computer with M amount of memory must run for at least m/M time steps to compute a function that has memory-time m. If the latency of the algorithm is too small, it cannot accommodate the memory-time required to process all the jobs.

Backpropagation on a pipeline requires the activations x_s^b to stay live until the backward pass has executed. So x_s^b must remain live for at least $2(S - s) + 1$ time steps. To illustrate, here is the compute graph for the backpropagation equations for a four stage pipeline:



Each batch therefore requires $\sum_{s=0}^{S-1} 2(S-s)-1 = S^2$ memory-time, so processing B batches requires at least BS^2 memory-time. A schedule with latency L with W workers can provide at most LWM memory-time. We must therefore have $LWM \geq BS^2$. Plugging in the definition for ρ gives $\rho \geq M/S$. □

Appendix: Training a pipeline with back-propagation

To train a neural network, we compute the gradient of a loss function of the output of the neural network with respect to the parameters of each stage of the neural network's pipeline. We'd like compute the gradients of output of an S stage pipeline with respect to the weights of each of the stages. Each stage s is a function f_s parameterized by weights w_s. Each stage maps its input x_s to an output x_{s+1}:

$$x_{s+1} = f_s(x_s, w_s).$$

The input of the pipeline is x_0, and x_S is the resulting scalar loss (meaning the final stage computes the loss). To compute the gradient of x_{S-1} with respect to each $w_0 \ldots w_{S-1}$, we execute a backward pass where each stage s computes, recursively, the gradient of the loss with respect to its activations:

$$\frac{\partial x_S}{\partial x_s} = \frac{\partial x_S}{\partial x_{s+1}} \frac{\partial x_{s+1}}{\partial x_s},$$

From this, each stage computes the gradient of the loss with respect to the stage's parameters:

$$\frac{\partial x_S}{\partial w_s} = \frac{\partial x_S}{\partial x_{s+1}} \frac{\partial x_{s+1}}{\partial w_s}.$$

These operations can be written in a compact operator form:

$$\begin{aligned} x_{s+1} &= F_s \; x_s \\ z_s &= B_s(x_s) \; z_{s+1} \end{aligned}$$

The forward operator F_s applies the function $f_s(\cdot, w_s)$. For the backward pass, defined $z_s \equiv (\frac{\partial x_T}{\partial x_s}, \frac{\partial x_T}{\partial w_s})$ to capture the state of the backward iteration, and an operator $B_s(x_s)$ parametrized by the forward activations x_s that right-multiplies z_{s+1} by the matrix $\begin{bmatrix} \frac{\partial}{\partial x_s} f_s(x_s, w_s) & \frac{\partial}{\partial w_s} f_s(x_s, w_s) \\ 0 & 0 \end{bmatrix}$.

We are to apply the above pipeline on B mini-batches of data at once without changing the parameters of the pipeline in the interim. We'll use a superscript on the inputs, activations, and results generated during the backward pass to denote each mini-batch, with x_s^b denoting the input of stage s from the bth mini-batch.

Appendix: One code to schedule them all

This section sketches out pseudocode for the generic task scheduler. The pseudocode is written in a math-inspired version of Python. Like in Python, ranges are inclusive of their start and exclusive of their end (so `0..W` includes 0 but not `W`). The `match` operator is inspired by Haskell and Rust's match statement. The set syntax follows established mathematical notation.

Before the round of work starts, we globally initialize a list of available work:

```
# A unit of work is a tuple of a batch id and an operator F[s] or B[s].
Direction = 'forward' | 'backward'
Stage = 0..S
Batch = 0..B
Work = (Stage, Batch, Direction)
Worker = 0..W

# Initially, the first stage of all batches is ready to execute.
ready : Set[Work] = {(-1, b, 'forward') : b   Batch}

# Nothing is currently executing.
working_on : Set[Work] = {}
```

Then each worker goes in a loop picking off available work that it can process:

```
def available_work(worker: Worker, ready: Set[Work]) → (Work, Work):
    # Find jobs that are ready to be executed by the worker. This blocks
    # until a job is available.
    candidates =  {(job, new_job)   ready x ready :
                   w_compute(new_job) = worker, new_job = pred(job)}

    # Among the candidates, return the pair with the highest priority.
    return find_smallest(candidates, key=lambda (job, new_job): n(new_job))
```

```
def fetch_work(w: Worker, ready: Set[Work]) → (Work, Work):
    atomically:
        finished_work, work_to_do = available_work(w, ready)
        remove finished_work from ready
        return (finished_work, work_to_do)

def worker_compute_thread(w: Worker):
    while True:
        finished_work, work_to_do = fetch_work(w, ready)

        match work_to_do:
            stage, batch, 'forward':
                # Initiate prefetch
                insert work_to_do into working_on

                # Start computing
                new_activations = F[stage](
                    await_weights(stage),
                    await_activations(stage - 1, batch)
                )
                store_activations(stage, batach, new_activations)
                insert work_to_do into ready

            stage, batch, 'backward':
                # Initiate prefetch
                insert work_to_do into working_on

                # Start computing
                new_grad = B[stage](
                   (stage < S) and await_gradients(stage+1, batch),
                   await_weights(stage),
                   await_activations(stage, batch)
                )
                store_gradient(stage, b, new_grad)


def worker_prefetch_thread(w: Worker):
    # Optional thread that hides the fetching latency in the compute thread
    # by prefetching weights and activations.
    while True:
        finished_work, work_to_do = fetch_work(w, working_on)
        match work_to_do:
            stage, batch, 'forward':
                prefetch_weights(stage)
                prefetch_activations(stage - 1, batch)
            stage, batch, 'backward':
                (stage < S) and prefetch_gradients(stage + 1)
                prefetch_weights(stage)
                prefetch_activations(stage, batch)
```

The code above depends on w_{compute} only through the `available_work` function. It depends on w_{weights} through the `await_gradients`, `await_activations` and their prefetch varaiants.