Scalable Deep Neural Network Training with Distributed K-FAC

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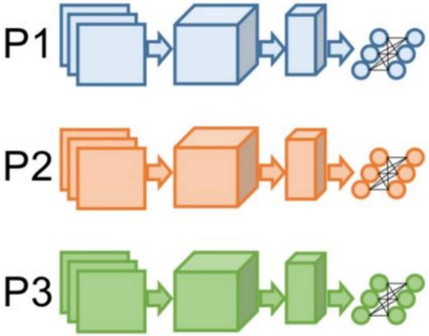
Outline

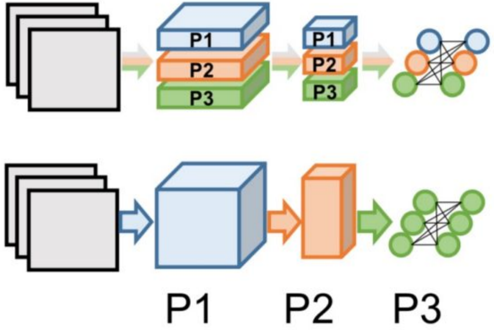
1. Challenges in large scale deep learning training
2. Optimization methods: first-order vs. second-order
3. Prior work in distributed K-FAC
4. Communication optimized distributed K-FAC [*SC ‘20, TPDS ‘22*]
5. KAISA: generalizing distributed second-order optimization [*SC ‘21*]
6. Implementation
7. Evaluation

Large Scale Training

Faster ➡ *Data Parallelism*



Larger Models ➡ *Model Parallelism*



Can we keep scaling the batch size to use more processors?

Published as a conference paper at ICLR 2017

ON LARGE-BATCH TRAINING FOR DEEP LEARNING: GENERALIZATION GAP AND SHARP MINIMA

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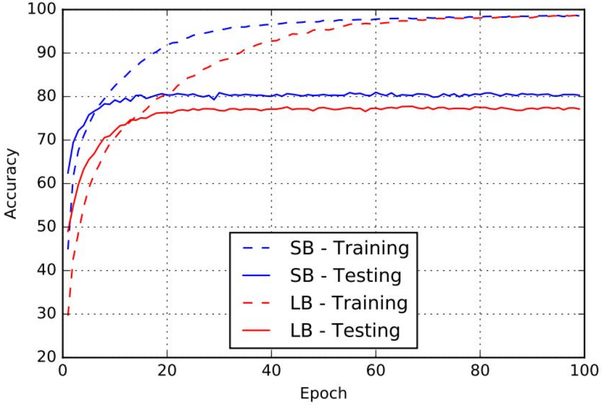


HPC and Machine Learning

Large batch sizes (e.g., 100K to 1M)...

- ++ Used to **scale out** to more nodes.
- -- Leads to **worse generalization** performance and **higher communication** costs.

How can we better enable large batch training on HPC (generalization performance and scaling)?

Previous Efforts

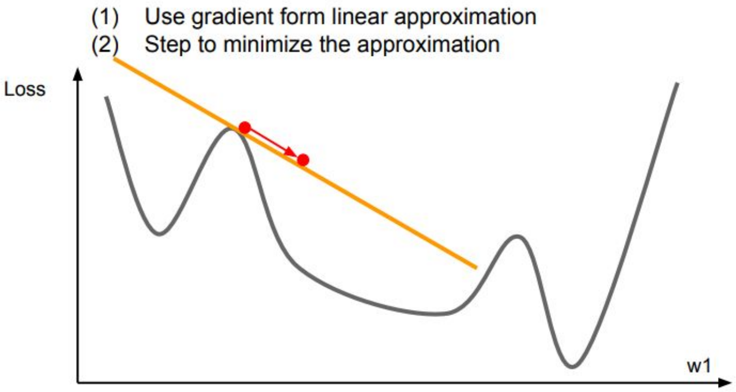
Generalization Gap

- Learning Rate Warmup
- Learning Rate Scaling
- Batch Size Warmup
- Layer-wise Adaptive Learning Rate (LARS/LAMB)
- Distributed Batch Normalization
- . . . and many more

Better Scaling

- Gradient Compression
- Lower Precision (FP16)
- Network Topology Aware Operations
- Layer Pipelining/Hybrid-Parallelism
- Asynchronous SGD
- Custom Fused Kernels
- Gradient Checkpointing
- . . . and many more

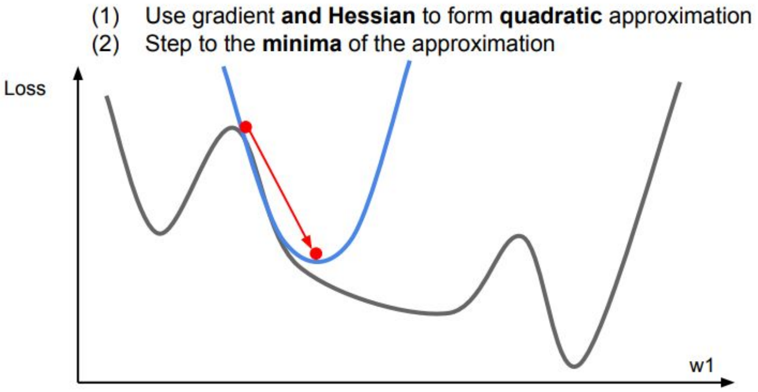
First-Order Optimization



1. Use gradient form linear approximation
2. Step to minimize the approximation

$$\text{SGD: } w_{k+1} = w_k - \alpha \nabla L(w_k)$$

Second-Order Optimization



1. Use gradient **and Hessian** to form **quadratic** approximation
2. Step to the **minima** of the approximation

$$\text{Newton: } w_{k+1} = w_k - \alpha \underbrace{H^{-1} \nabla L(w_k)}_{\text{Precondition}}$$

Hessian has $O(n^2)$ elements
Inversion is $O(n^3)$ operations

http://cs231n.stanford.edu/slides/2018/cs231n_2018_lecture07.pdf

Second-Order Optimization

A good candidate for large batch, distributed training!

1. Larger batches are more representative of the dataset's distribution.

   → *infrequent second-order information updates*

2. Gradient noise limits batch size and increases throughout training (McCandlish, 2018).

   → *second-order methods optimize noise-independent terms better* (Martens, 2014)

3. Higher computation-to-communication ratio in second-order methods.

   → *enables more advanced distribution schemes*

Kronecker-Factored Approximate Curvature

- Second-order methods incorporate the curvature of the parameter space.
  - ++ More progress optimizing the objective function per-iteration
  - -- **Expensive to compute!**

- K-FAC **efficiently approximates** the Fisher Information Matrix (FIM) for preconditioning the gradients (Martens+, 2015).

$$\text{SGD: } w^{(k+1)} = w^{(k)} - \frac{\alpha^{(k)}}{n} \sum_{i=1}^{n} \nabla L_i(w^{(k)}) \qquad \text{K-FAC: } w^{(k+1)} = w^{(k)} - \frac{\alpha^{(k)} \boxed{F^{-1}(w^{(k)})}}{n} \sum_{i=1}^{n} \nabla L_i(w^{(k)})$$

- Generalizes better with **large batch sizes** and **converges in fewer iterations** than first-order methods (Ba+, 2017)
  - Scales to extremely large batch sizes, e.g., 131k for ImageNet training (Osawa+, 2019)

Kronecker Product

$$A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{bmatrix}$$

$$m \times n \otimes p \times q \longrightarrow mp \times nq$$

$$\begin{bmatrix} 1 & \boxed{2} \\ 3 & 4 \end{bmatrix} \otimes \boxed{\begin{bmatrix} 5 & 6 \\ 7 & 8 \\ 9 & 0 \end{bmatrix}} = \begin{bmatrix} 1 \times 5 & 1 \times 6 & \boxed{2} \times 5 & \boxed{2} \times 6 \\ 1 \times 7 & 1 \times 8 & \boxed{2} \times 7 & \boxed{2} \times 8 \\ 1 \times 9 & 1 \times 0 & \boxed{2} \times 9 & \boxed{2} \times 0 \\ 3 \times 5 & 3 \times 6 & 4 \times 5 & 4 \times 6 \\ 3 \times 7 & 3 \times 8 & 4 \times 7 & 4 \times 8 \\ 3 \times 9 & 3 \times 0 & 4 \times 9 & 4 \times 0 \end{bmatrix}$$

$$2 \times 2 \otimes 3 \times 2 \longrightarrow 6 \times 4$$

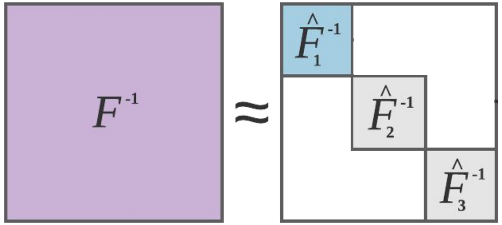
Efficient F Approximation

Step 1: Approximate the FIM as a block diagonal matrix*

$$\hat{F} = \mathtt{diag}(\hat{F}_1, \ldots, \hat{F}_i, \ldots, \hat{F}_L)$$

Step 2: Decompose each block as the Kronecker Product of the activations of the previous layer with the gradient w.r.t. the output of the current layer

$$\hat{F}_i = a_{i-1}a_{i-1}^\top \otimes g_i g_i^\top = A_{i-1} \otimes G_i$$



**Recall inverse of block diagonal matrix is composed of the inverses of each block*

Efficient Gradient Preconditioning

Step 3: Apply properties of Kronecker Product to weight update equation

Properties: $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$ $\quad (A \otimes B)\vec{c} = B^{\top}\vec{c}A$

Weight Update: $w_i^{(k+1)} = w_i^{(k)} - \alpha^{(k)} \boxed{\hat{F}_i^{-1} \nabla L_i(w_i^{(k)})}$

$$\begin{aligned}
\hat{F}_i^{-1} \nabla L_i(w_i^{(k)}) &= (A_{i-1} \otimes G_i)^{-1} \nabla L_i(w_i^{(k)}) \\
&= (A_{i-1}^{-1} \otimes G_i^{-1}) \nabla L_i(w_i^{(k)}) \\
&= G_i^{-1} \nabla L_i(w_i^{(k)}) A_{i-1}^{-1}
\end{aligned}$$

Preconditioned Gradient

Computing Inverses

. . . can be difficult

Tikhonov Regularization: $(\hat{F}_i + \gamma I)^{-1} = (A_{i-1} + \gamma I)^{-1} \otimes (G_i + \gamma I)^{-1}$

Use Eigen Decompositions:

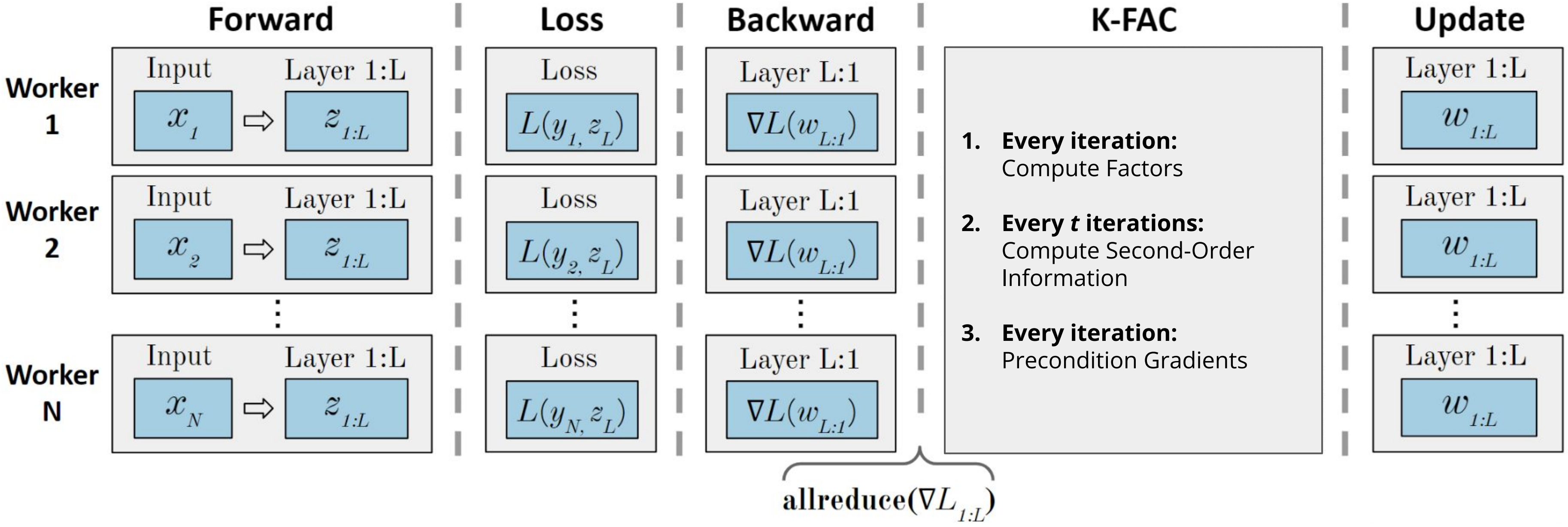
$$V_1 = Q_G^\top \nabla L(w_i^{(k)}) Q_A$$

$$V_2 = V_1 / (v_G v_A^\top + \gamma)$$

$$(\hat{F}_i + \gamma I)^{-1} \nabla L(w_i^{(k)}) = Q_G V_2 Q_A^\top$$

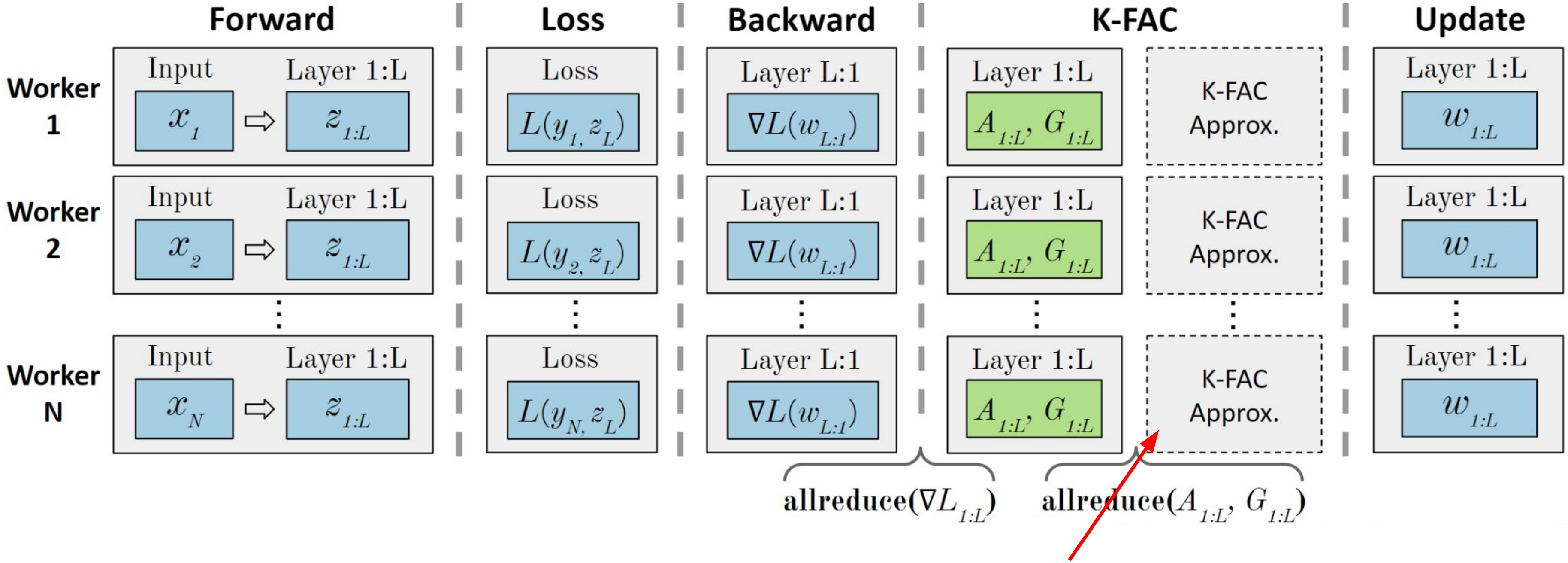
Batch Size	256	512	1024
SGD	92.77%	92.58%	92.69%
K-FAC with Inverse	92.58%	92.36%	91.71%
K-FAC with Eigen-decomp.	92.76%	92.90%	92.92%

Data Parallel Training with K-FAC



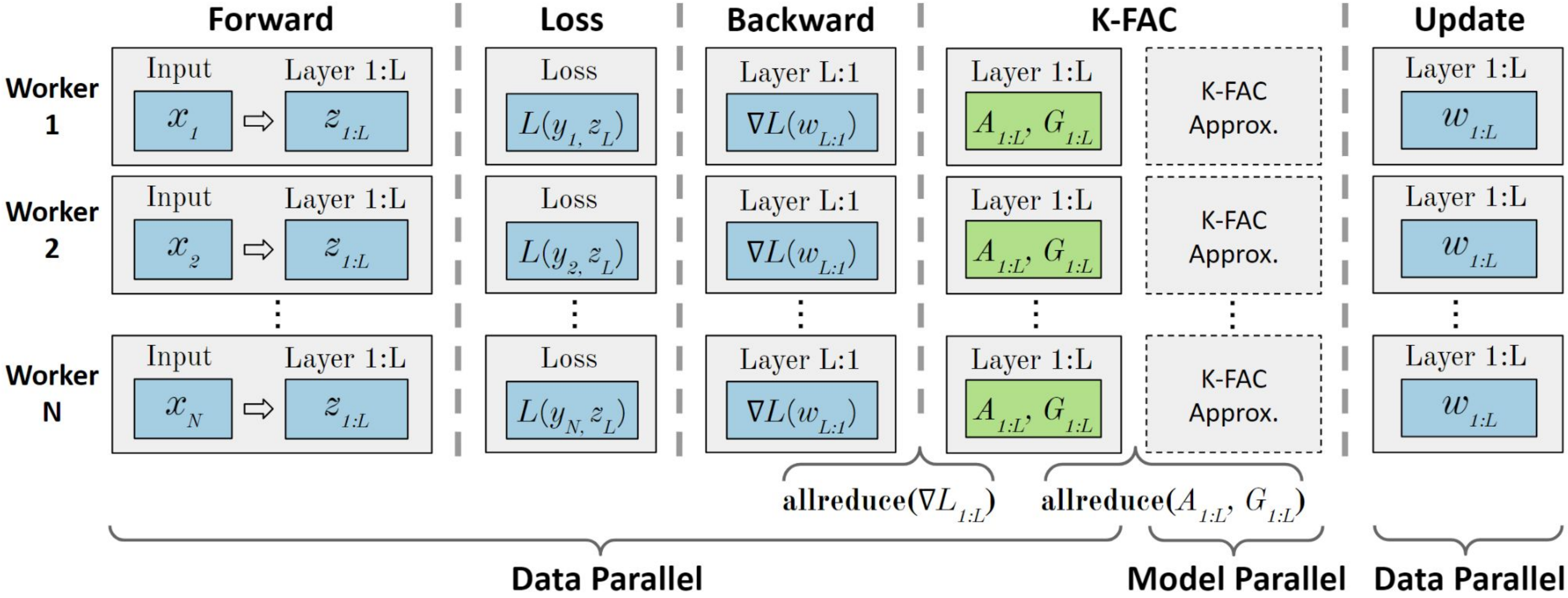
1. **Every iteration:** Compute Factors
2. **Every *t* iterations:** Compute Second-Order Information
3. **Every iteration:** Precondition Gradients

Data Parallel Training with K-FAC



Redundant expensive second-order computations

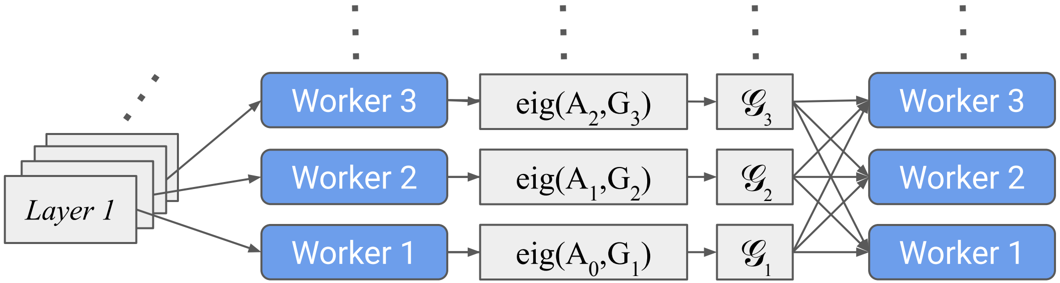
Data Parallel Training with K-FAC



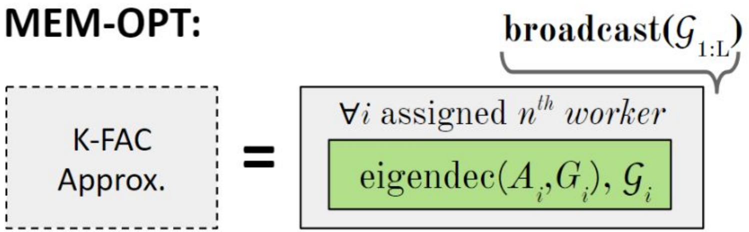
Model Parallel K-FAC Stage

MEM-OPT

Osawa et al. (CVPR 2019)



- ++ Lower memory usage
- -- Communication required every iteration



MEM-OPT:

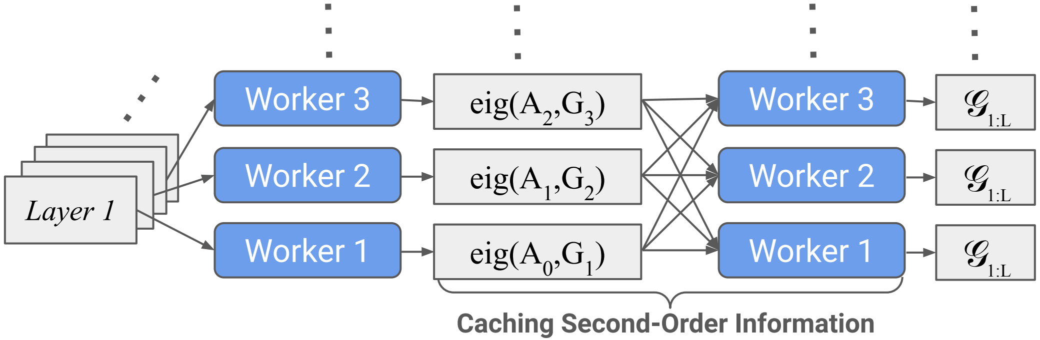
$$\boxed{\text{K-FAC Approx.}} = \overbrace{\forall i \text{ assigned } n^{th} \; worker \;\; \mathrm{eigendec}(A_i,G_i),\ \mathcal{G}_i}^{\mathbf{broadcast}(\mathcal{G}_{1:L})}$$

Can we make the communication frequency a function of the second-order computation frequency?

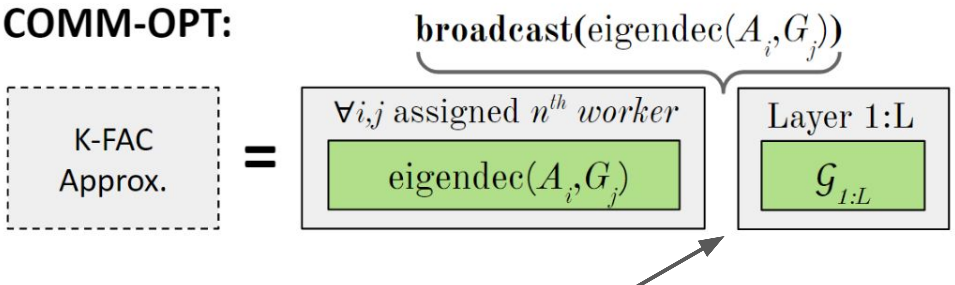
Model Parallel K-FAC Stage

COMM-OPT

Pauloski et al. (SC20)



- ++ Communication every *t* iterations
- -- Higher memory usage due to caching



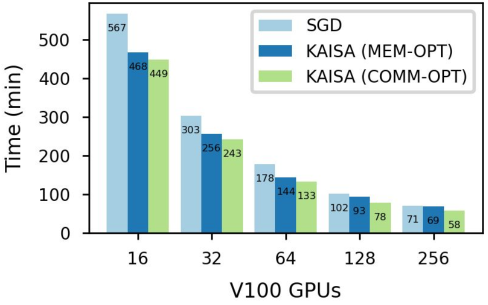
COMM-OPT:

$$\boxed{\text{K-FAC Approx.}} = \overbrace{\boxed{\forall i,j \text{ assigned } n^{th}\ \mathit{worker}\quad \boxed{\mathrm{eigendec}(A_i,G_j)}}}^{\mathbf{broadcast}(\mathrm{eigendec}(A_i,G_j))}\ \boxed{\text{Layer 1:L}\quad \boxed{\mathcal{G}_{1:L}}}$$

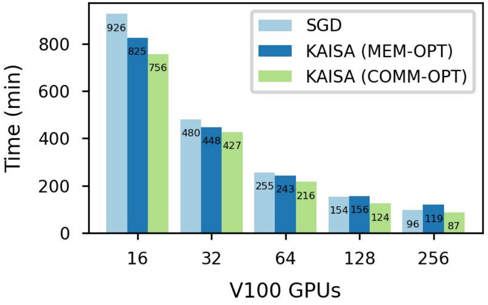
Preconditioning is cheap compared to eigen decomposition

MEM-OPT vs COMM-OPT

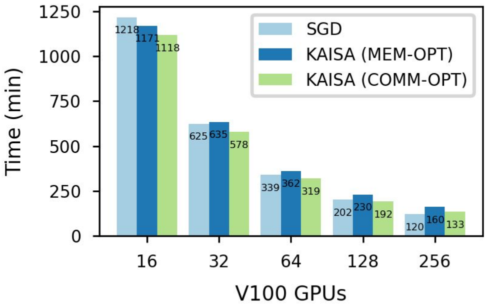
Communication Operation Interval				
	Gradients	**Factors**	**Preconditioned Gradients**	**Inverses/Eigen Decomps**
	`Allreduce`	`Allreduce`	`Broadcast/Allgather`	`Broadcast/Allgather`
MEM-OPT	**1**	***t***	**1**	**N/A**
COMM-OPT	**1**	***t***	**N/A**	***t***



(a) ***ResNet-50***

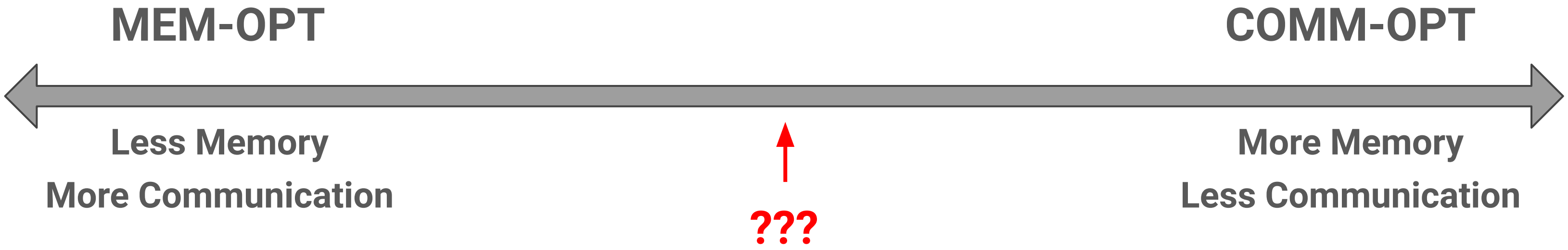


(a) ***ResNet-101***



(a) ***ResNet-152***

Communication vs Memory



MEM-OPT

COMM-OPT

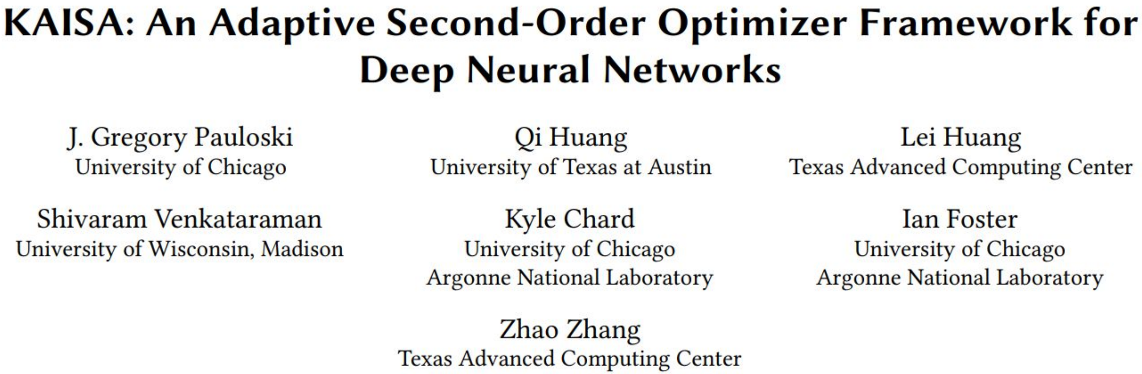
Less Memory

More Communication

???

More Memory

Less Communication



KAISA: An Adaptive Second-Order Optimizer Framework for Deep Neural Networks

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Distribution of Work

Worker Types for a Layer (*N* workers)

Second-Order Worker	Gradient Worker	Gradient Receivers
Compute second-order information (one of the gradient workers)	Compute preconditioned gradient with second-order information	Receives preconditioned gradients from a gradient worker
1 per layer	***m*** per layer	***N* - *m*** per layer

Gradient Worker Fraction (*grad_worker_frac*) = ***m / N***

MEM-OPT: *grad_worker_frac* = **1/N**
COMM-OPT: *grad_worker_frac* = **1**

Gradient Worker Fraction

MEM-OPT

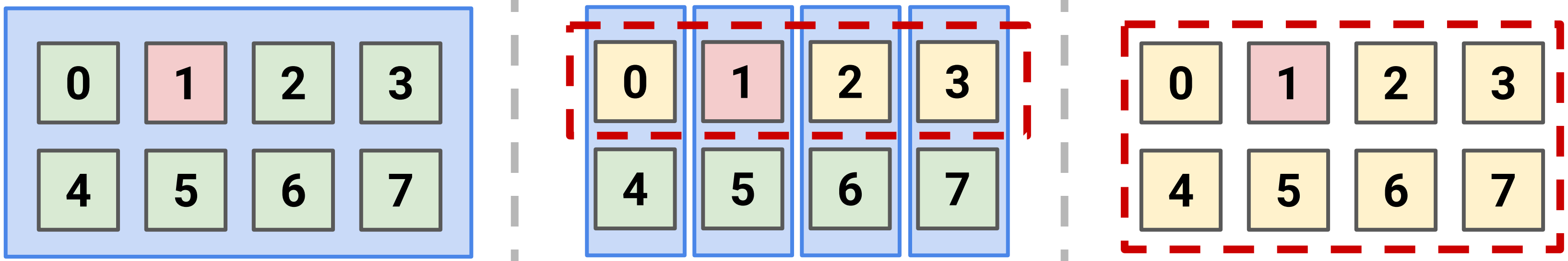
grad_worker_frac = 1/8

HYBRID-OPT

grad_worker_frac = 1/2

COMM-OPT

grad_worker_frac = 1



🟥 1 : second-order (gradient worker)

🟨 0 : gradient worker

🟩 0 : gradient receiver

🟦 : preconditioned gradient communication group (every iteration)

⬚ : second-order information communication group (every *t* iterations)

Gradient Worker Fraction

MEM-OPT

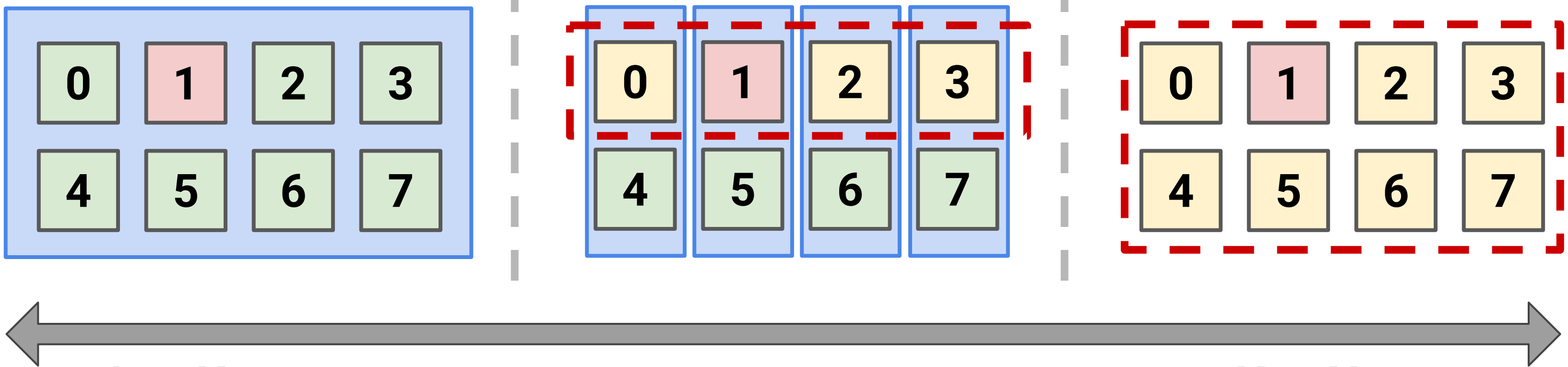
grad_worker_frac = 1/8

HYBRID-OPT

grad_worker_frac = 1/2

COMM-OPT

grad_worker_frac = 1

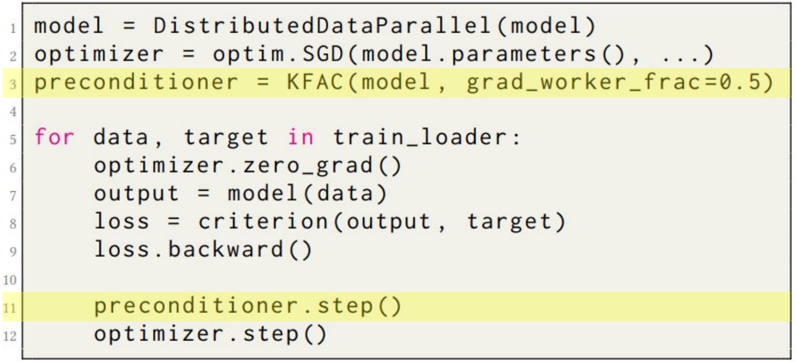


Less Memory
More Communication

More Memory
Less Communication

KAISA: Design Goals

- PyTorch **gradient preconditioner**
- **K-FAC** for second-order method
- **Adaptable** distribution scheme
- Understand the memory and communication **tradeoffs** in distributed second-order optimization
- Show KAISA is **faster** than default optimizers



```
model = DistributedDataParallel(model)
optimizer = optim.SGD(model.parameters(), ...)
preconditioner = KFAC(model, grad_worker_frac=0.5)

for data, target in train_loader:
    optimizer.zero_grad()
    output = model(data)
    loss = criterion(output, target)
    loss.backward()

    preconditioner.step()
    optimizer.step()
```

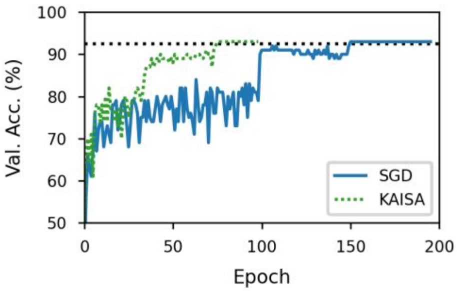
Listing 1: Example K-FAC usage.

https://github.com/gpauloski/kfac_pytorch

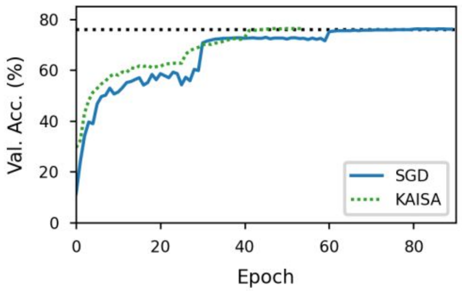
KAISA: Features

- Inverse or Eigen decomposition (default) K-FAC preconditioning
  - Linear and Conv2D layers
- Data Parallel Training Frameworks: PyTorch, DeepSpeed, NVIDIA Apex
- Adaptable distribution scheme (gradient worker fraction)
- Mixed Precision Training
- Gradient Accumulation
- Other Minor Optimizations:
  - Symmetry aware communication and communication bucketing
  - Preconditioning precomputation

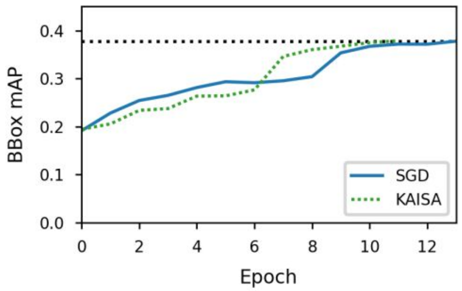
Evaluation: Convergence



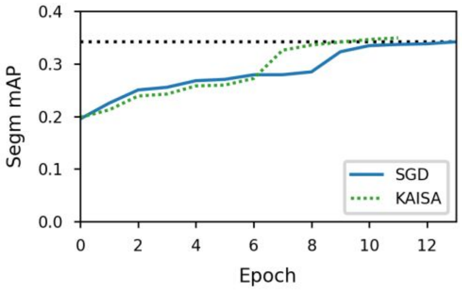
(a) ResNet-34 Accuracy



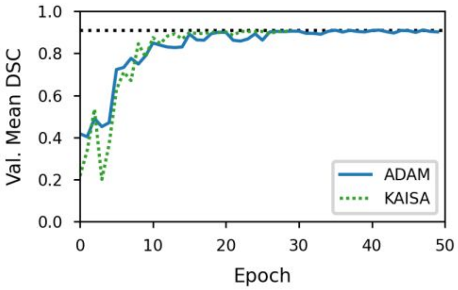
(b) ResNet-50 Accuracy



(c) Mask R-CNN BBox mAP



(d) Mask R-CNN Segm mAP



(e) U-Net Dice Score

Evaluation: Time-to-Convergence w/ Fixed Batch Size

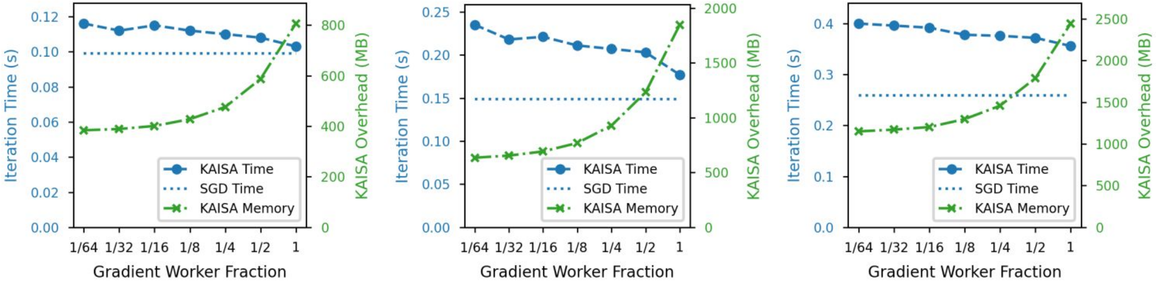
App	Default Optimizer	Baseline	# GPUs	Global Batch Size	Precision	KAISA Time-to-Convergence Improvement
ResNet-50	SGD	75.9% Val. Acc.	8 A100	2048	FP16	**24.3%**
Mask R-CNN	SGD	0.377 bbox mAP 0.342 segm mAP	64 V100	64	FP32	**18.1%**
U-Net	ADAM	91.0% Val. DSC	4 A100	64	FP32	**25.4%**
BERT-Large (Phase 2)	LAMB	90.8% SQuAD v1.1 F1	8 A100	65,636	FP16	**36.3%**

Evaluation: Time-to-Convergence w/ Fixed Memory Budget

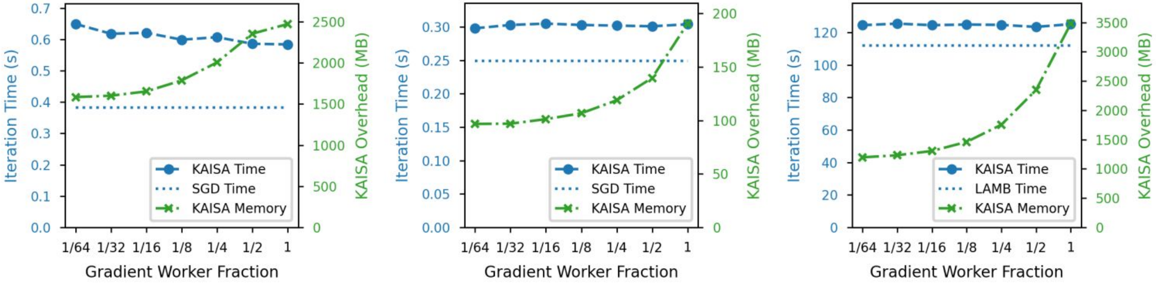
App	Optimizer	GPUs	Grad. Worker Frac.	Local Batch Size	Time-to-Convergence (minutes)
ResNet-50	SGD	64 V100	--	128	**123 (DNC)**
	KAISA		1/64	80	**96**
	KAISA		1/2	80	**83**
BERT-Large (Phase 2)	LAMB	8 A100	--	12	**2918**
	KAISA		1/2	8	**1703**
	KAISA		1	8	**1704**

* Use max possible local batch size for each experiment and measure time-to-convergence.

Evaluation: Memory vs. Communication



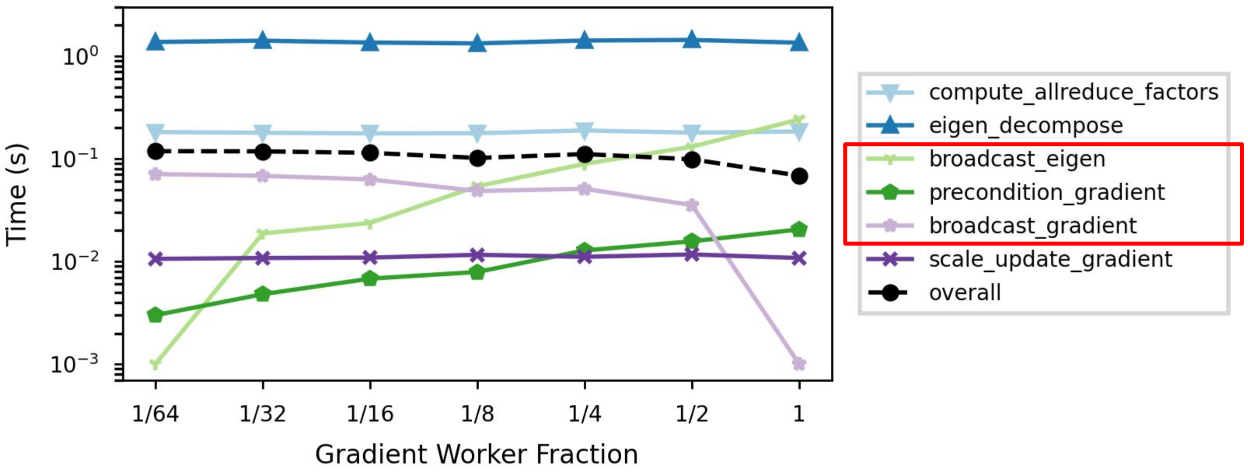
(a) ResNet-18 (FP32) (b) ResNet-50 (FP32) (c) ResNet-101 (FP32)



(d) ResNet-152 (FP32) (e) Mask R-CNN (FP32) (f) BERT-Large Phase 2 (FP16)

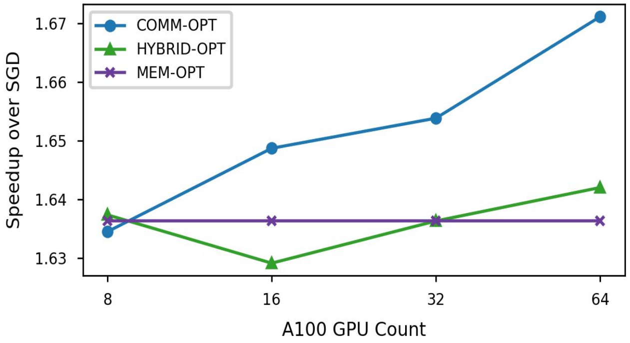
Figure 6.3: Average iteration time and K-FAC memory overhead across *grad-worker-frac* values on 64 V100 GPUs. Dotted lines are the baseline iteration times without K-FAC.

Evaluation: Memory vs. Communication

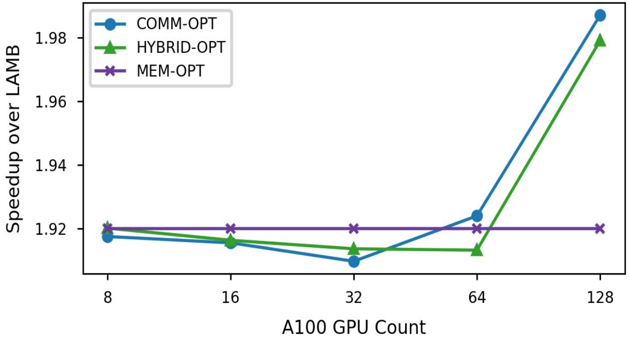


Evaluation: Scaling

- 27-29% **faster than SGD** with ResNet-50
- 41-44% **faster than LAMB** for BERT-Large
- MEM-OPT has constant speedup
- HYBRID/COMM-OPT **improve with scale**
- HYBRID-OPT **best balance** of memory usage and scaling with BERT-Large



(a) ResNet-50



(b) BERT-Large

Takeaways

Second-order optimization is **viable** for distributed training

- Converges to **same target** metrics as first-order methods
- Converges in **less wall time** with minimal configuration

Second-order optimization enables more **creative hybrid-parallel** schemes

KAISA's provides a framework for distributed training with **future second-order methods**

Questions?

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`github.com/gpauloski/kfac_pytorch`

J. Gregory Pauloski, Zhao Zhang, Lei Huang, Weijia Xu, and Ian T. Foster. 2020. *Convolutional Neural Network Training with Distributed K-FAC*. International Conference for High Performance Computing, Networking, Storage and Analysis (SC '20).

J. Gregory Pauloski, Qi Huang, Lei Huang, Shivaram Venkataraman, Kyle Chard, Ian Foster, and Zhao Zhang. 2021. *KAISA: An Adaptive Second-order Optimizer Framework for Deep Neural Networks*. International Conference for High Performance Computing, Networking, Storage and Analysis (SC '21).

J. Gregory Pauloski, Lei Huang, Weijia Xu, Kyle Chard, Ian T. Foster, and Zhao Zhang. 2022. *Deep Neural Network Training with Distributed K-FAC*. To appear in Transactions on Parallel and Distributed Systems (TPDS).