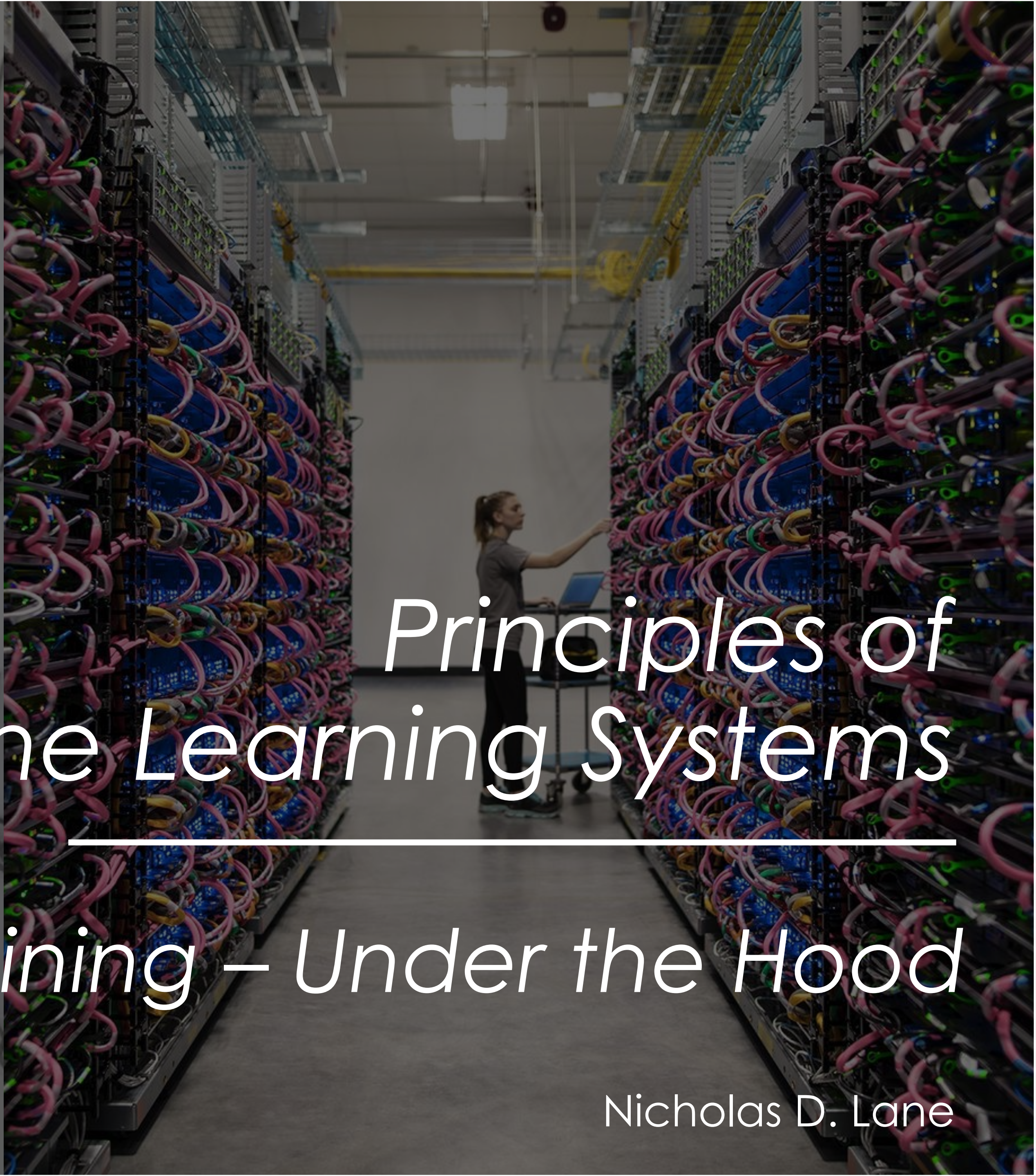

Principles of Machine Learning Systems

4: Training – Under the Hood

v1.5

Nicholas D. Lane

Roadmap for Today

1. The fundamentals of DL training
    1. DL model as a compute graph
    2. Training algorithm specifics
    3. NumPy implementation
    4. Exploitable parallelism
2. Resource management
    1. Characterising resource requirements
    2. Speed-up strategies

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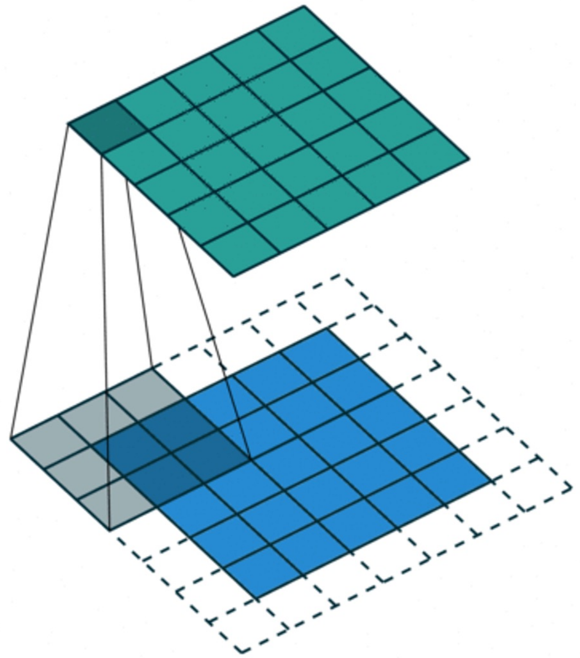
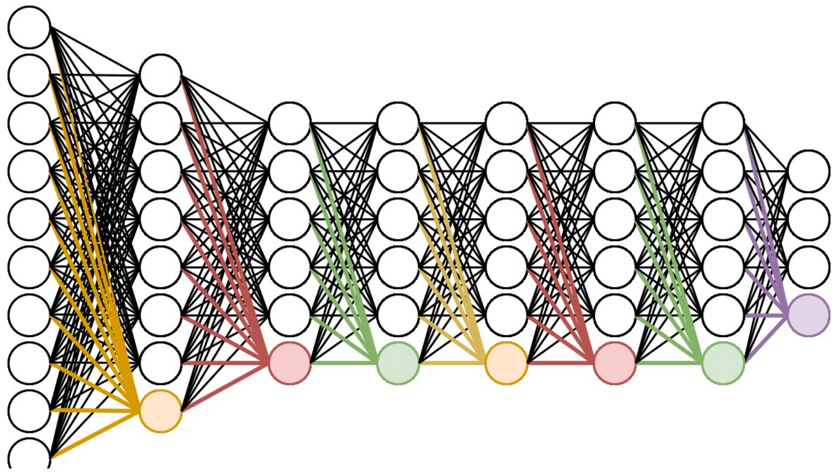
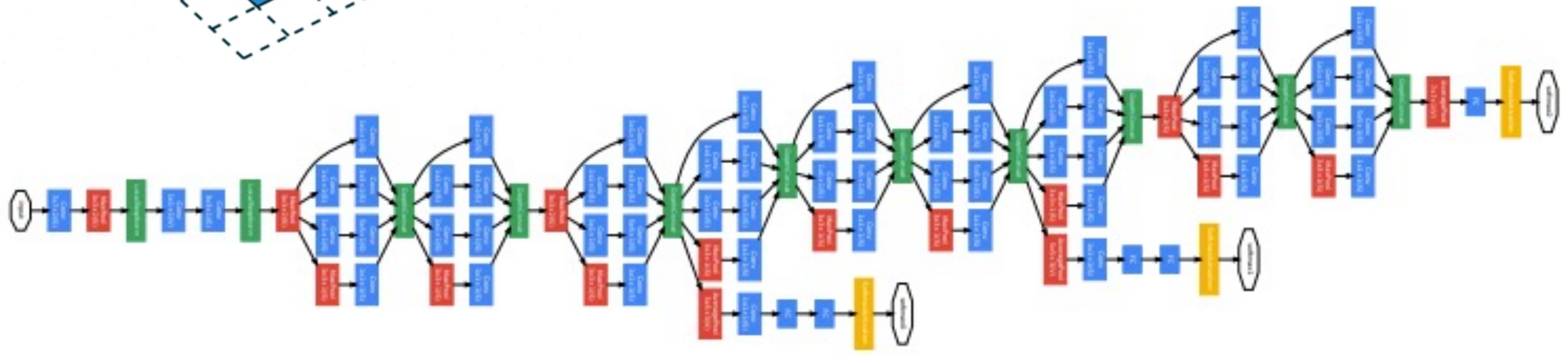
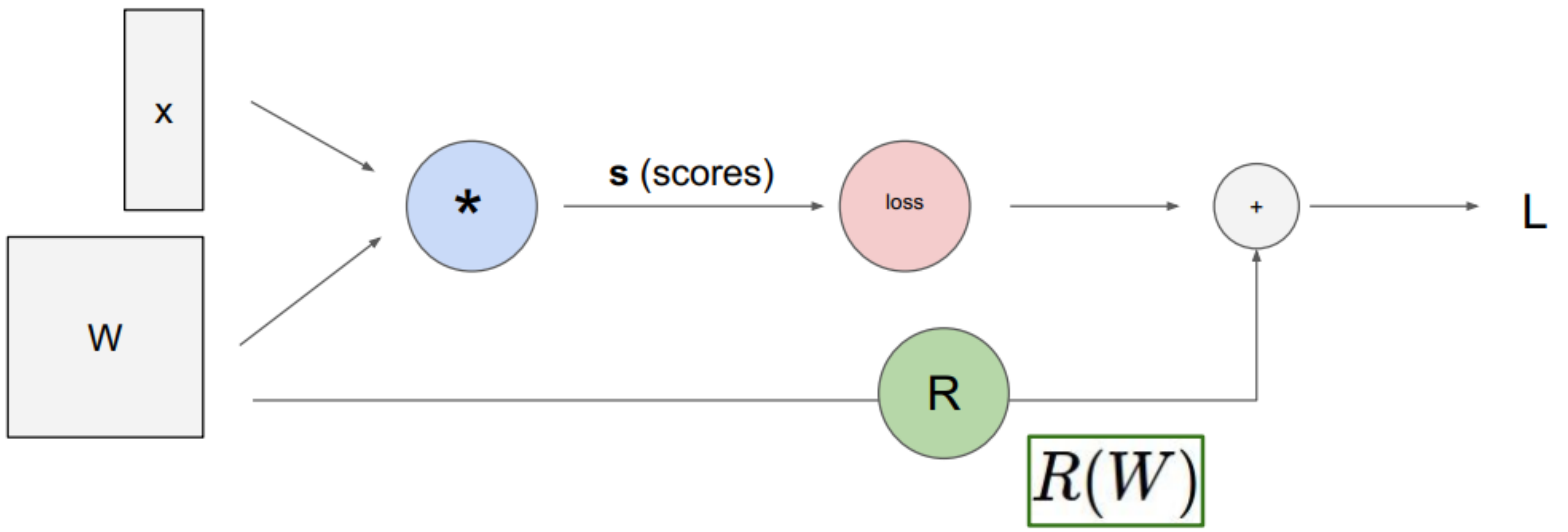
DL model recap



DL compute graph

$$L(\theta) = \frac{1}{N}\sum_{i=1}^{N}\left(-\left(y_i log(\tilde{y}_i) + (1 - y_i) log(1 - \tilde{y}_i)\right)\right) + \|\theta\|_2$$



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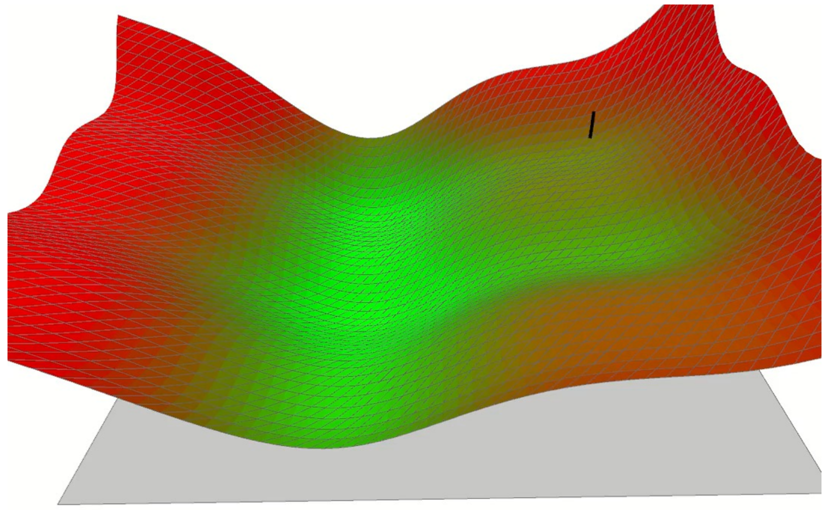
Gradient descent – update rule

A common sense tells us to repetitively take a small step in the most downhill direction until a bottom is reached.

That is precisely what we do! The **most downhill direction is defined as the negative** of the loss function's **gradient**.



Gradient descent – update rule

More formally

at the layer l any parameter i is updated at step s like so:

- Weights: $$w_{l,i}^{s+1} = w_{l,i}^{s} - r \cdot g_{l,i}^{s}$$
- Biases: $$b_{l,i}^{s+1} = b_{l,i}^{s} - r \cdot g_{l,i}^{s}$$

Generally, the same holds for any parameter θ:

$$\theta_{l,i}^{s+1} = \theta_{l,i}^{s} - \overset{\text{step size}}{r} \cdot \underset{\text{gradient}}{g_{l,i}^{s}}$$

GD, SGD & mini-batches

1. **Gradient Descent (GD):** *Exact Gradients*
   - Use all training set examples to compute the true gradient.
   - Very slow and very memory intensive.
2. **Stochastic GD (SGD):** *Approximate Gradients*
   - Use only one example to compute the true gradient.
   - Very imprecise, but fast.
3. **Mini-batched SGD (SGD):** *Mini-batch gradients*
   - Middle ground – use N uniformly sampled examples.
   - Can be sped up significantly through parallelization – so not much faster than approximate gradient methods.
   - Much more stable and much better converging than approximate gradient methods.

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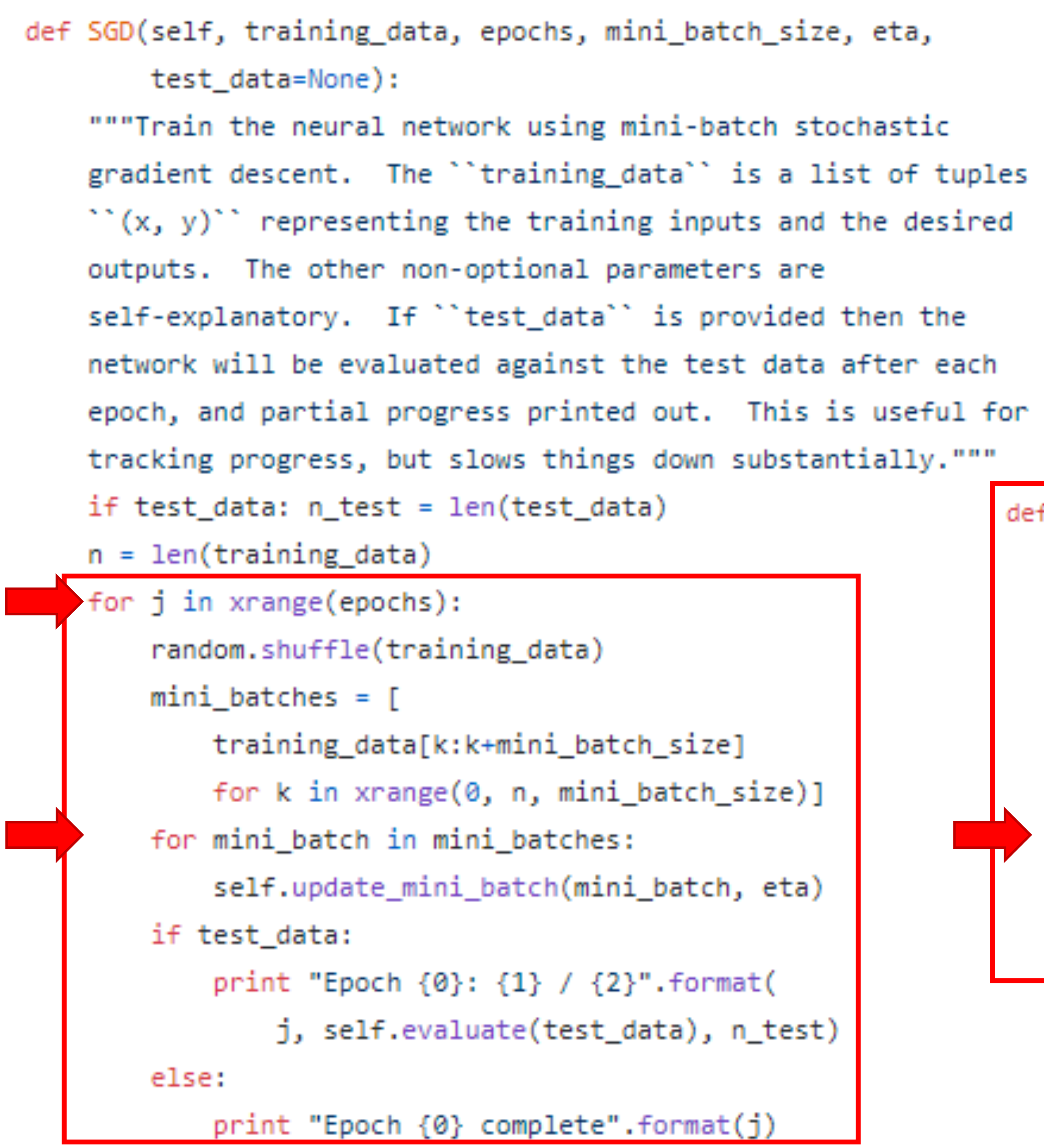
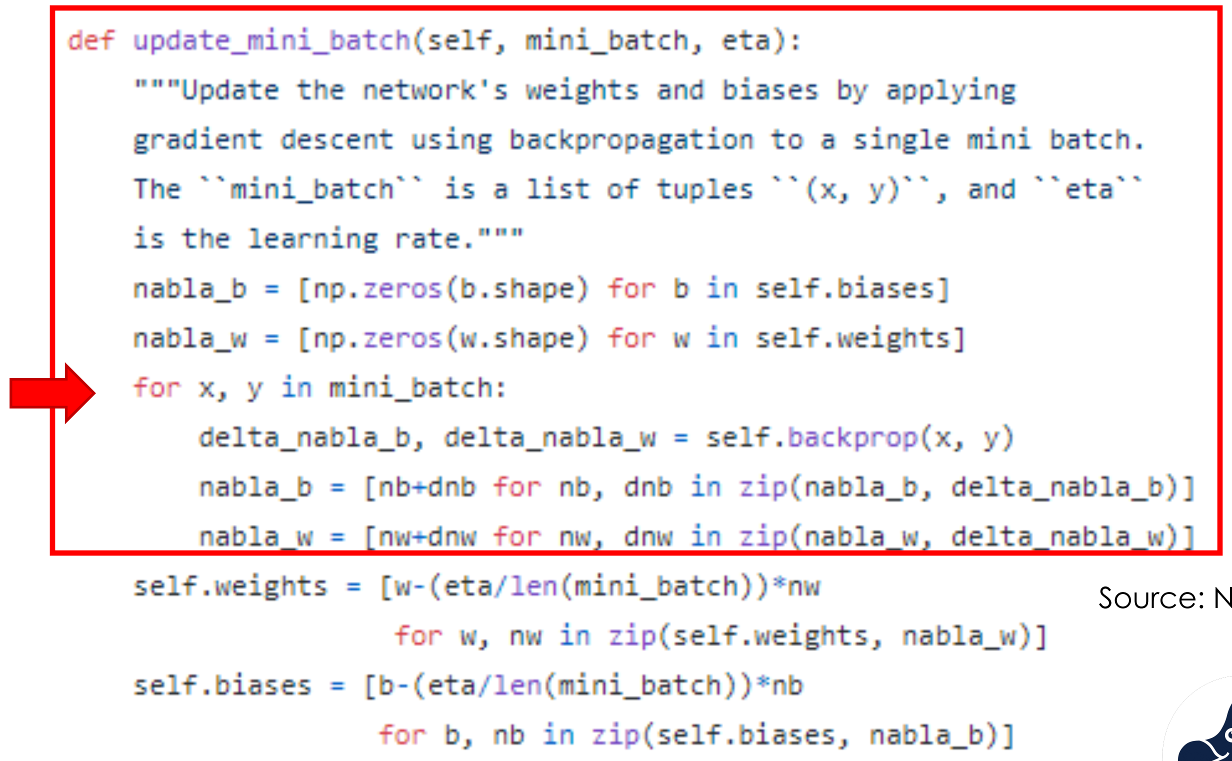
NumPy: training loop



```
def SGD(self, training_data, epochs, mini_batch_size, eta,
        test_data=None):
    """Train the neural network using mini-batch stochastic
    gradient descent.  The ``training_data`` is a list of tuples
    ``(x, y)`` representing the training inputs and the desired
    outputs.  The other non-optional parameters are
    self-explanatory.  If ``test_data`` is provided then the
    network will be evaluated against the test data after each
    epoch, and partial progress printed out.  This is useful for
    tracking progress, but slows things down substantially."""
    if test_data: n_test = len(test_data)
    n = len(training_data)
    for j in xrange(epochs):
        random.shuffle(training_data)
        mini_batches = [
            training_data[k:k+mini_batch_size]
            for k in xrange(0, n, mini_batch_size)]
        for mini_batch in mini_batches:
            self.update_mini_batch(mini_batch, eta)
        if test_data:
            print "Epoch {0}: {1} / {2}".format(
                j, self.evaluate(test_data), n_test)
        else:
            print "Epoch {0} complete".format(j)
```



```
def update_mini_batch(self, mini_batch, eta):
    """Update the network's weights and biases by applying
    gradient descent using backpropagation to a single mini batch.
    The ``mini_batch`` is a list of tuples ``(x, y)``, and ``eta``
    is the learning rate."""
    nabla_b = [np.zeros(b.shape) for b in self.biases]
    nabla_w = [np.zeros(w.shape) for w in self.weights]
    for x, y in mini_batch:
        delta_nabla_b, delta_nabla_w = self.backprop(x, y)
        nabla_b = [nb+dnb for nb, dnb in zip(nabla_b, delta_nabla_b)]
        nabla_w = [nw+dnw for nw, dnw in zip(nabla_w, delta_nabla_w)]
    self.weights = [w-(eta/len(mini_batch))*nw
                    for w, nw in zip(self.weights, nabla_w)]
    self.biases = [b-(eta/len(mini_batch))*nb
                   for b, nb in zip(self.biases, nabla_b)]
```

Source: Nielsen

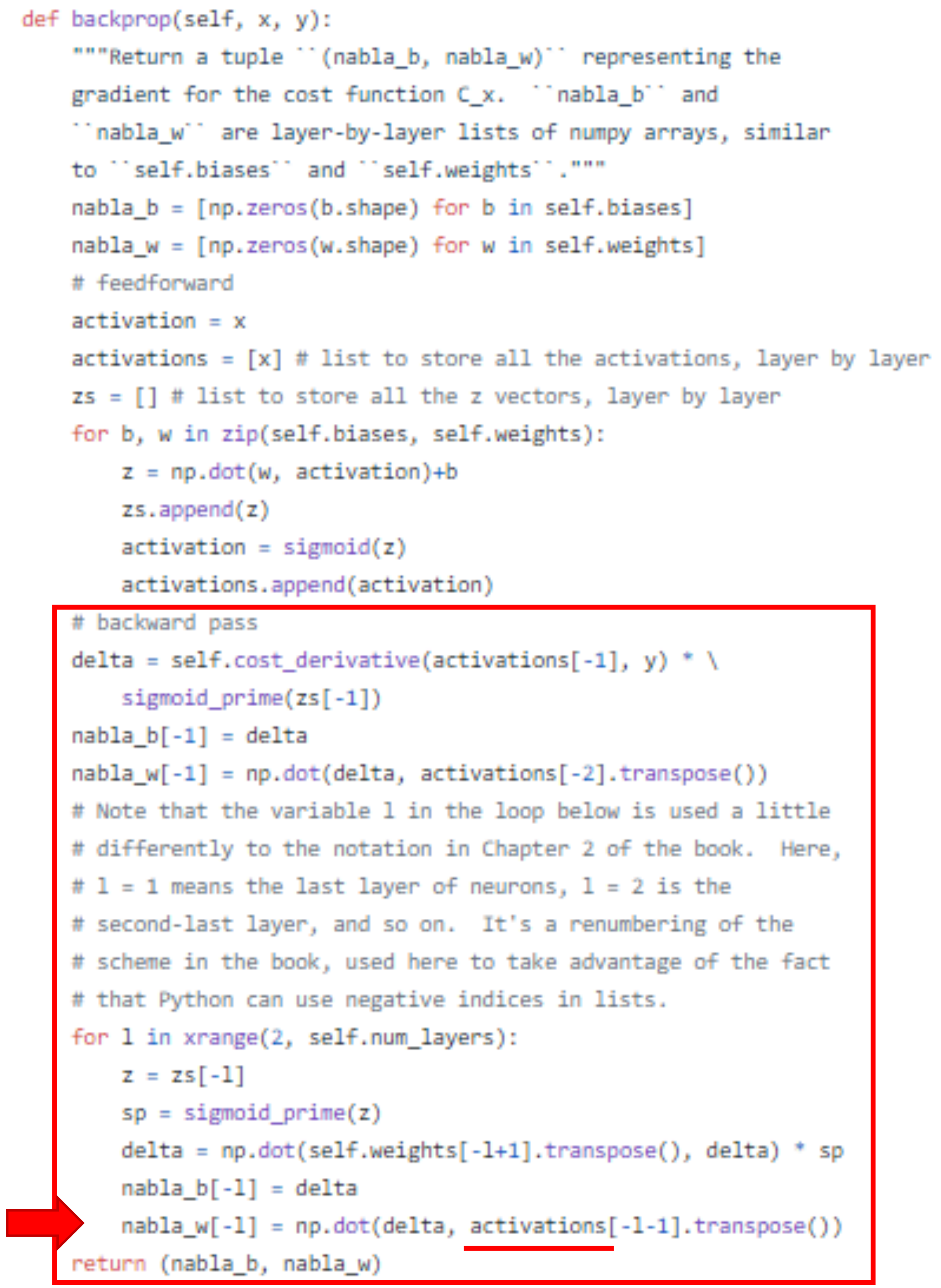
https://github.com/mnielsen/neural-networks-and-deep-learning/blob/master/src/network.py

NumPy: FC forward

```
def backprop(self, x, y):
    """Return a tuple ``(nabla_b, nabla_w)`` representing the
    gradient for the cost function C_x.  ``nabla_b`` and
    ``nabla_w`` are layer-by-layer lists of numpy arrays, similar
    to ``self.biases`` and ``self.weights``."""
    nabla_b = [np.zeros(b.shape) for b in self.biases]
    nabla_w = [np.zeros(w.shape) for w in self.weights]
    # feedforward
    activation = x
    activations = [x] # list to store all the activations, layer by layer
    zs = [] # list to store all the z vectors, layer by layer
    for b, w in zip(self.biases, self.weights):
        z = np.dot(w, activation)+b
        zs.append(z)
        activation = sigmoid(z)
        activations.append(activation)
    # backward pass
```

Source: Nielsen

NumPy: FC backward



```python
def backprop(self, x, y):
    """Return a tuple ``(nabla_b, nabla_w)`` representing the
    gradient for the cost function C_x.  ``nabla_b`` and
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    # feedforward
    activation = x
    activations = [x] # list to store all the activations, layer by layer
    zs = [] # list to store all the z vectors, layer by layer
    for b, w in zip(self.biases, self.weights):
        z = np.dot(w, activation)+b
        zs.append(z)
        activation = sigmoid(z)
        activations.append(activation)
    # backward pass
    delta = self.cost_derivative(activations[-1], y) * \
        sigmoid_prime(zs[-1])
    nabla_b[-1] = delta
    nabla_w[-1] = np.dot(delta, activations[-2].transpose())
    # Note that the variable l in the loop below is used a little
    # differently to the notation in Chapter 2 of the book.  Here,
    # l = 1 means the last layer of neurons, l = 2 is the
    # second-last layer, and so on.  It's a renumbering of the
    # scheme in the book, used here to take advantage of the fact
    # that Python can use negative indices in lists.
    for l in xrange(2, self.num_layers):
        z = zs[-l]
        sp = sigmoid_prime(z)
        delta = np.dot(self.weights[-l+1].transpose(), delta) * sp
        nabla_b[-l] = delta
        nabla_w[-l] = np.dot(delta, activations[-l-1].transpose())
    return (nabla_b, nabla_w)
```

Source: Nielsen

NumPy: FC updates

```python
def SGD(self, training_data, epochs, mini_batch_size, eta,
        test_data=None):
    """Train the neural network using mini-batch stochastic
    gradient descent.  The ``training_data`` is a list of tuples
    ``(x, y)`` representing the training inputs and the desired
    outputs.  The other non-optional parameters are
    self-explanatory.  If ``test_data`` is provided then the
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    tracking progress, but slows things down substantially."""
    if test_data: n_test = len(test_data)
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        mini_batches = [
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        if test_data:
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        else:
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```python
def update_mini_batch(self, mini_batch, eta):
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        nabla_b = [nb+dnb for nb, dnb in zip(nabla_b, delta_nabla_b)]
        nabla_w = [nw+dnw for nw, dnw in zip(nabla_w, delta_nabla_w)]
    self.weights = [w-(eta/len(mini_batch))*nw
                    for w, nw in zip(self.weights, nabla_w)]
    self.biases = [b-(eta/len(mini_batch))*nb
                   for b, nb in zip(self.biases, nabla_b)]
```

Source: Nielsen

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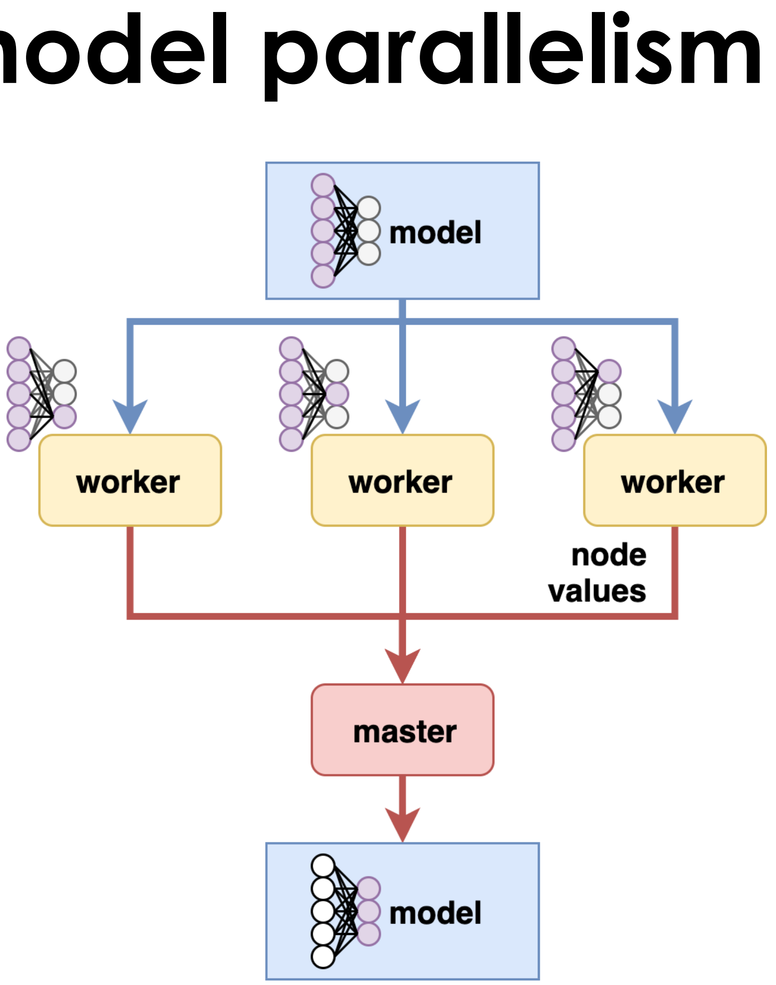
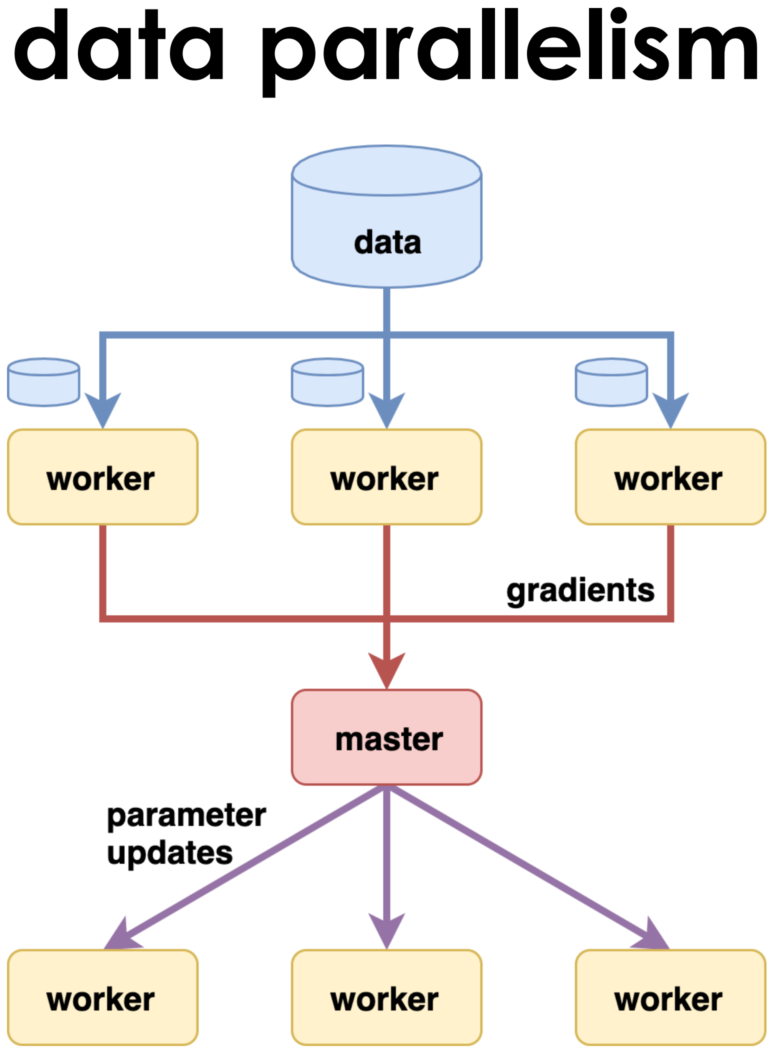
Types of parallelism





SGD sources of data parallelism

Minibatch model update:

$$\theta_{l,i}^{s+1} = \theta_{l,i}^{s} - \frac{r}{B}\sum_{b=1}^{B} g_{l,i,b}^{s}$$

where,$\theta_{l,i}^{s}$ is a parameter i of a layer l at step s in the training process, r is the learning rate, B is the batch size, and $g_{l,i,b}^{s}$ is the gradient of a parameter i of a layer l at step s coming from example b of the mini-batch of size B.

SGD sources of data parallelism

Parallelize gradient samples:

$$\theta_{l,i}^{s+1} = \theta_{l,i}^{s} - \frac{r}{B} \sum_{b=1}^{B} \boxed{g_{l,i,b}^{s}}$$

Matrix multiplications in the computation of the example-level gradient samples can be parallelized.

SGD sources of data parallelism

Parallelize minibatch sum:

$$\theta_{l,i}^{s+1} = \theta_{l,i}^{s} - \frac{r}{B}\boxed{\sum_{b=1}^{B} g_{l,i,b}^{s}}$$

The individual example-level gradient estimates can be parallelized before they are averaged and applied in the model update.

SGD sources of data parallelism

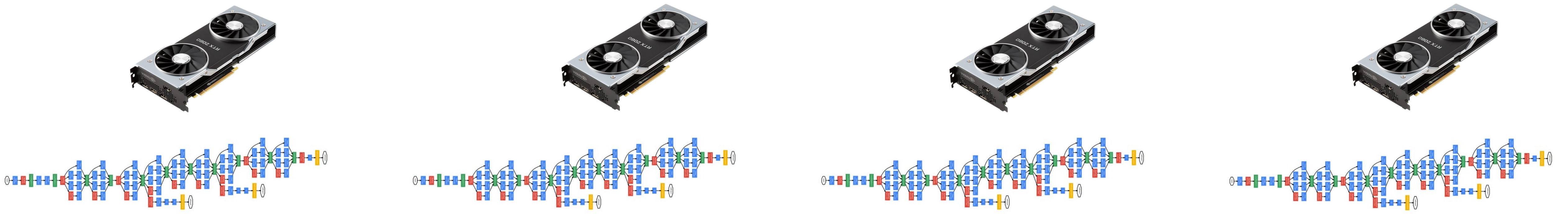
Parallelize multiple iterations of the update:

$$\theta_{l,i}^{s+1} = \theta_{l,i}^{s} - \boxed{\frac{r}{B}\sum_{b=1}^{B} g_{l,i,b}^{s}}$$

Separate model updates can be initialized and computed in parallel.

SGD sources of data parallelism

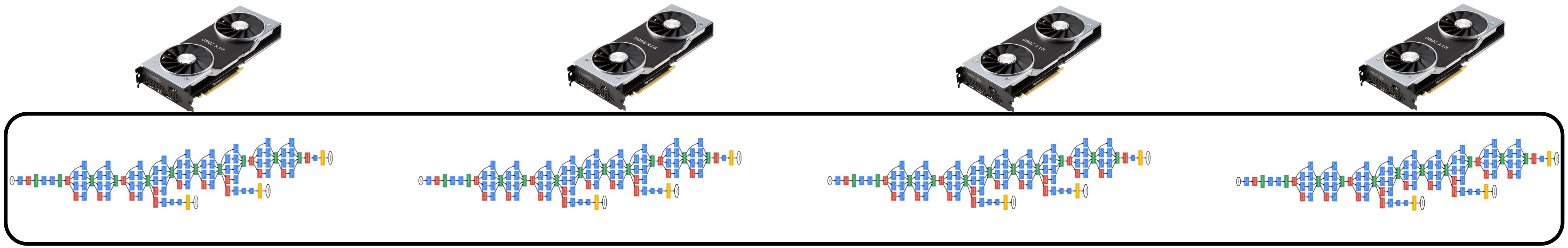
Parallelize hyperparameter optimization (model):



The search of hyperparameter search can, and should, be distributed between separate workers whenever possible.

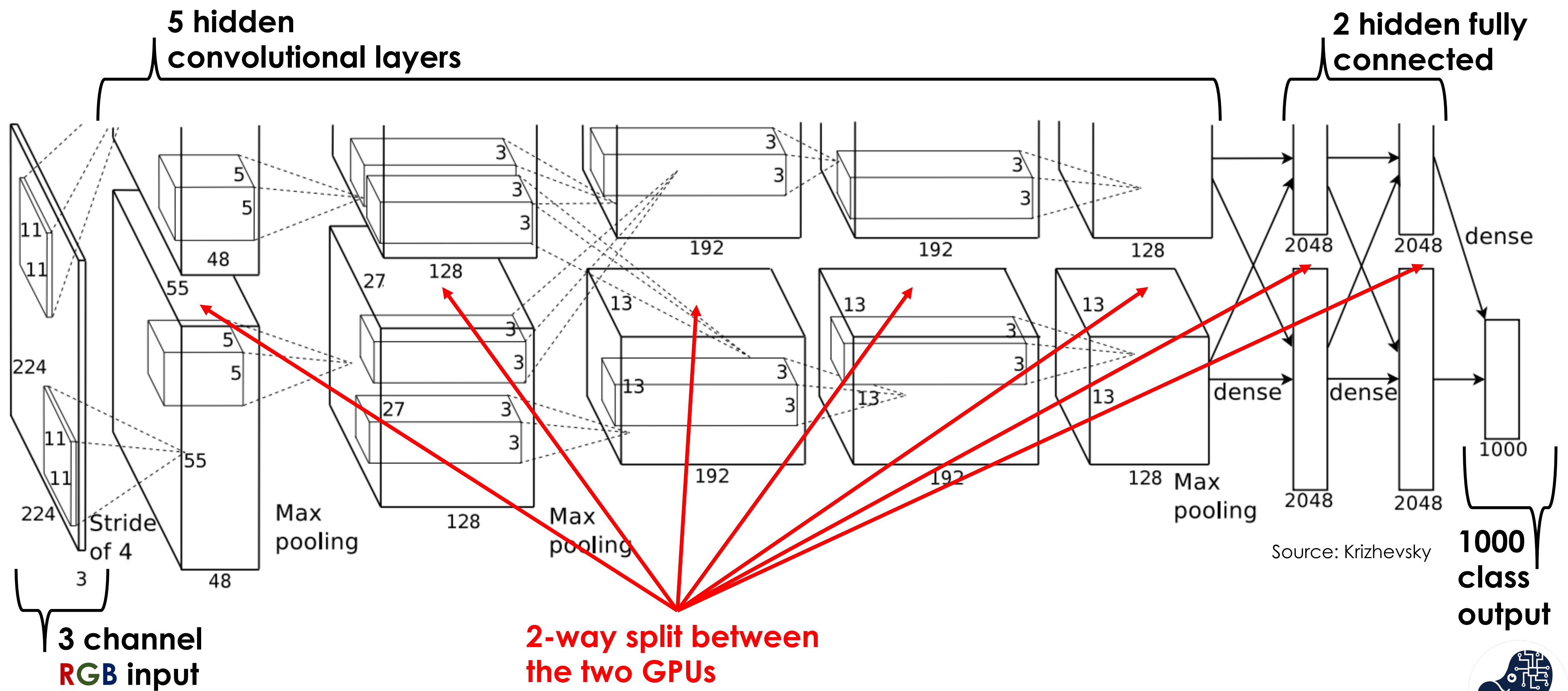
SGD sources of data parallelism

Parallelize ensembles (model):



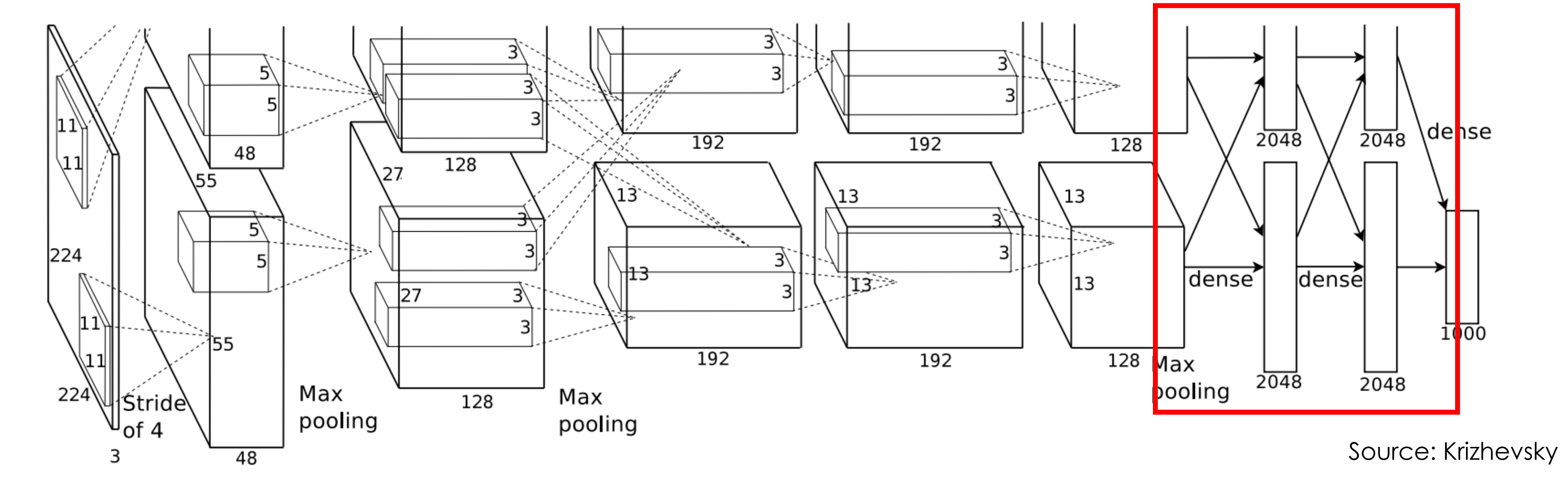
Ensembles are collections of independently trained DL models that vote on a joint output. Both the training and the inference can be significantly sped up by parallelizing.

AlexNet on GPU



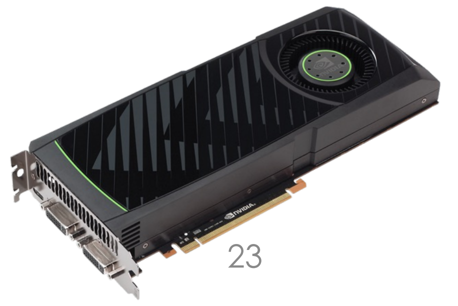
Source: Krizhevsky

AlexNet on GPU so why the split?



Source: Krizhevsky

- The **4096 neuron long layers** alone account for almost **1GB** of parameters needed to be stored in memory. This is before the storage of activations is accounted for.
- The authors chose to split the network between two **GTX 580 GPUs which have 3GB** device memory each.



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arXiv:1904.10631v1 [cs.LG] 24 Apr 2019

Low-Memory Neural Network Training:
A Technical Report

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April 25, 2019

Abstract

Memory is increasingly often the bottleneck when training neural network models. Despite this, techniques to lower the overall memory requirements of training have been less widely studied compared to the extensive literature on reducing the memory requirements of inference. In this paper we study a fundamental question: *How much memory is actually needed to train a neural network?* To answer this question, we profile the overall memory usage of training on two representative deep learning benchmarks — the WideResNet model for image classification and the DynamicConv Transformer model for machine translation — and comprehensively evaluate four standard techniques for reducing the training memory requirements: (1) imposing sparsity on the model, (2) using low precision, (3) microbatching, and (4) gradient checkpointing. We explore how each of these techniques in isolation affects both the peak memory usage of training and the quality of the end model, and explore the memory, accuracy, and computation tradeoffs incurred when combining these techniques. Using appropriate combinations of these techniques, we show that it is possible to the reduce the memory required to train a WideResNet-28-2 on CIFAR-10 by up to 60.7x with a 0.4% loss in accuracy, and reduce the memory required to train a DynamicConv model on IWSLT'14 German to English translation by up to 8.7x with a BLEU score drop of 0.15.

1 Introduction

Recently, there has been an explosion of interest around techniques to reduce the memory requirements of neural network inference [Han et al., 2016a, Zhu and Gupta, 2017]. A central driver for this work is the fact that deep neural networks are notoriously parameter-hungry, typically containing several millions or even billions of parameters [Radford et al., 2019], making memory a significant hardware bottleneck for even storing and evaluating these models. Unfortunately, *training* is inherently more memory-intensive than inference (often by orders of magnitude), because it requires the storage of much more than just the network itself. However, the majority of state-of-the-art techniques to reduce inference memory are inapplicable to reducing training memory, as they often require first training a full-size model that is later compressed. As a result, training still requires

1

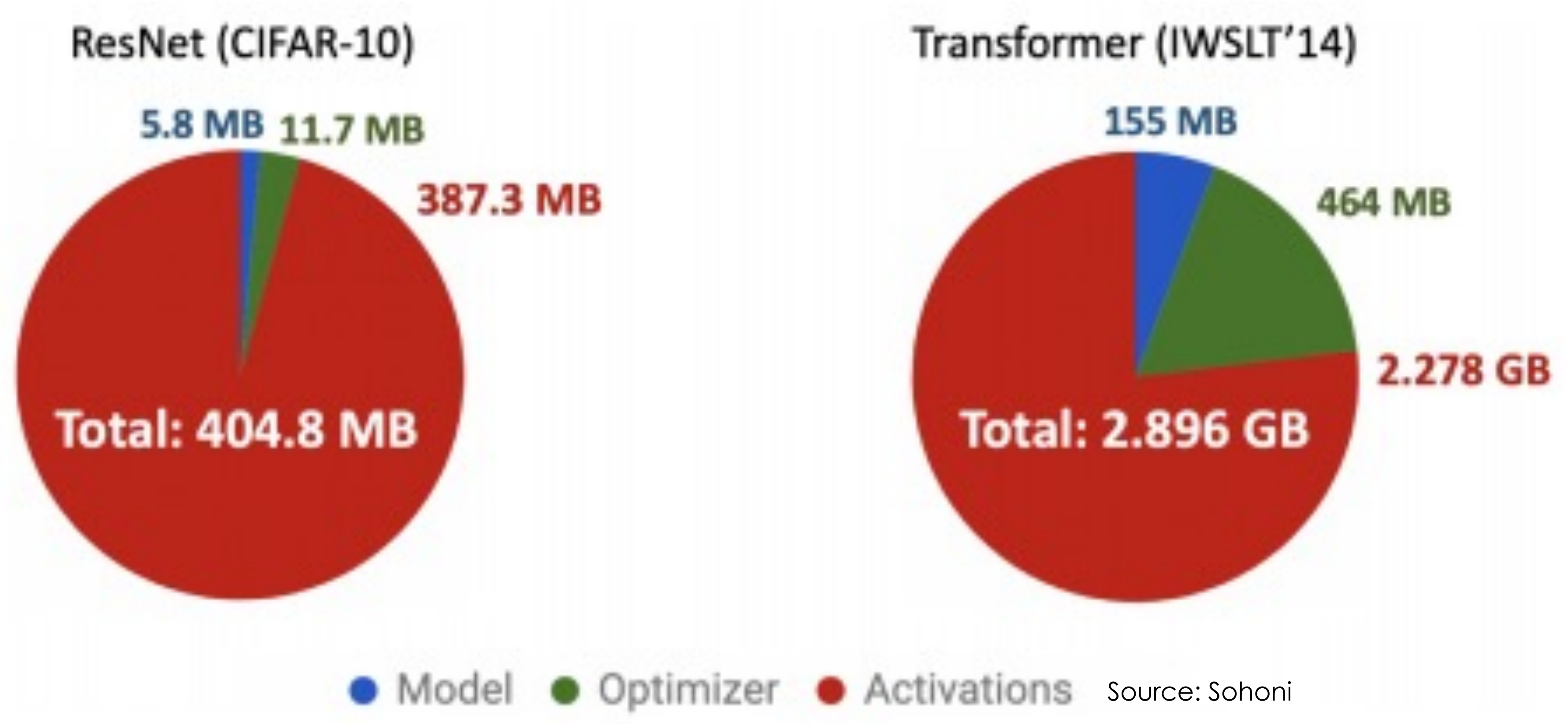
Types of memory

1. **Model Memory** stores the model parameters, i.e. the weights and biases of each layer in the network.

2. **Optimizer Memory** stores the gradients and any momentum buffers during training. For instance, standard SGD with momentum saves one momentum value corresponding to each weight in the model.

3. **Activation Memory** stores the activations of each layer in the network – that is the outputs of each layer in the net.

Profiling



Source: Sohoni

Figure 1: Pie charts of training memory consumption for (a) WideResNet on CIFAR-10 [left] and (b) DC-Transformer on IWSLT'14 German to English [right].

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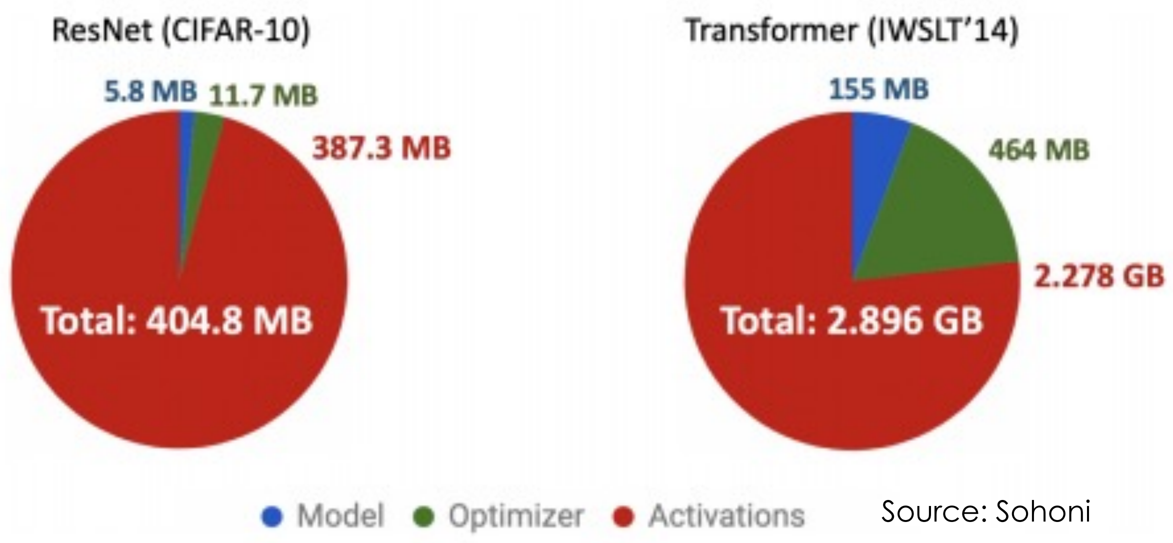
Overview

- Sparse training – Model & **Activations memory**
- Quantization – Model & **Activations memory**
- Microbatching – **Activations memory**
- Gradient checkpointing – **Activations memory**



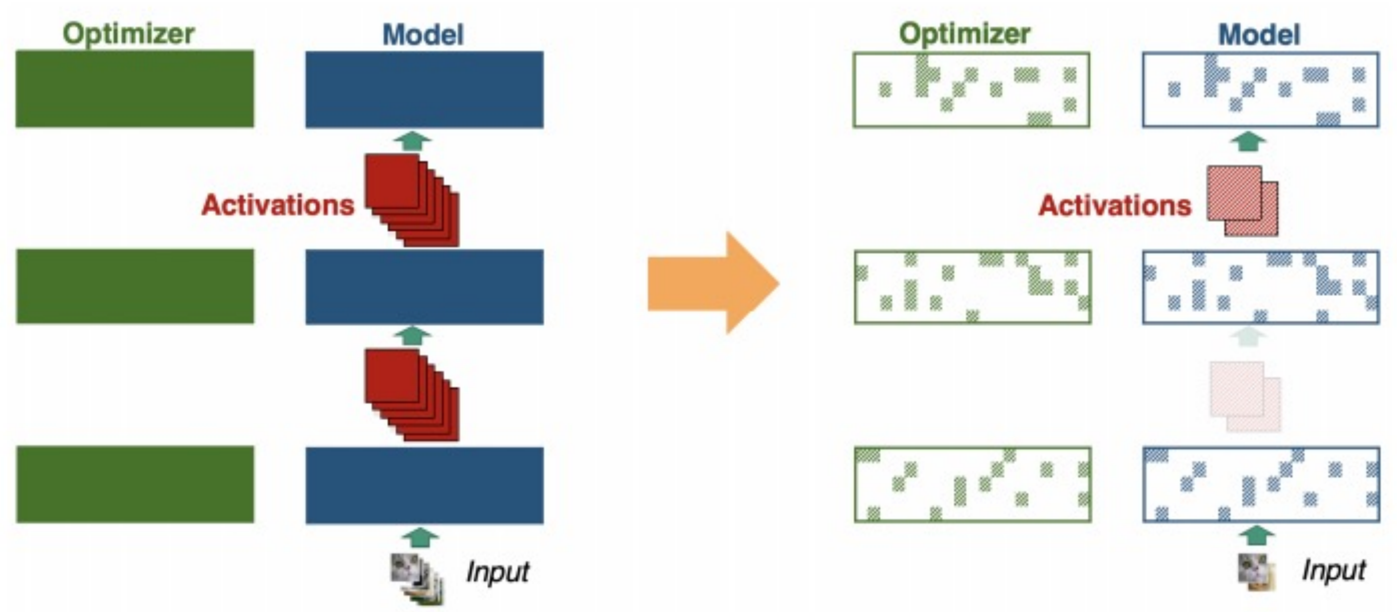
Source: Sohoni

Sparse training

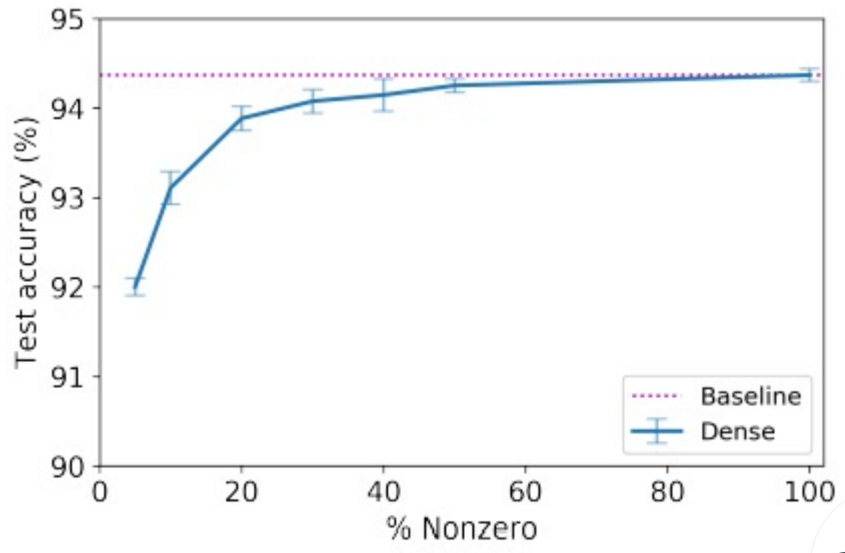
Dynamic Sparse Reparameterization

1. initializes the network with a fixed sparsity pattern,
2. during training the smallest-magnitude weights are pruned
3. same number of nonzeros are introduced back in the net

$\left.\begin{array}{l} 2. \\ 3. \end{array}\right\}$ rewiring



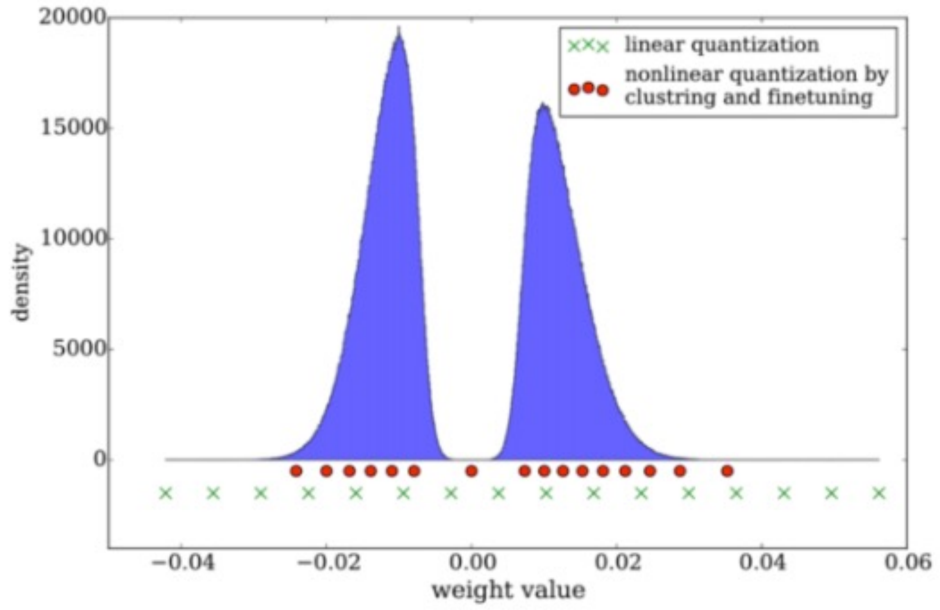
Source: Mostafa



Quantization (recap)

Quantized training

1. keep weights (and activations) in low precision numerical formats
2. perform updates in full precision (usually single precision float32)
3. quantize before next forward pass: stochastic rounding



Source: Han

Microbatching

Minibatch size directly translates one-to-one to activations size.

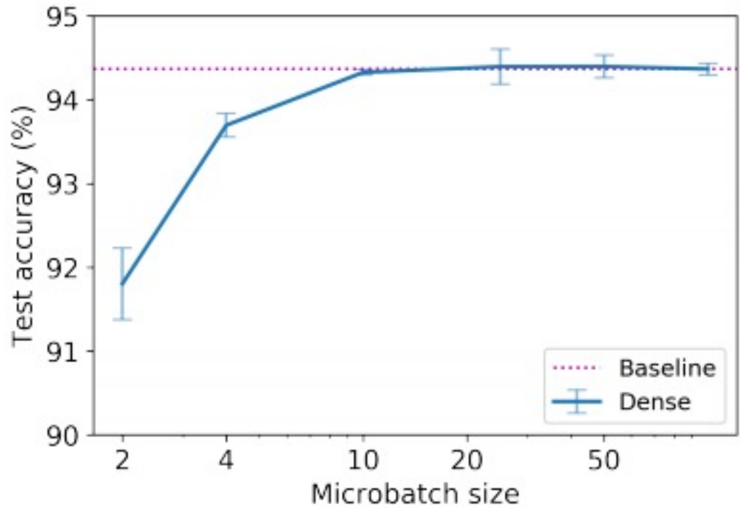


Figure 4: Test accuracy vs. microbatch size, for WRN-28-2 on CIFAR-10. Vertical lines denote 95% confidence intervals. Dotted line is the baseline with a single microbatch, i.e. same minibatch and microbatch size of 100.

Source: Sohoni

Sparse, Quant., Microbatching eval.

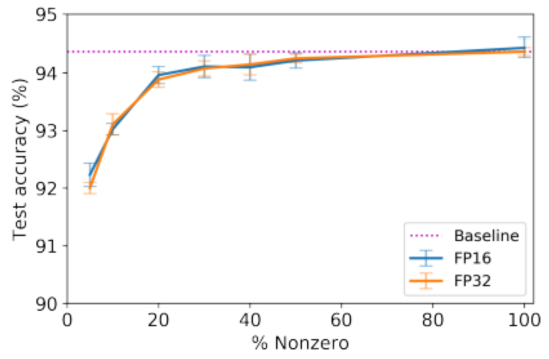


Figure 6: Plot of test accuracy vs. sparsity for WRN-28-2 on CIFAR-10, for FP16 and FP32. The lines align extremely closely with one another, meaning that half precision does not significantly affect the accuracy.

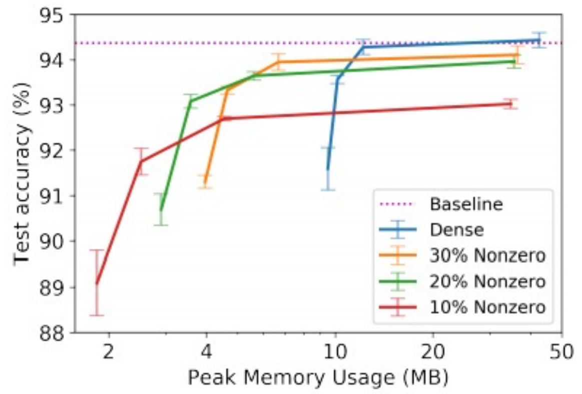


Figure 7: Plot of test accuracy vs. training memory usage for WRN-28-2 on CIFAR-10. Each curve represents a different sparsity level, while different points on a given curve represent different microbatch sizes (100, 10, 4, and 2). All settings use FP16 and CHECKPOINT-RESIDUAL-2*.

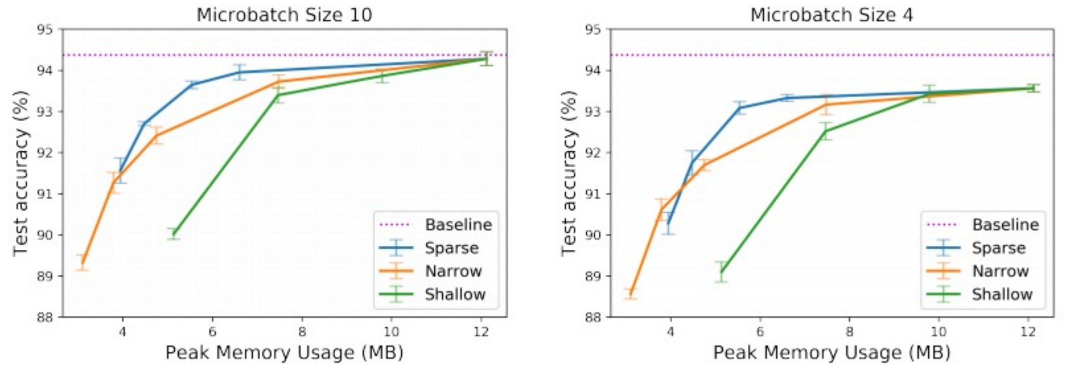


Figure 8: Plot of test accuracy vs. training memory usage for WideResNet on CIFAR-10, when using a microbatch size of 10 (left) or 4 (right). The three curves in each plot are generated by varying the number of layers ("shallow"), the width of the layers ("narrow"), or the sparsity level of the layers ("sparse"). All settings use FP16 and CHECKPOINT-RESIDUAL-2*.

Nonzero %	Microbatch Size	Memory	Mem. Reduction	Test Acc.
100	100	404.8 MB	-	94.37 ± 0.07
100	100	42.6 MB	9.5x	94.43 ± 0.17
100	10	12.2 MB	33.2x	94.28 ± 0.17
30	10	6.7 MB	60.7x	93.95 ± 0.18
20	10	5.6 MB	72.2x	93.64 ± 0.09
20	4	3.6 MB	113.0x	93.08 ± 0.15
10	4	2.5 MB	160.8x	91.75 ± 0.29

Table 3: Pareto-optimal settings for CIFAR-10 WideResNet training. The baseline, which is dense (100% nonzero) and uses 32-bit precision, a minibatch size of 100, no microbatching, and no checkpointing, is the top row. Memory reduction is computed relative to this baseline. All other settings use 16-bit precision, and CHECKPOINT-RESIDUAL-2*. Accuracies are reported as percentages; accuracies exceeding the standard-length training baseline are bolded. (Note: N % refers to the percentage of nonzeros in convolutions.)

Source: Sohoni

Summary & evaluation

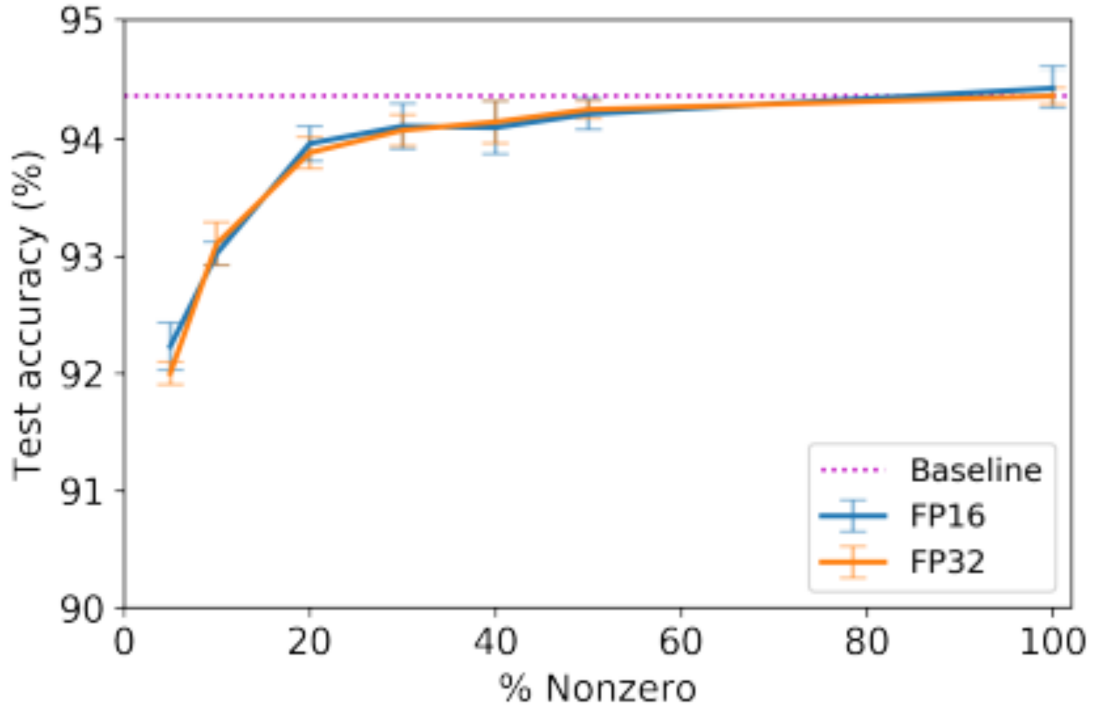


Figure 6: Plot of test accuracy vs. sparsity for WRN-28-2 on CIFAR-10, for FP16 and FP32. The lines align extremely closely with one another, meaning that half precision does not significantly affect the accuracy.

Source: Sohoni

Summary & evaluation

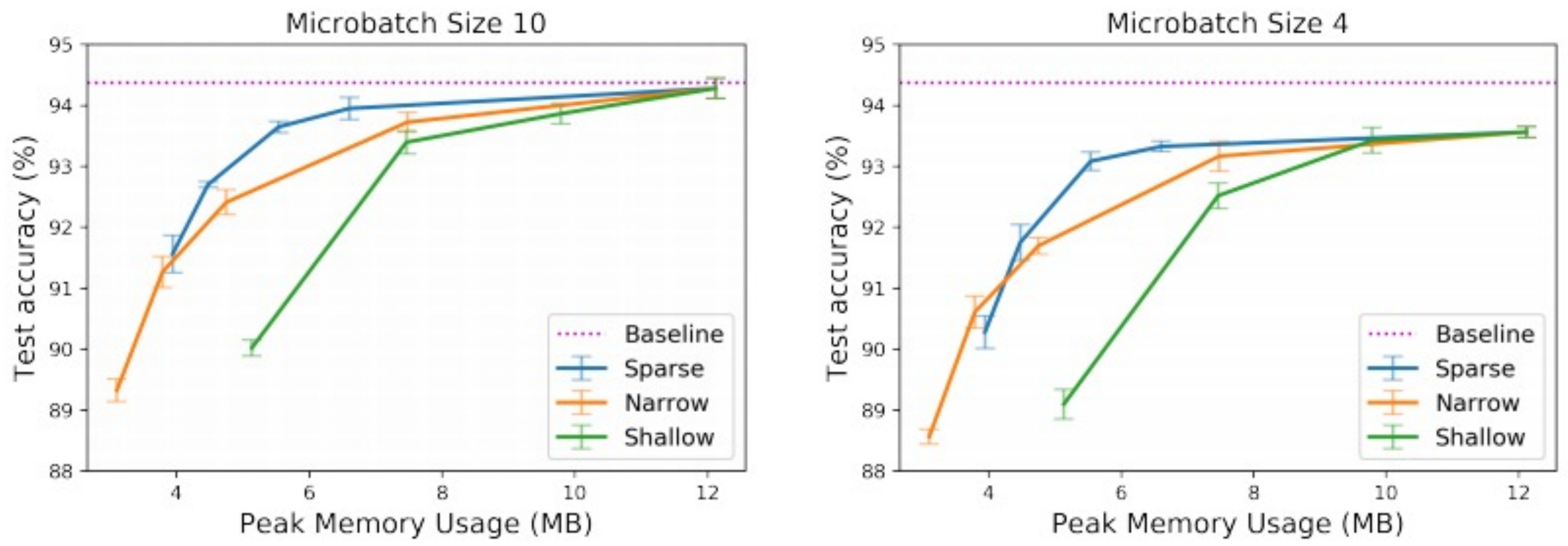


Figure 8: Plot of test accuracy vs. training memory usage for WideResNet on CIFAR-10, when using a microbatch size of 10 (left) or 4 (right). The three curves in each plot are generated by varying the number of layers ("shallow"), the width of the layers ("narrow"), or the sparsity level of the layers ("sparse"). All settings use FP16 and CHECKPOINT-RESIDUAL-2*.

Source: Sohoni

Summary & evaluation

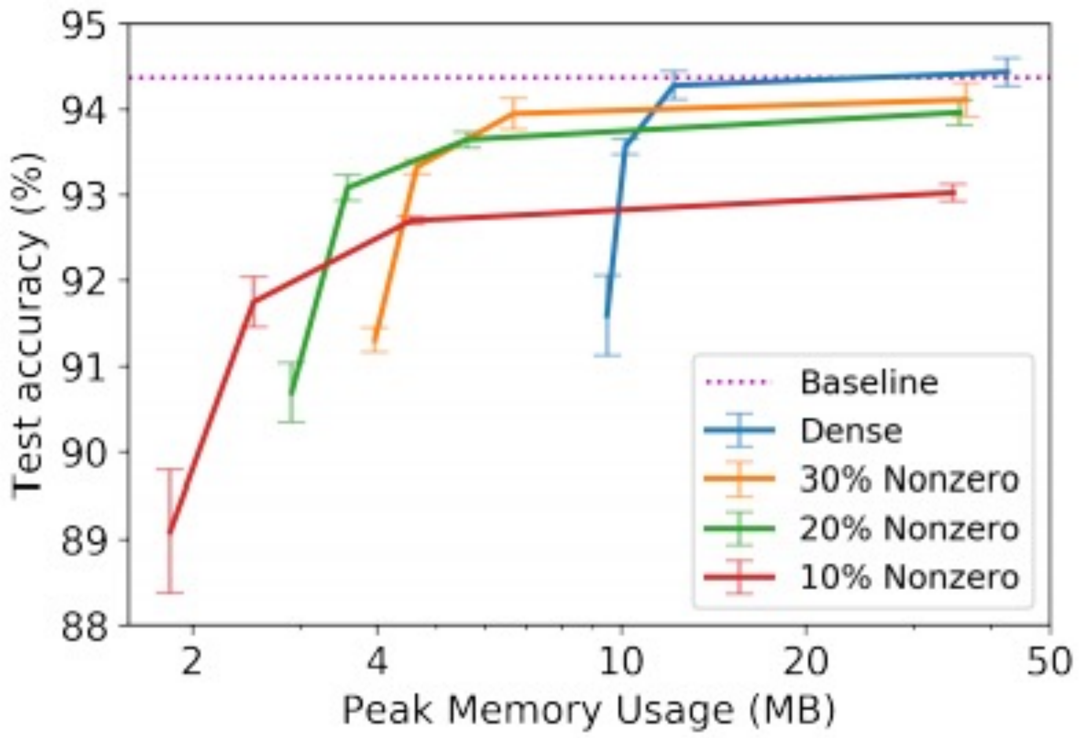
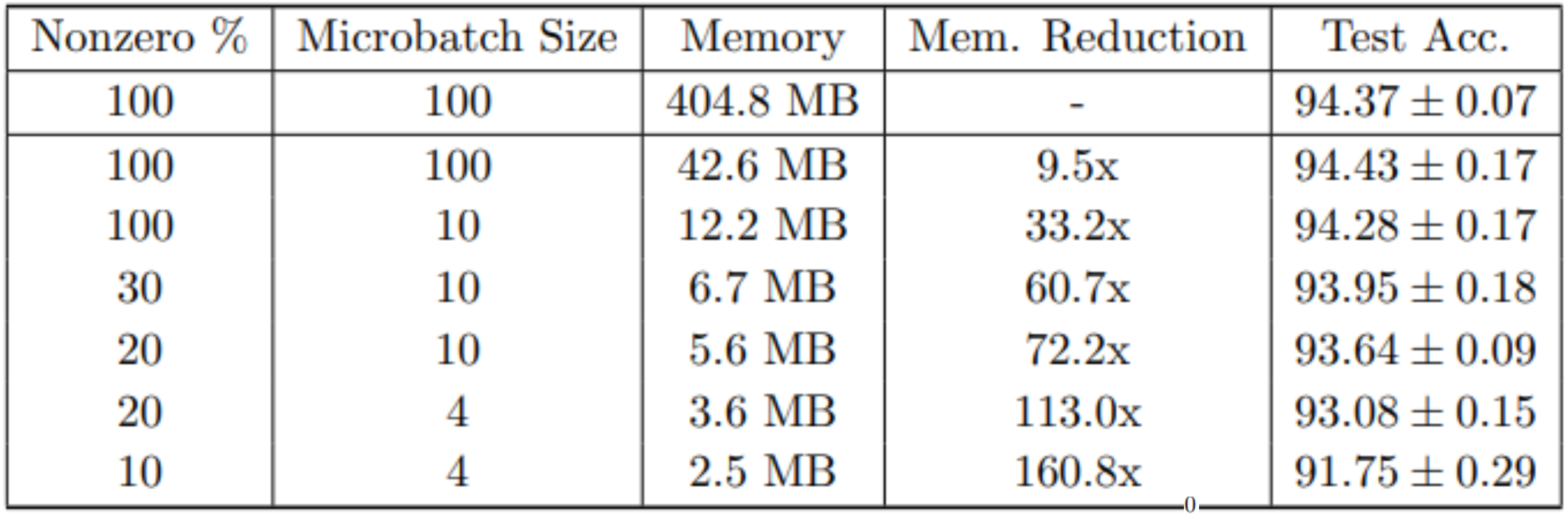


Figure 7: Plot of test accuracy vs. training memory usage for WRN-28-2 on CIFAR-10. Each curve represents a different sparsity level, while different points on a given curve represent different microbatch sizes (100, 10, 4, and 2). All settings use FP16 and CHECKPOINT-RESIDUAL-2*.

Source: Sohoni

Summary & evaluation



Nonzero %	Microbatch Size	Memory	Mem. Reduction	Test Acc.
100	100	404.8 MB	-	94.37 ± 0.07
100	100	42.6 MB	9.5x	94.43 ± 0.17
100	10	12.2 MB	33.2x	94.28 ± 0.17
30	10	6.7 MB	60.7x	93.95 ± 0.18
20	10	5.6 MB	72.2x	93.64 ± 0.09
20	4	3.6 MB	113.0x	93.08 ± 0.15
10	4	2.5 MB	160.8x	91.75 ± 0.29

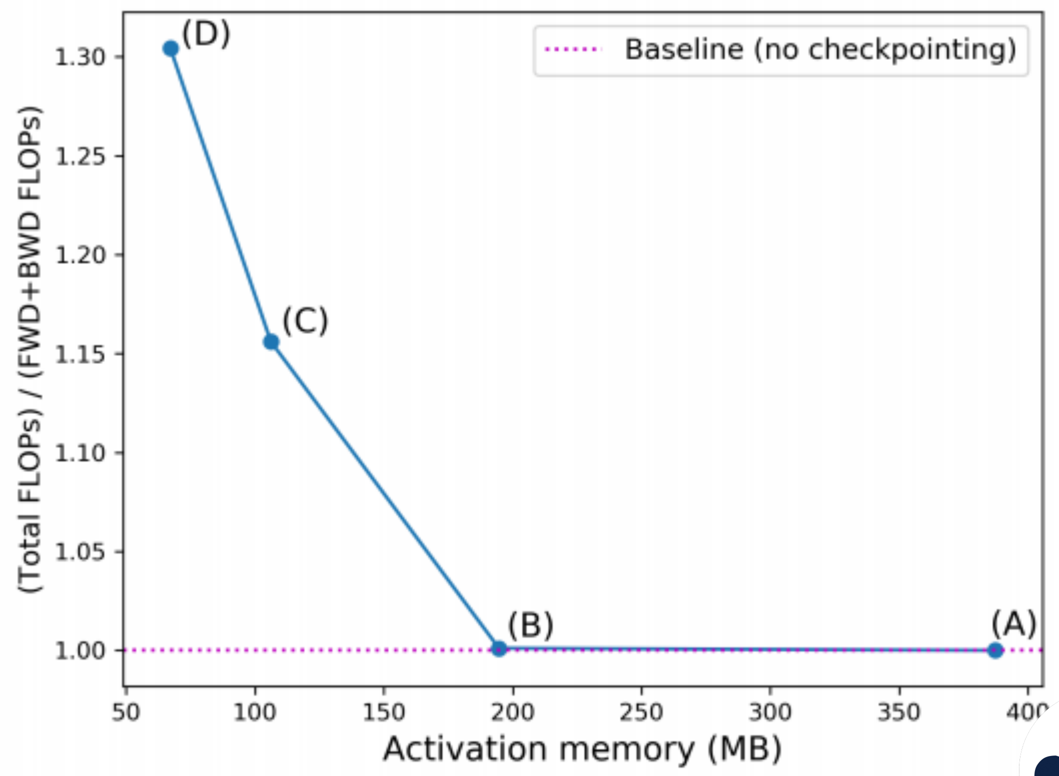
Table 3: Pareto-optimal settings for CIFAR-10 WideResNet training. The baseline, which is dense (100% nonzero) and uses 32-bit precision, a minibatch size of 100, no microbatching, and no checkpointing, is the top row. Memory reduction is computed relative to this baseline. All other settings use 16-bit precision, and CHECKPOINT-RESIDUAL-2*. Accuracies are reported as percentages; accuracies exceeding the standard-length training baseline are bolded. (Note: Nonzero % refers to the percentage of nonzeros in convolutions.)

Source: Sohoni

Gradient checkpointing

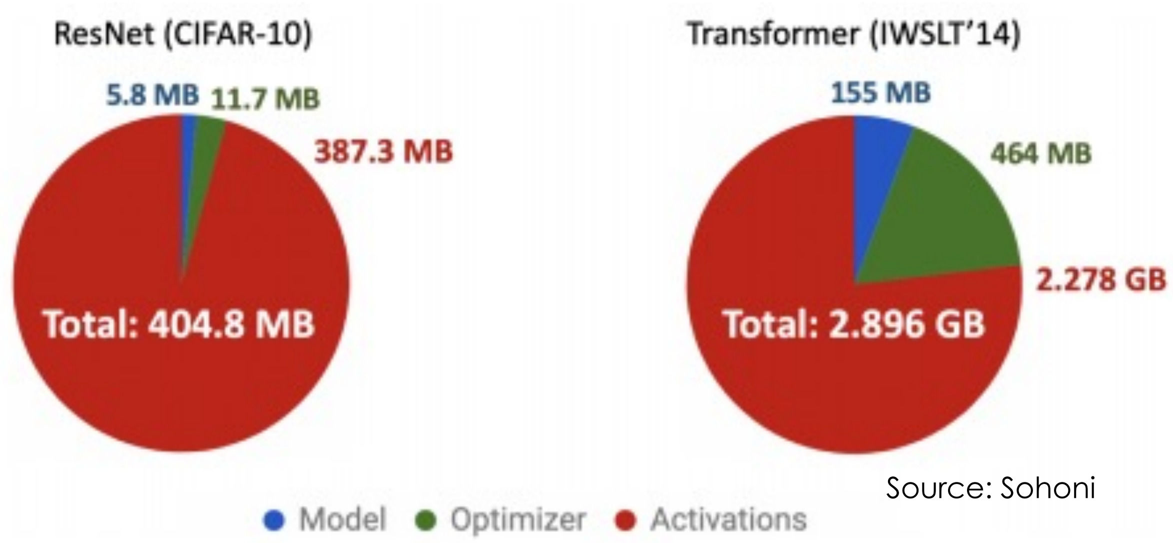
Main idea: *save memory at the cost of re-doing some of the forward passes by only storing a subset of the network activations and recomputing the rest when they are needed.*

- No accuracy trade-off: re-computed and original activations are mathematically and numerically the same!
- Pure trade-off between FLOPs and memory.
- Fig. FLOPs/original FLOPs vs. MB.



Source: Sohoni

Putting it all together



Source: Sohoni

		Sparsity	Low Precision	Microbatching	Checkpointing
Memory	*Model*	↓	↓		
	Optimizer	↓	↓		
	Activations		↓	↓	↓
Computation		↓	↓		↑

Summary of the Day

1. The fundamentals of DL training
    1. DL model as a compute graph
    2. Training algorithm specifics
    3. NumPy implementation
    4. Exploitable parallelism
2. Resource management
    1. Characterising resource requirements
    2. Speed-up strategies