Introduction to Computation Technologies in Deep Learning

Kai Jia

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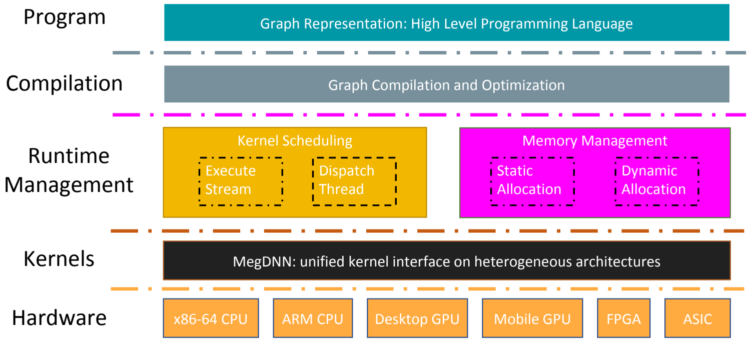
About Me

Name	Kai Jia
Education	OIer => Tsinghua University
Email	`jiakai@megvii.com`
@Megvii	1. First API website (`http://faceplusplus.com`) 2. Face detection: from traditional methods to deep learning (Twice FDDB No.1) 3. Deep learning framework: MegBrain

Overview of a Deep Learning Framework

MegBrain Architecture



Computation Graph

$$y = \mathrm{conv}(x, w) + b$$

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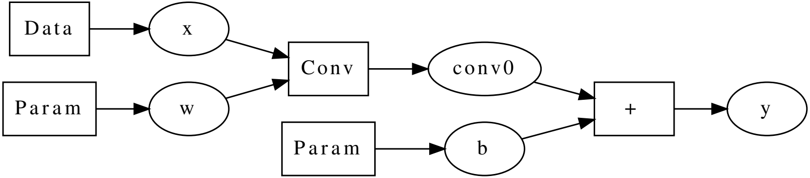


Graph Structure

It is a directed acyclic bipartite graph composed of variables and operators.

Variable

- Corresponding to a tensor[1] during graph execution
- Shape attribute: important for NN design and automatic weight initialization

Example

```
assert x.shape == (128, 50)
y = fully_connected(x, output_dim=100)
assert y.shape == (128, 100)
```

The weight matrix of this `FullyConnected` operator can be initialized to `np.random.normal((50, 100))`.

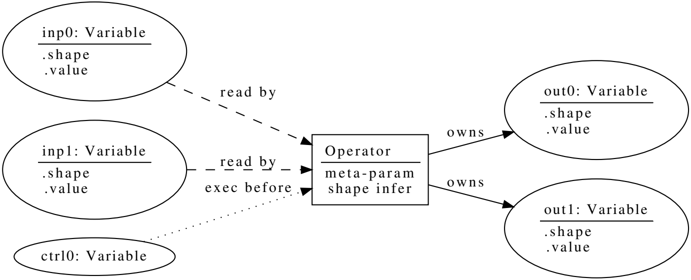
[1] a high-dimensional array

Graph Structure

It is a directed acyclic bipartite graph composed of variables and operators.

Operator
- Connecting multiple input/output variables
- Representing the operation to be applied on input tensors
- Defining shape inference rules
- Carrying meta-parameters: e.g. `stride` and `padding` for `Conv`

Edge
- Data dependency: read input data
- Control dependency: require input operator to have finished



Operator Granularity

An on-going debate: how much should a single operator do?

Category	Example	Advantage	Framework
Coarse-grained	$y = \mathrm{BatchNorm}(x)$	Parsimony; Easy performance tuning	Caffe
Fine-grained	$y = \frac{x - \mathrm{mean}(x)}{\mathrm{std}(x)}$	Flexibility	Theano

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Our philosophy:

- Prefer flexibility: this can not be changed once the framework has been designed
- Utilize multi-level API for simplifying graph representation
- Speed can be continuously improved by graph optimizer

Auto Differentiation

Gradient-based training is a crucial part for deep learning.

Straight-forward approach: each operator provides two methods: `fprop` and `bprop`.

[1] Ishaan Gulrajani et al. "Improved training of wasserstein gans". In: *arXiv preprint arXiv:1704.00028* (2017).

Auto Differentiation

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Limitations

- Graph optimizer can not be uniformly applied on both forward and backward passes
- Difficult to implement gradient of gradient ($\frac{\partial f(\frac{\partial L}{\partial x})}{\partial y}$, in WGAN training [1]) or higher-order gradients ($\frac{\partial^2 L}{\partial x^2}$).
- Difficult to modify/manipulate gradients (e.g. for low-bit training).

[1] Ishaan Gulrajani et al. "Improved training of wasserstein gans". In: *arXiv preprint arXiv:1704.00028* (2017).

Auto Differentiation

Gradient-based training is a crucial part for deep learning.

Unified approach: extending the graph with operators computing gradients of specific variables, via the chain rule.

$$y_1, \cdots, y_m = f(x_1, \cdots, x_n)$$

Gradient operator g for f:

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Gradient operator g for f:

$$\frac{\partial L}{\partial x_1}, \cdots, \frac{\partial L}{\partial x_n} = g\left(\frac{\partial L}{\partial y_1}, \cdots, \frac{\partial L}{\partial y_m}, x_1, \cdots, x_n, y_1, \cdots, y_m\right)$$

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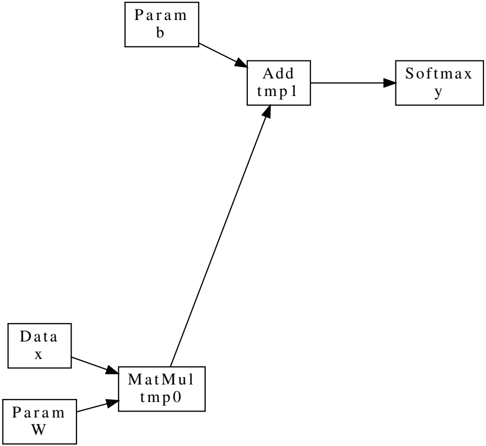

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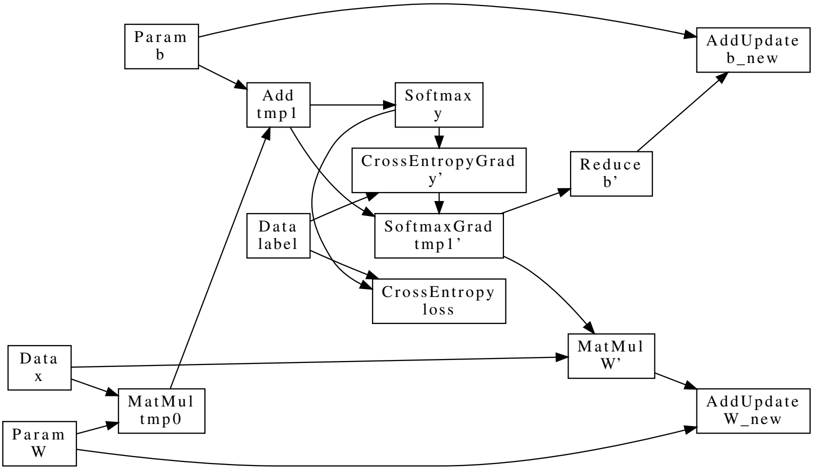
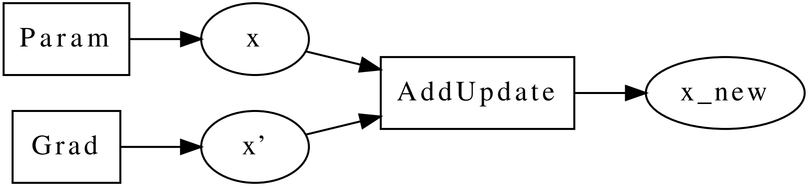


Mutable State

How to express the SGD algorithm within the graph?



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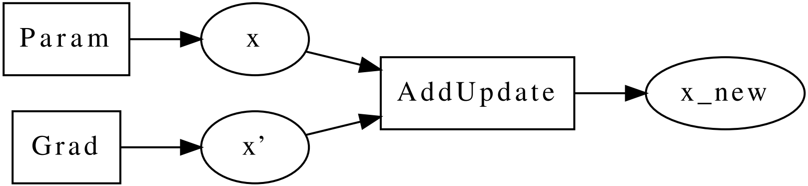

Note

- `x` and `x_new` share the underlying storage and should not be simultaneously read by one operator. Equivalently speaking, `AddUpdate` separates the graph.

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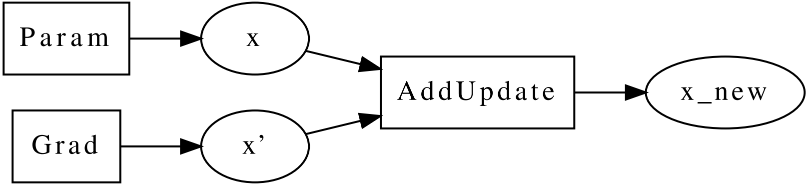


Note

- `x` and `x_new` share the underlying storage and should not be simultaneously read by one operator. Equivalently speaking, `AddUpdate` separates the graph.
- Readers of `x` must have finished (impl. by control dependency)

Symbolic Shape

Shapes of variables can also be involved in the computation

Example

Maxout[1]:

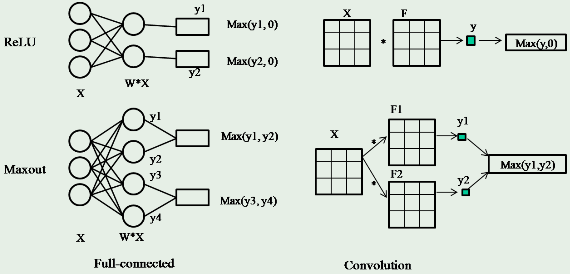


Image from [2]

[2] Hai Dai Nguyen, Anh Duc Le, and Masaki Nakagawa. "Recognition of Online Handwritten Math Symbols Using Deep Neural Networks". In: *IEICE Trans. Inf.& Syst.* 99.12 (2016), pp. 3110–3118.

[1] Ian J Goodfellow et al. "Maxout networks". In: *arXiv preprint*

Symbolic Shape

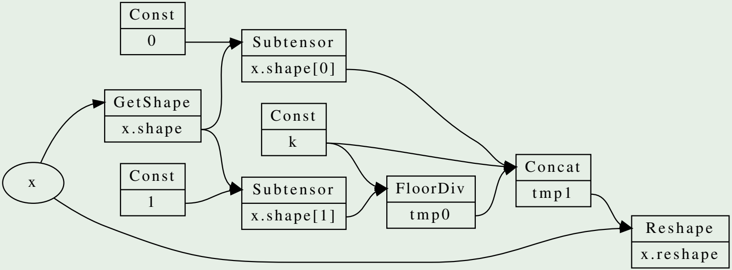
Shapes of variables can also be involved in the computation

Example

Maxout[1]:

```
y = x.reshape(x.shape[0], x.shape[1] // k, k).max(axis=2)
```

where `x.shape` is also a symbol whose value is evaluated at runtime, so the computation adapts to different input shapes.



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Symbolic Shape

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Example

Maxout[1]:

```
y = x.reshape(x.shape[0], x.shape[1] // k, k).max(axis=2)
```

- Helps dealing with non-constant batch size or input image size
- Requires dynamic shape support: some shapes may remain unknown until graph execution

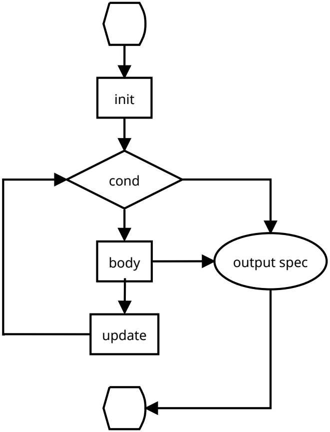
[1] Ian J Goodfellow et al. "Maxout networks". In: *arXiv preprint arXiv:1302.4389* (2013).

Control Flow Operators

What can be computed by a computation graph?

Loop operator:

`scan` in Theano, `while_loop` in TensorFlow and `loop` in MegBrain.



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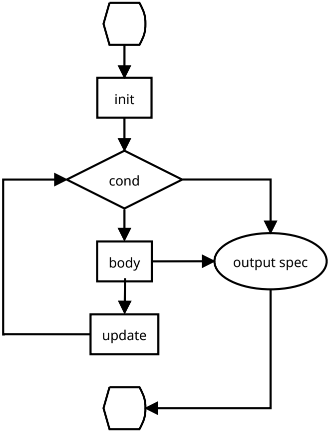

- With symbolic shapes and control flow operators, a computation graph is Turing-complete!
- Useful for RNN and iterative algorithms

Dynamic Computation Graph

Is Turing-completeness enough?

Static Computation Graph

- **Unfamiliar programming model**:
  Stateless, functional: `y = x.setsub[1:3](xs)`
  rather than imperative: `x[1:3] = xs`

Dynamic Computation Graph

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Static Computation Graph

- **Unfamiliar programming model**:
  Stateless, functional: `y = x.setsub[1:3](xs)`
  rather than imperative: `x[1:3] = xs`
- **Difficult to debug**: code is written for graph contruction but tensor values can only be known during graph execution
  `y = printop(y)` rather than `print(y)`

Dynamic Computation Graph

Is Turing-completeness enough?

Dynamic Computation Graph

- Implemented by eager evaluation:

```
while (a.dot(x) - I).max().getvalue() > eps:
    x = x.dot(2 * I - a.dot(x))
print(grad(loss, x).getvalue())
```

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- Auto differentiation: keep symbolic track of computation path
- Drawbacks:
    - hard to optimize: lack of global information
    - hard to deploy: graph depends on code

Graph Execution

Use executors to hide architecture details.

- Map from variables to tensor values

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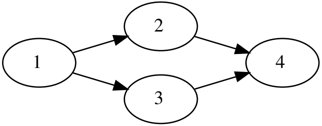
- Map from operators to executors on some specific architecture
- Execute operators according to topological order



$(1, 2, 3, 4)$ or $(1, 3, 2, 4)$

Optimizing by Graph Transformation

- Expression simplifying: $x + 1 - 2 + x \;\Rightarrow\; 2x - 1$

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Optimizing by Graph Transformation

- Expression simplifying: $x + 1 - 2 + x \Rightarrow 2x - 1$
- Operation reordering
  tensors: x and y
  scalars: a and b
  $x + a + y + b \Rightarrow a + b + x + y$
- Operator fusion: $x \cdot y + z \Rightarrow \text{fma}(x, y, z)$
  - static fusion: predefined fusion rules
  - dynamic fusion: Just-in-time compilation (JIT) for actual computation graph

Runtime Memory Management

- Baseline: reference counting + some classical memory allocator

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- Readonly forwarding: reuse input storage for operators like `reshape` and `subtensor`
- Writable forwarding (a.k.a. inplace operation): overwrite input storage
  Caution: must ensure no other readers exist (i.e. `refcnt` equals 1)

Sublinear Memory

Observation

- Long-term dependency for gradient computing consumes lots of memory.
- Assume $x_{i+1} = \mathrm{conv}(x_i, w_i)$, then x_{i+1} can only be discarded after $\frac{\partial L}{\partial w_i}$ and $\frac{\partial L}{\partial x_i}$ have been computed.

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Method

- Split the sequence into blocks consisting of consecutive operators and keep only the first variable in any block
- Recompute internal values in a block when gradient is needed
- In the above example, discard x_{km+j} for all $0 < j < m$ and recompute them when needed.

Sublinear Memory

Reduce memory usage to $O(\sqrt{n})$ with extra $O(n)$ time cost in the ideal case.

For a graph with 10000 convolutions and their gradients:

comp_node	alloc	lower_bound	upper_bound
gpu0:0	15624.37MiB(16383336448bytes)	15624.37MiB(100.00%)	31889.13MiB(204.10%)

comp_node	alloc	lower_bound	upper_bound
gpu0:0	173.03MiB(181430784bytes)	168.76MiB(97.53%)	47251.78MiB(27309.08%)

Note: this idea is also published in[2].

[2] Tianqi Chen et al. "Training deep nets with sublinear memory cost". In: *arXiv preprint arXiv:1604.06174* (2016).

Instruction: The Hardware/Software Interface

What is a program?

```
int sum(int *x) {
    return x[0] + x[1];
}
```

```
0000000000000000 <sum>:
   0:     8b 47 04                mov     0x4(%rdi),%eax
   3:     03 07                   add     (%rdi),%eax
   5:     c3                      retq
```

Modern CPU Technologies

Instr. No.	Pipeline Stage						
1	IF	ID	EX	MEM	WB		
2		IF	ID	EX	MEM	WB	
3			IF	ID	EX	MEM	WB
4				IF	ID	EX	MEM
5					IF	ID	EX
Clock Cycle	**1**	**2**	**3**	**4**	**5**	**6**	**7**

- **Pipeline** [3]
- **Superpipelining** increases stage number and simplifies each stage
- **Superscalar** dispatches multiple instructions to implement instruction-level parallelism
- **Out-of-order execution** executes according to availability of input data rather than original program order

[3] Image from https://en.wikipedia.org/wiki/Instruction_pipelining

Memory Hierarchy

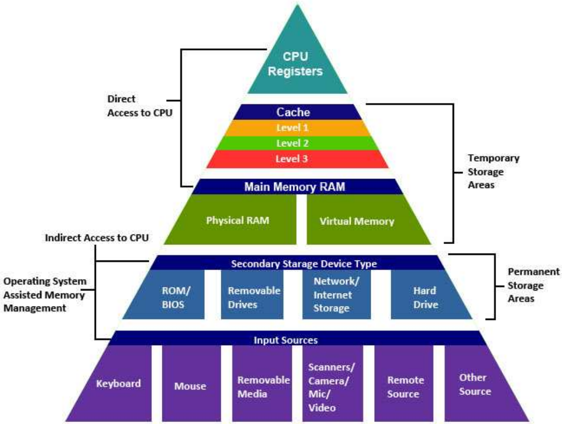
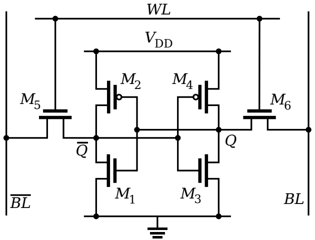


Image from `http://cse1.net/recaps/4-memory.html`

RAM Implementation
Static Random-Access Memory (SRAM)



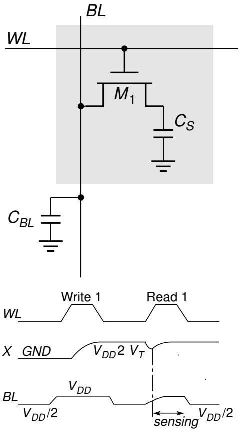
Advantages:

1. Fast
2. Low power consumption
3. No refresh circuit

Image from https://en.wikipedia.org/wiki/Static_random-access_memory

RAM Implementation

Dynamic Random-Access Memory (DRAM)



Advantages:

1. High density
2. Cheap

Refresh: periodically read blocks and write back.

Image from `http://docencia.ac.upc.edu/master/MIRI/NCD/docs/04-Memory%20Structures-2.pdf`

Cache Hierarchy

A hierarchical design for better trade-off between memory capacity and latency.

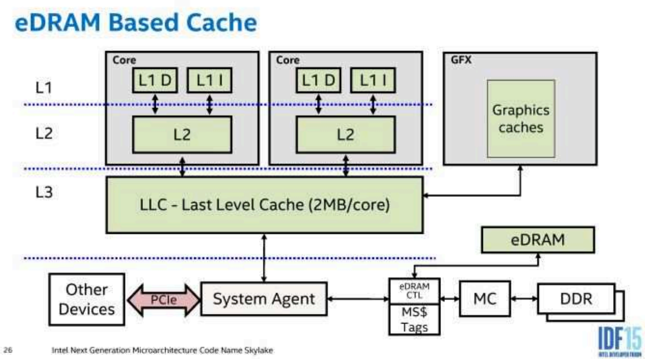


Image from

`https://www.anandtech.com/show/9582/intel-skylake-mobile-desktop-launch-architecture-analysis/5`

Cache Hierarchy

A hierarchical design for better trade-off between memory capacity and latency.

Core i7 Xeon 5500 Series

L1 hit	$\sim$ 4 cycles
L2 hit	$\sim$ 10 cycles
L3 hit line unshared	$\sim$ 40 cycles
L3 hit, shared line in another core	$\sim$ 65 cycles
L3 hit, modified in another core	$\sim$ 75 cycles
Remote L3	$\sim$ $100 - 300$ cycles
Local DRAM	$\sim$ 60 ns
Remote DRAM	$\sim$ 100 ns

source:

https://software.intel.com/sites/products/collateral/hpc/vtune/performance_analysis_guide.pdf

CPU Cache Structure

- Cache line

tag	data block	flag bits (valid, dirty)

- Indexing

tag	index	block offset

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tag	data block	flag bits (valid, dirty)

- Indexing

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- Associativity
  Number of different tags to be kept under the same index
- Addressing
  Virtually indexed, physically tagged (VIPT): simultaneous cache and TLB lookup

Interesting reading: http://igoro.com/archive/gallery-of-processor-cache-effects/

CPU Cache Structure

Example

```
$ grep -m1 name /proc/cpuinfo
model name      : Intel(R) Core(TM) i5-6200U CPU @ 2.30GHz

$ cat /sys/devices/system/cpu/cpu0/cache/index0/{size,ways_of_associativity,coherency_line_size}
32K
8
64
```

- block offset: $\log_2 64 = 6\text{bit}$
- index: $\log_2(32\text{KiB}/64\text{B}/8) = 6\text{bit}$
- tag: $52 - 6 - 6 = 40\text{bit}$ (48-bit virtual memory and 52-bit physical memory)

Note that *block offset* and *index* together take 12 bits, which is equal to page size (4KiB), so VIPT can be easily implemented.

SIMD

Single instruction, multiple data

Store multiple data items in one register and process them in a single instruction.

Calculation of theoretical FLOPS[4]

$$FLOPS = f \cdot w \cdot IPC$$

$$\begin{aligned} f &: \text{frequency} \\ w &: \text{SIMD width (number of floats per register)} \\ IPC &: \text{SIMD instructions per cycle} \end{aligned}$$

[4] floating point operations per second

SIMD

Single instruction, multiple data

Example

Intel® CPUs usually have $IPC = 2$. However if FMA is supported, IPC should be counted as 4 since 2 FMA instructions is essentially 4 floating point operations.

Intel® Xeon® Platinum 8180M[4]

# of Cores	28
Processor Base Frequency	2.50 GHz
Max Turbo Frequency	3.80 GHz
# of AVX-512 FMA Units	2

$$FLOPS = 3.8Gcyc/s \times 4instr/cyc \times 16float/instr$$
$$= 243.2GFLOPS$$
$$FLOPS\_TOT = FLOPS \times 28 = 6.8TFLOPS$$

[4] data available at https://ark.intel.com/products/120498/Intel-Xeon-Platinum-8180M-Processor-38_5M-Cache-2_50-GHz

A MatMul Example

```
void matmul(float *a, float *b, float *c, int n) {
    for (int i = 0; i < n; ++ i) {
        for (int j = 0; j < n; ++ j) {
            float sum = 0;
            for (int k = 0; k < n; ++ k) {
                sum += a[i * n + k] * b[k * n + j];
            }
            c[i * n + j] = sum;
        }
    }
}
```

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        }
    }
}
```

Swap the loops on j and k

NVIDIA GPU

A single instruction, multiple thread architecture

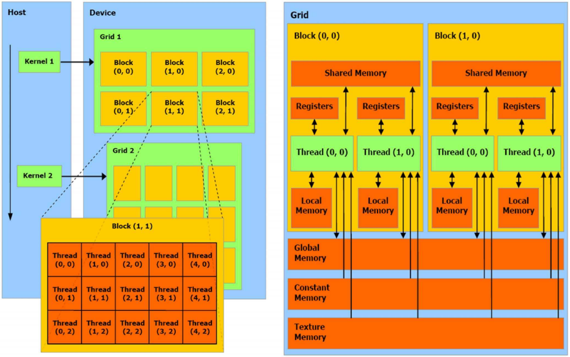

Image from[5]

[5] Marco Nobile et al. "cuTauLeaping: A GPU-Powered Tau-Leaping Stochastic Simulator for Massive Parallel Analyses of Biological Systems". In: 9 (Mar. 2014), e91963.

NVIDIA GPU

A single instruction, multiple thread architecture

```
__global__ void add(float *a, float *b, float *c, int n) {
    int id = blockIdx.x*blockDim.x+threadIdx.x;
    if (id < n)
        c[id] = a[id] + b[id];
}
```

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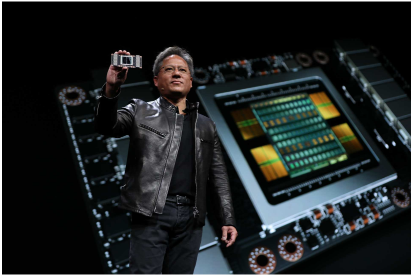


Tesla V100 for NVLink

- 15.7 *TFLOPS* for single-precision
- 125 *TFLOPS* for half-precision

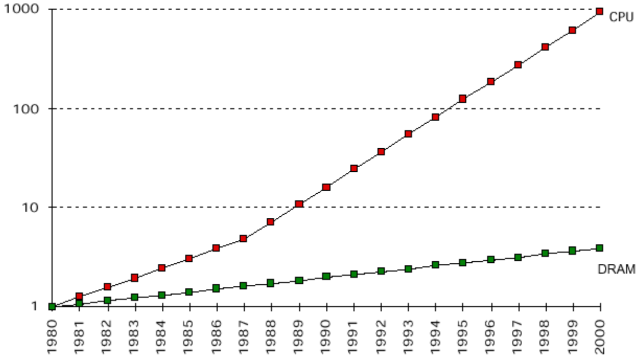
Image from https://arstechnica.com/gadgets/2017/05/nvidia-tesla-v100-gpu-details/

New Devices

- Google TPU: systolic array, 45 TFLOPS (presumably fp16)
- Huawei NPU in Kirin 970 (Cambricon[5]): 1.92 TFLOPS fp16
- Mobile: CPU + GPU + DSP

[5] Yunji Chen et al. "Dadiannao: A machine-learning supercomputer". In: *MICRO*. 2014, pp. 609–622.

Unbalanced Development of Processor and Memory



Graph from[6]

[6] Carlos Carvalho. "The gap between processor and memory speeds". In: *Proc. of IEEE International Conference on Control and Automation*. 2002.

Challenges from NN Architecture

Computation-sparse structure seems to be beneficial.

Architecture	**Computation**	**Memory**
Small kernel	$\frac{k2^2}{k1^2}$	Param $\frac{k1^2}{k2^2}$
Large stride	$\frac{1}{s^2}$	Output $\frac{1}{s^2}$
Group/depthwise conv	$\frac{1}{g^2}$	Param $\frac{1}{g}$
Shuffle/concat	0	1

Roofline Model

A visualization method to characterize computation/memory

Performance P (FLOPS) is approximately a function of arithmetic intensity I (FLOP/byte) for a particular architecture[7].

Naïve Roofline

$$P = \min \begin{cases} \pi \\ \beta \times I \end{cases}$$

where π is the peak computing performance and β is the peak bandwidth.

[7] Samuel Webb Williams. *Auto-tuning performance on multicore computers.* University of California, Berkeley, 2008.

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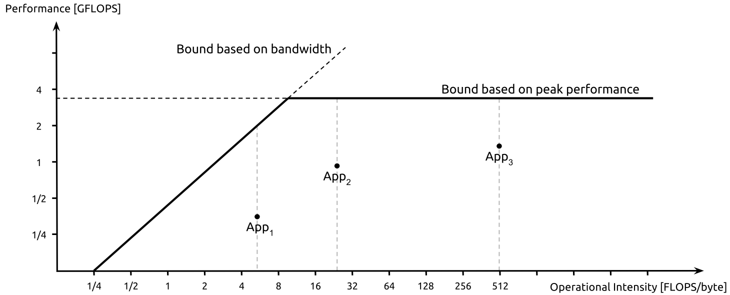

Image from `https://en.wikipedia.org/wiki/Roofline_model`

Communication System: Single Node

- PCI-e: connection between GPUs, network adaptors and others
  - Switches may be needed
  - 985 MiB/s each PCI-e 3.0 lane
  - LGA-2011 socket: 40 lanes
- NVLink: GPU interconnect by NVIDIA

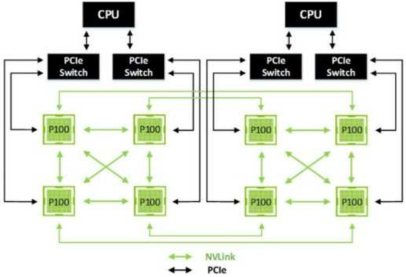

Image from https://www.nextplatform.com/2016/05/04/nvlink-takes-gpu-acceleration-next-level/

Communication System: LAN

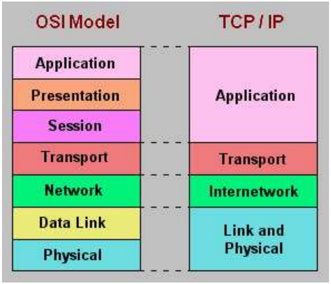

Image from `http://www.just2good.co.uk/tcpipStack.php`

- Ethernet: 10M to 100G, latency 100 - 20 μs
- InfiniBand: 2.5 to 250G, latency 5 - 0.5 μs

RDMA

Remote Direct Memory Access

Bypass the TCP/IP stack and free CPU from handling packets.

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Bypass the TCP/IP stack and free CPU from handling packets.

- RoCE: RDMA over Converged Ethernet
- InfiniBand: RDMA supported
- NVIDIA GPUDirect: RDMA between GPUs

1. Symbolic Computation
   - Representation
   - Execution & Optimization
2. Dense Numerical Computation
   - CPU Computation
   - Other Computation Devices
   - Computation & Memory Gap
3. Distributed Computation
   - System
   - **Optimzation Algorithms**
   - Communication Algorithms

Synchronous SGD
Basics

Each worker processes a part of the whole batch; params and grads must be synchronized

$$L(\{d_0, d_1\}, W) = \alpha_0 L(\{d_0\}, W) + \alpha_1 L(\{d_1\}, W)$$

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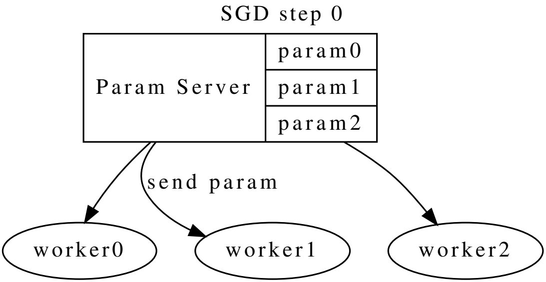

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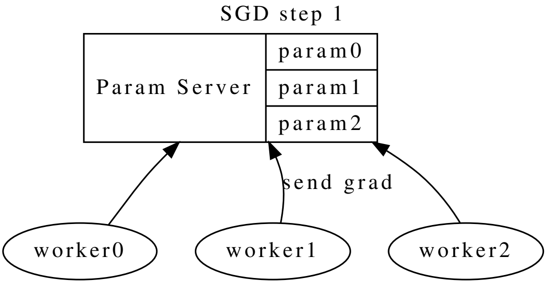

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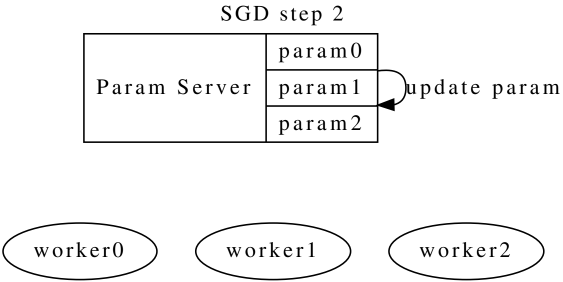

Asynchronous SGD

Basics

Each worker has an outdated local copy of params and updates central param storage asynchronously. Friendly for parallel speedup.

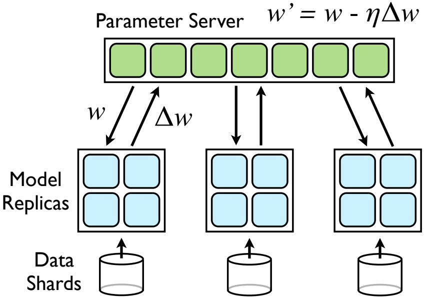

Image from[7]

[7] Jeffrey Dean et al. "Large scale distributed deep networks". In: *NIPS*. 2012, pp. 1223–1231.

Asynchronous SGD
Difficulties

ASGD is not equivalent to SGD and it is hard to tune due to noisy gradients. Many works exist on analyzing convergence and improving performance[8][9][10].

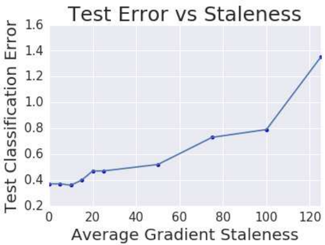

Image from[11]

[8] Xiangru Lian et al. "Asynchronous Parallel Stochastic Gradient for Nonconvex Optimization". In: *NIPS*. 2015, pp. 2737–2745.

[9] Wei Zhang et al. "Staleness-aware async-SGD for Distributed Deep Learning". In: *IJCAI*. 2016, pp. 2350–2356.

[10] Sixin Zhang, Anna E Choromanska, and Yann LeCun. "Deep learning with elastic averaging SGD". In: *NIPS*. 2015, pp. 685–693.

[11] Jianmin Chen et al. "Revisiting distributed synchronous SGD". In: *arXiv preprint arXiv:1604.00981* (2016).

Synchronous SGD
Improvements

- Reduce communication by compressing gradients[12]
- Handle straggling workers by backup workers[13]
- Ensure performance by careful hyperparam tuning[14]

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[12] Ryota Tomioka and Milan Vojnovic. "QSGD: Communication-Efficient Stochastic Gradient Descent, with Applications to Training Neural Networks". In: *arXiv preprint arXiv:1610.02132* (2016).

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Synchronous SGD
Improvements

- Reduce communication by compressing gradients[12]

$$Q_s(v_i) = \|\boldsymbol{v}\|_2 \cdot \mathrm{sgn}(v_i) \cdot \xi(\frac{|v_i|}{\|\boldsymbol{v}\|_2}, s)$$

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Synchronous SGD
Improvements

- Reduce communication by compressing gradients[12]
- Handle straggling workers by backup workers[13]
  Use $N + b$ workers but only receive gradients from any N of them and do not wait for the slowest b workers.
- Ensure performance by careful hyperparam tuning[14]

[12] Ryota Tomioka and Milan Vojnovic. "QSGD: Communication-Efficient Stochastic Gradient Descent, with Applications to Training Neural Networks". In: *arXiv preprint arXiv:1610.02132* (2016).

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Synchronous SGD
Improvements

- Reduce communication by compressing gradients[12]
- Handle straggling workers by backup workers[13]
- Ensure performance by careful hyperparam tuning[14]
  8192 minibatch size on 256 GPUs:

$$\hat{\eta} = k\eta$$
$$m = \frac{\eta_{t+1}}{\eta_t}$$

[12] Ryota Tomioka and Milan Vojnovic. "QSGD: Communication-Efficient Stochastic Gradient Descent, with Applications to Training Neural Networks". In: *arXiv preprint arXiv:1610.02132* (2016).

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MPI Primitives

Collective communication routines in MPI are common in distributed DL

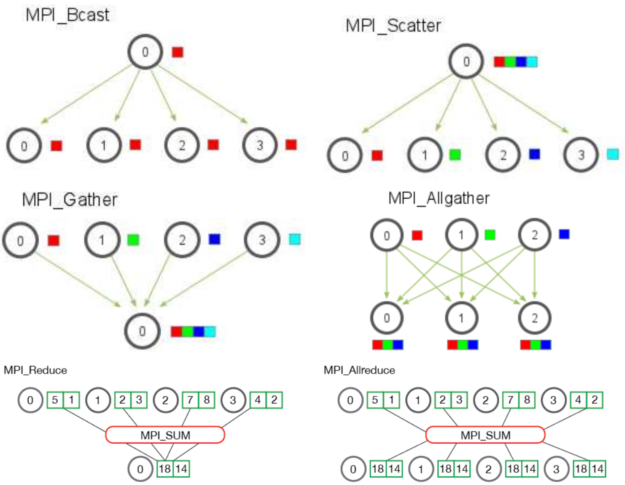

Image source: `http://mpitutorial.com`

An AllReduce Algorithm

Assume message size K and number of workers N

- Reduce to a worker (assume W_{N-1} here):
  W_i sends to W_{i+1} at step i; communication per worker is N
- Broadcast from a worker: as above

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- AllReduce:
  1. Split the message into N parts
  2. Reduce the ith part to W_i; all reductions run in parallel
  3. Broadcast each reduced part to all workers in parallel

  Communication cost for each worker is $2(N-1)\frac{K}{N}$, independent of N.

More details and discussions are given in[15] [16].

[15] Rajeev Thakur, Rolf Rabenseifner, and William Gropp. "Optimization of collective communication operations in MPICH". In: *The International Journal of High Performance Computing Applications* 19.1 (2005), pp. 49–66.

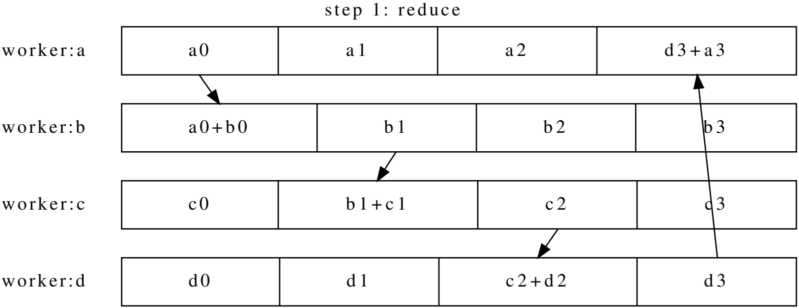
[16] http://research.baidu.com/bringing-hpc-techniques-deep-learning

An AllReduce Algorithm

step 0: init

worker:a	a0	a1	a2	a3
worker:b	b0	b1	b2	b3
worker:c	c0	c1	c2	c3
worker:d	d0	d1	d2	d3

An AllReduce Algorithm



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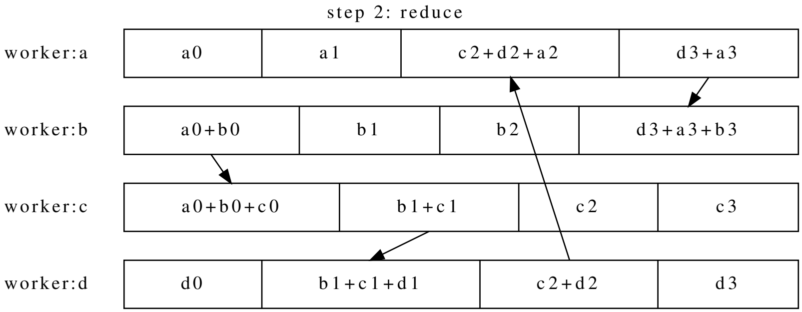

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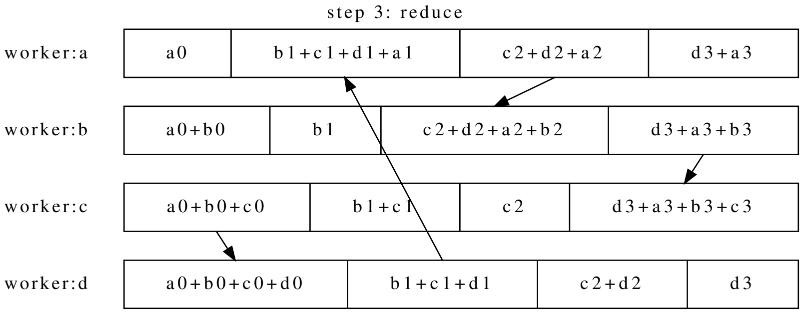

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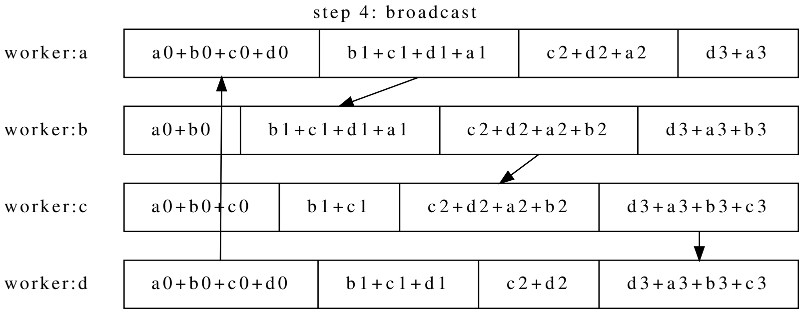

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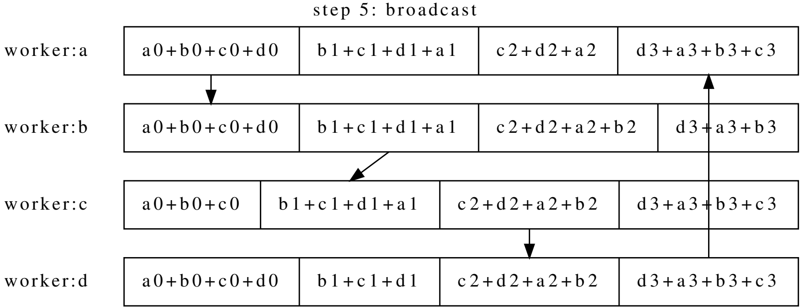

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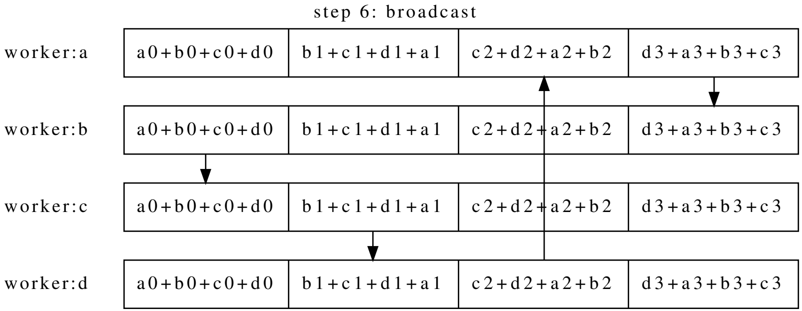

Thanks!

Questions are welcome