

DEEP LEARNING

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From the beginning of 2016, I decided to cease all explicit crowdfunding for any of my materials on physics, math. I failed to raise *any* funds from previous crowdfunding efforts. I decided that if I was going to live in *abundance*, I must lose a scarcity attitude. I am committed to keeping all of my material **open-sourced**. I give all my stuff *for free*.

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ABSTRACT. Everything about Machine Learning, Deep Learning.

Part 1. Neural Networks

1. LOSS FUNCTIONS

1.1. **L1**. From Pytorch Docs, torch.nn, [L1Loss Pytorch](#)

$$\ell(x, y) = L = \{l_1, \dots, l_N\}^\top, \quad l_n = |x_n - y_n|$$

where  $N$  is the batch size. If ‘reduction’ is not ‘none’ (default ‘mean’), then:

$$\ell(x, y) = \begin{cases} \text{mean}(L), & \text{if reduction = ‘mean’;} \\ \text{sum}(L), & \text{if reduction = ‘sum’}. \end{cases}$$

Instead, consider the following: let  $\mathbf{x}, \mathbf{y} \in \mathbf{R}^N$  where  $\mathbf{R}$  is some ring (integers and floating point types in computer science are at least rings).

Let  $\mathbf{x}$  be the predicted values and  $\mathbf{y}$  be the true values.

If

$$l(x, y) = L = \{l_1, \dots, l_N\}^T, \quad l_n = |x_n - y_n|$$

then

$$\frac{\partial}{\partial x^i} L = \frac{\partial}{\partial x^i} \begin{cases} x_j - y_j & \text{if } x_j \geq y_j \\ y_j - x_j & \text{if } x_j < y_j \end{cases} = \begin{cases} 1 & \text{if } x_j \geq y_j \\ -1 & \text{if } x_j < y_j \end{cases}$$

If

$$l(x, y) = L = \frac{1}{N} \sum_{j=1}^N l_j$$

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Then

$$\frac{\partial}{\partial x_i}L = \frac{1}{N} \begin{cases} 1 & \text{if } x_j \geq y_j \\ -1 & \text{if } x_j < y_j \end{cases}$$

If

$$l(x,y) = L = \sum_{j=1}^N l_j$$

Then

$$\frac{\partial}{\partial x_i}L = \begin{cases} 1 & \text{if } x_j \geq y_j \\ -1 & \text{if } x_j < y_j \end{cases}$$

**Part 2. CUDA**

Keep in mind that CUDA won’t be the end-all, be-all for optimized deep learning. Consider Open XLA and consider LLVM.

2. THREADS, BLOCKS, GRIDS

cf. Chapter 5 Thread Cooperation, Section 5.2. Splitting Parallel Blocks of Sanders and Kandrot (2010) [42].

Consider first a 1-dimensional block.

- `threadIdx.x`  $\Leftarrow M_x \equiv$  number of threads per block in  $x$ -direction. Let  $j_x = 0 \dots M_x - 1$  be the index for the thread. Note that  $1 \leq M_x \leq M_x^{\max}$ , where  $M_x^{\max} = 1024$  is the maximum number of threads per block that can be allocated, which is a hard hardware limit (I presume).
- `blockIdx.x`  $\Leftarrow N_x \equiv$  number of blocks in  $x$ -direction. Let  $i_x = 0 \dots N_x - 1$
- `blockDim.x` stores number of threads along each dimension of the block  $M_x$ .

Then if we were to “linearize” or “flatten” in this  $x$ -direction,

(1) 
$$k = j_x + i_x M_x$$

where  $k$  is the  $k$ th thread.  $k = 0 \dots N_x M_x - 1$ .

Take a look at [heattexture1.cu](#) which uses the GPU texture memory. Look at how `threadIdx/blockIdx` is mapped to pixel position.

As an exercise, let’s again rewrite the code in mathematical notation:

- `threadIdx.x`  $\Leftarrow j_x, 0 \leq j_x \leq M_x - 1$
- `blockIdx.x`  $\Leftarrow i_x, 0 \leq i_x \leq N_x - 1$
- `blockDim.x`  $\Leftarrow M_x$ , number of threads along each dimension (here dimension  $x$ ) of a block,  $1 \leq M_x \leq M_x^{\max} = 1024$
- `gridDim.x`  $\Leftarrow N_x, 1 \leq N_x$

resulting in

- $k_x = j_x + i_x M_x \implies$   
$$\text{int } x = \text{threadIdx.x} + \text{blockIdx.x} * \text{blockDim.x} ;$$
- $k_y = j_y + i_y M_y \implies$   
$$\text{int } y = \text{threadIdx.y} + \text{blockIdx.y} * \text{blockDim.y} ;$$

and so for a “flattened” thread index  $J \in \mathbb{N}$ ,

$$J = k_x + N_x \cdot M_x \cdot k_y$$

$\implies$

$$\text{offset} = x + y * \text{blockDim.x} * \text{gridDim.x} ;$$

Suppose vector is of length  $N$ . So we *need*  $N$  parallel threads to launch, in total.

e.g. if  $M_x = 128$  threads per block,  $N/128 = N/M_x$  blocks to get our total of  $N$  threads running.

Wrinkle: integer division! e.g. if  $N = 127$ ,  $\frac{N}{128} = 0$ .

Solution: consider  $\frac{N+127}{128}$  blocks. If  $N = l \cdot 128 + r, l \in \mathbb{N}, r = 0 \dots 127$ .

$$\begin{aligned} \frac{N + 127}{128} &= \frac{l \cdot 128 + r + 127}{128} = \frac{(l + 1)128 + r - 1}{128} = \\ &= l + 1 + \frac{r - 1}{128} = \begin{cases} l & \text{if } r = 0 \\ l + 1 & \text{if } r = 1 \dots 127 \end{cases} \\ \frac{N + (M_x - 1)}{M_x} &= \frac{l \cdot M_x + r + M_x - 1}{M_x} = \frac{(l + 1)M_x + r - 1}{M_x} = \\ &= l + 1 + \frac{r - 1}{M_x} = \begin{cases} l & \text{if } r = 0 \\ l + 1 & \text{if } r = 1 \dots M_x - 1 \end{cases} \end{aligned}$$

So  $\frac{N+(M_x-1)}{M_x}$  is the smallest multiple of  $M_x$  greater than or equal to  $N$ , so  $\frac{N+(M_x-1)}{M_x}$  **blocks are needed or more than needed to run a total of  $N$  threads.**

Problem: Max. grid dim. in 1-direction is 65535,  $\equiv N_i^{\max}$ .

So  $\frac{N+(M_x-1)}{M_x} = N_i^{\max} \implies N = N_i^{\max} M_x - (M_x - 1) \leq N_i^{\max} M_x$ . i.e. number of threads  $N$  is limited by  $N_i^{\max} M_x$ .

Solution.

- number of threads per block in  $x$ -direction  $\equiv M_x \implies \text{blockDim.x}$
- number of blocks in grid  $\equiv N_x \implies \text{gridDim.x}$
- $N_x M_x$  total number of threads in  $x$ -direction. Increment by  $N_x M_x$ . So next scheduled execution by GPU at the  $k = N_x M_x$  thread.

Sanders and Kandrot (2010) [42] made an important note, on pp. 176-177 Ch. 9 Atomics of Section 9.4 Computing Histograms, an important *rule of thumb* on the number of blocks.

First, consider  $N^{\text{threads}}$  total threads. The extremes are either  $N^{\text{threads}}$  threads on a single block, or  $N^{\text{threads}}$  blocks, each with a single thread.

Sanders and Kandrot gave this tip:

number of blocks, i.e. `gridDim.x`  $\Leftarrow N_x \sim 2 \times$  number of GPU multiprocessors, i.e. twice the number of GPU multiprocessors. In the case of my GeForce GTX 980 Ti, it has 22 Multiprocessors.

**2.1. global thread Indexing: 1-dim., 2-dim., 3-dim.** Consider the problem of *global thread indexing*. This was asked on the NVIDIA Developer’s board (cf. [Calculate GLOBAL thread Id](#)). Also, there exists a “cheatsheet” (cf. [CUDA Thread Indexing Cheatsheet](#)). Let’s consider a (mathematical) generalization.

Consider again (cf. [2](#)) the following notation:

- `threadIdx.x`  $\Leftarrow i_x, 0 \leq i_x \leq M_x - 1$ ,  $i_x \in \{0 \dots M_x - 1\} \equiv I_x$ , of “cardinal length/size” of  $|I_x| = M_x$
- `blockIdx.x`  $\Leftarrow j_x, 0 \leq j_x \leq N_x - 1$ ,  $j_x \in \{0 \dots N_x - 1\} \equiv J_x$ , of “cardinal length/size” of  $|J_x| = N_x$
- `blockDim.x`  $\Leftarrow M_x$
- `gridDim.x`  $\Leftarrow N_x$

Now consider formulating the various cases, of a grid of dimensions from 1 to 3, and blocks of dimensions from 1 to 3 (for a total of 9 different cases) mathematically, as the [CUDA Thread Indexing Cheatsheet](#) did, similarly:

- *1-dim. grid of 1-dim. blocks.* Consider  $J_x \times I_x$ . For  $j_x \in J_x, i_x \in I_x$ , then  $k_x = j_x M_x + i_x, k_x \in \{0 \dots N_x M_x - 1\} \equiv K_x$ . The condition that  $k_x$  be a valid global thread index is that  $K_x$  has equal cardinality or size as  $J_x \times I_x$ , i.e.

$$|J_x \times I_x| = |K_x|$$

(this must be true). This can be checked by checking the most extreme, maximal, case of  $j_x = N_x - 1$ ,  $i_x = M_x - 1$ :

$$k_x = j_x M_x + i_x = (N_x - 1)M_x + M_x - 1 = N_x M_x - 1$$

and so  $k_x$  ranges from 0 to  $N_x M_x - 1$ , and so  $|K_x| = N_x M_x$ .

Summarizing all of this in the following manner:

$$J_x \times I_x \longrightarrow K_x \equiv K^{N_x M_x} = \{0 \dots N_x M_x - 1\}$$

$$(j_x, i_x) \longmapsto k_x = j_x M_x + i_x$$

For the other cases, this generalization we've just done is implied.

- *1-dim. grid of 2-dim. blocks*

$$J_x \times (I_x \times I_y) \longrightarrow K^{N_x M_x M_y} \equiv \{0 \dots N_x M_x M_y - 1\}$$

$$(j_x, (i_x, i_y)) \longmapsto k = j_x M_x M_y + (i_x + i_y M_x) = j_x |I_x \times I_y| + (i_x + i_y M_x) \in \{0 \dots N_x M_x M_y - 1\}$$

The “most extreme, maximal” case that can be checked to check that the “cardinal size” of  $K^{N_x M_x M_y}$  is equal to  $J_x \times (I_x \times I_y)$  is the following, and for the other cases, will be implied (unless explicitly written or checked out):

$$k = j_x M_x M_y + (i_x + i_y M_x) = (N_x - 1)M_x M_y + ((M_x - 1) + (M_y - 1)M_x) = (N_x M_x M_y - 1)$$

The thing to notice is this emerging, general pattern, what could be called a “global view” of understanding the threads and blocks model of the GPU (cf. [njuffa's answer](#)):

total number of threads = block index (Id) · total number of threads per blocok + thread index on the block

But as we'll see, that's not the only way of “flattening” the index, or transforming into a 1-dimensional index.

- *1-dim. grid of 3-dim. blocks*

$$J_x \times (I_x \times I_y \times I_z) \longrightarrow K^{N_x M_x M_y M_z}$$

$$(j_x, (i_x, i_y, i_z)) \longmapsto k = j_x (M_x M_y M_z) + (i_x + i_y M_x + i_z M_x M_y) \in \{0 \dots N_x M_x M_y M_z - 1\}$$

- *2-dim. grid of 1-dim. blocks*

$$(J_x \times J_y) \times I_x \longrightarrow L^{N_x N_y} \times I_x \longrightarrow K^{N_x N_y M_x}$$

$$((j_x, j_y), i_x) \longmapsto ((j_x + N_x j_y), i_x) \longmapsto k = (j_x + N_x j_y) \cdot M_x + i_x \in \{0 \dots N_x N_y M_x - 1\}$$

- *2-dim. grid of 2-dim. blocks*

$$(J_x \times J_y) \times (I_x, I_y) \longrightarrow L^{N_x N_y} \times (I_x, I_y) \longrightarrow K^{N_x N_y M_x}$$

$$((j_x, j_y), (i_x, i_y)) \longmapsto ((j_x + N_x j_y), (i_x, i_y)) \longmapsto k = (j_x + N_x j_y) \cdot M_x M_y + i_x + M_x i_y$$

But this *isn't the only way of obtaining* a “flattened index.” Exploit the commutativity and associativity of the Cartesian product:

$$J_x \times J_y \times I_x \times I_y = (J_x \times I_x) \times (J_y \times I_y) \longrightarrow K^{N_x M_x} \times K^{N_y M_y} \longrightarrow K^{N_x N_y M_x M_y}$$

$$((j_x, j_y, i_x, i_y) = ((j_x, i_x), (j_y, i_y)) \longmapsto (i_x + M_x j_x, i_y + M_y j_y) \equiv (k_x, k_y) \longmapsto k = k_x + k_y N_x M_x = (i_x + M_x j_x) + (i_y + M_y j_y) M_x N_x$$

Indeed, checking the “maximal, extreme” case,

$$k = k_x + k_y N_x M_x = M_x N_x - 1 + (M_y N_y - 1)(N_x M_x) = M_y M_y N_x M_x - 1$$

and so  $k$  ranges from 0 to  $M_y M_y N_x M_x - 1$ .

- *3-dim. grid of 3-dim. blocks*

$$(J_x \times J_y \times J_z) \times (I_x \times I_y \times I_z) = \longrightarrow K^{N_x M_x} \times K^{N_y M_y} \times K^{N_z M_z} \longrightarrow K^{N_x N_y N_z M_x M_y M_z}$$

$$((j_x, j_y, j_z), (i_x, i_y, i_z)) = \longmapsto (i_x + M_x j_x, i_y + M_y j_y, i_z + M_z j_z) \equiv \longmapsto k = k_x + k_y N_x M_x + k_z N_x M_x N_y M_y$$

$$= ((j_x, i_x), (j_y, i_y), (j_z, i_z)) \equiv (k_x, k_y, k_z)$$

Indeed, checking the “extreme, maximal” case for  $k$ :

$$k = k_x + k_y N_x M_x + k_z N_x M_x N_y N_y = (N_x M_x - 1) + (N_y M_y - 1)N_x M_x + (N_z M_z - 1)N_x M_x N_y M_y = N_x N_y N_z M_x M_y M_z - 1$$

**2.2. With Stride.** Consider this code for the **L1 loss function** and **L2 loss function**. It introduces the idea of a ”stride.” Let's figure out what the stride means mathematically.

Given Eq. 1, recall that

$$k = j_x + i_x M_x, \quad \begin{matrix} 0 \leq j_x < M_x \\ 0 \leq i_x < N_x \end{matrix}, \quad 0 \leq k < N_x M_x$$

Let  $S \equiv$  stride.

Following the code we mentioned above for L1 and L2 loss functions, it seems that the following 2 indices were introduced, with inter roughly meaning ”outside” or ”outward” and intra meaning ”within” or ”internal”, presumably:

$$i_{\text{intra}} = k \bmod S \in \{0, 1, \dots, S - 1\}$$

$$i_{\text{inter}} = \lfloor k/S \rfloor \in \{0, 1, \dots, (N_x M_x - 1)/S\}$$

Now let  $D =$  number of dimensions.

Continuing with the code, it seems that  $i_{\text{intra}} < D$  is what's expected. Otherwise, if  $i_{\text{intra}} \geq D$ , then we effectively don't compute.

$$l \equiv i_{\text{inter}} D + i_{\text{intra}}, \quad 0 \leq l \leq \left( \frac{N_x M_x - 1}{S} \right) D + S - 1$$

Let's try some examples. If  $S = 1$ ,  $i_{\text{intra}} = 0$ , always (the modulus of a number by 1 is always 0 because any number can be divided by 1 ”evenly” (no remainder)), and  $i_{\text{inter}} = k$ . So  $l = kD$ . If  $D = 1$  we get a 1 to 1 mapping which is what I'd typically expect if given arrays. If  $D = 2$ , then  $l$  would be all the even indices it seems implied that the ”target” array that's using  $l$  as an index would have at least twice the size of the input array!

If  $S = 2$ ,  $i_{\text{intra}} \in \{0, 1\}$ ,  $i_{\text{inter}} \in \{0, 1, \dots, \lfloor \frac{N_x M_x - 1}{2} \rfloor\}$  and so  $l \in \{0, 1, \dots, (\frac{N_x M_x - 1}{2}) D + 1\}$ .

3. ROW-MAJOR ORDERING VS. COLUMN MAJOR ORDERING, AS FLATTEN

So-called row-major ordering and column major ordering should be formalized, to deal with continguous memory access in reading or writing to a matrix, or lack thereof.

Given

$$\begin{aligned} A &\in \text{Mat}_{\mathbb{R}}(m, n) \\ A &: \{1, 2, \dots m\} \times \{1, 2, \dots n\} \rightarrow \mathbb{R} \\ A &: (i, j) \mapsto A(i, j) \in \mathbb{R} \\ A &: \{0, 1, \dots m-1\} \times \{0, 1, \dots n-1\} \rightarrow \mathbb{R} \\ \text{or} \quad A &: (i, j) \mapsto A(i, j) \in \mathbb{R} \end{aligned}$$

Consider isomorphism ”flatten”:

$$\begin{aligned} \text{Mat}_{\mathbb{R}}(m, n) &\xrightarrow{\text{flatten}} \mathbb{R}^{mn} \\ (2) \quad \{1, 2, \dots m\} \times \{1, 2, \dots n\} &\rightarrow \{1, 2, \dots mn\} \\ \{0, 1, \dots m-1\} \times \{0, 1, \dots n-1\} &\rightarrow \{0, 1, \dots mn-1\} \end{aligned}$$

There are 2 kinds of flatten:

Row-major ordering is the one we’re (psychologically) used to, if we read continguously from left to right, horizontally, along a row.

**Definition 1** (row-major ordering).

$$\begin{aligned} \{0, 1, \dots m-1\} \times \{0, 1, \dots n-1\} &\rightarrow \{0, 1, \dots mn-1\} & \{0, 1, \dots mn-1\} &\rightarrow \{0, 1, \dots m-1\} \times \{0, 1, \dots n-1\} \\ (i, j) &\mapsto in + j & k &\mapsto (k/n, k \bmod n) \\ (3) \quad \{1, 2, \dots m\} \times \{1, 2, \dots n\} &\rightarrow \{1, 2, \dots mn\} & \{1, 2, \dots mn\} &\rightarrow \{1, 2, \dots m\} \times \{1, 2, \dots n\} \\ (i, j) &\mapsto (i-1)n + j & k &\mapsto (\lceil k/n \rceil, k \bmod n) \end{aligned}$$

**Definition 2** (column-major ordering).

$$\begin{aligned} \{0, 1, \dots m-1\} \times \{0, 1, \dots n-1\} &\rightarrow \{0, 1, \dots mn-1\} & \{0, 1, \dots mn-1\} &\rightarrow \{0, 1, \dots m-1\} \times \{0, 1, \dots n-1\} \\ (i, j) &\mapsto i + jm & k &\mapsto (k \bmod m, k/m) \\ (4) \quad \{1, 2, \dots m\} \times \{1, 2, \dots n\} &\rightarrow \{1, 2, \dots mn\} & \{1, 2, \dots mn\} &\rightarrow \{1, 2, \dots m\} \times \{1, 2, \dots n\} \\ (i, j) &\mapsto i + (j-1)m & k &\mapsto (k \bmod m, \lceil k/m \rceil) \end{aligned}$$

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