

Based on the provided sources, here is a detailed explanation of the chapters and topics you requested, organized by week:

## Week 16: Deep Learning and Convolutional Neural Networks (Chapter 16)

This chapter serves as an application case study on deep learning, a branch of machine learning using artificial neural networks 1 . Machine learning involves training application logic based on experience from datasets, and deep learning uses neural networks for this purpose 1 . The goal is to understand and develop kernels for deep learning approaches to machine learning tasks 2 ... .

### • Convolutional Neural Networks (CNNs): An Introduction

- CNNs are a popular deep learning algorithm with a high compute-to-memory access ratio and high levels of parallelism, making them well-suited for GPU acceleration 4 .
- The computation in a convolutional network is organized as a sequence of layers 5 . These layers process inputs and outputs, often called feature maps or features 5 .
- LeNet-5 is a historical example of a CNN, composed of three types of layers: **convolutional layers, subsampling layers, and fully connected layers** 6 . These are still key components of modern neural networks 6 .
- The input to a CNN is typically an image 5 . The last layer computes an output, often representing probabilities for different categories (e.g., digits in handwriting recognition) 5 .
- **Convolutional layers** generate output feature maps from input feature maps 7 . Each pixel in an output feature map is produced by performing a **convolution** between a small local patch of pixels from the previous layer's feature map and a set of weights called a **filter bank** 7 . The convolution result is then fed into an activation function 7 .
- An output feature map can be the **sum of convolution results** from corresponding patches in *all* input feature maps 8 ... . Different pairs of input and output feature maps use different filter banks 8 .
- Input feature maps are often stored as a 3D array  $X[C, H, W]$ , where C is the number of input feature maps, H is height, and W is width 10 . Output feature maps are stored as  $Y[M, H_{out}, W_{out}]$ , where M is the number of output feature maps and  $H_{out}$ ,  $W_{out}$  depend on H, W, and the filter size K 11 . Filter banks are stored as  $W[M, C, K, K]$  11 . Filter bank  $W[m, c, \_, \_]$  is used when using input feature map  $X[c, \_, \_]$  to calculate output feature map  $Y[m, \_, \_]$  11 .
- **Subsampling layers (pooling layers)** reduce the size of image maps by combining pixels 12 ... . For instance, a 2x2 neighborhood in the input feature map might be averaged to form one pixel in the output feature map 13 . The number of output feature maps in a subsampling layer is the same as its input, but dimensions are reduced 14 . Subsampling layers often include an **activation function** 15 .
- **Fully connected layers** are layers where every output is a function of every input 16 . The process of evaluating outputs from inputs in a fully connected layer is a **matrix-vector multiplication** 17 . These layers become expensive for large inputs/outputs due to the size of the weight matrix 17 .

- CNNs reduce the cost of fully connected layers by reducing the number of inputs each classifier (like a perceptron) takes and **sharing the same weights** across classifiers in convolutional layers 18 . This allows for many classifiers (large M) without excessive weights 19 .

## • Kernel for Backpropagation and Forward Propagation

- **Forward Propagation:** The computation goes through layers sequentially 5 . Sequential C code for the forward pass of a convolutional layer involves nested loops iterating over output feature maps (m), output pixels (h, w), input feature maps (c), and filter weights (p, q) 9 ... .
- The innermost loops (c, p, q) perform the 3D convolution for one output pixel 12 . These loops can be kept serial to avoid atomic operations if not needed 22 .
- The four outer loop levels (n for batch, m for output feature map, h for output pixel row, w for output pixel column) offer significant parallelism:  $N * M * H_{out} * W_{out}$  parallel iterations 23 . This high degree of parallelism makes it excellent for GPU acceleration 23 .
- A CUDA kernel can be designed with threads mapped to compute one element of one output feature map pixel 24 . 2D thread blocks can compute a tile of pixels in one output feature map 24 . Blocks can be organized in a 3D grid to capture batch (N), output feature map (M), and tile location (h-w) parallelism 24 ... .
- One proposed thread organization uses grid dimensions for M (X), tile location (Y), and N (Z) 25 . The tile location in the Y dimension combines vertical and horizontal tile indices 26 ... .
- The host code for launching such a kernel sets grid dimensions based on M, the number of tiles ( $H_{grid} * W_{grid}$ ), and N 28 .

### ◦ **Forward Kernel Code Example:**

- *This kernel code iterates over input channels (c) and filter dimensions (p, q) serially for each output pixel (n, m, h, w) assigned to a thread 27 ... . This kernel consumes significant global memory bandwidth 31 . Optimizations like constant memory caching and shared memory tiling can reduce global memory traffic 31 .*

- **Backpropagation:** Training CNNs uses methods like stochastic gradient descent and backpropagation 32 . Backpropagation calculates gradients of the loss function with respect to parameters (@E/@w) and inputs (@E/@x) 33 ... .

- Calculating @E/@x for a convolutional layer involves a sum of "backward convolution" with the transposed filter bank (@E/@y convolved with wT) 35 ... . This is because each input element contributes to multiple output elements through weights, and its gradient receives contributions from the gradients of those output elements 35 ... .

- Calculating @E/@w for a convolutional layer involves accumulating gradients over all pixels in the corresponding output feature map 38 . This is essentially a convolution between the input feature map and @E/@y 38 .

### ◦ **Backward @E/@x Kernel (C code):**

- This code snippet header indicates a function for calculating input gradients. 39 ... . It assumes @E/@y for the current layer is available and space for @E/@x is allocated 37 ... .

- **Backward @E/@w Kernel (C code):**

- This code snippet header indicates a function for calculating weight gradients. 38 ... . It initializes the gradient accumulation to zero and then iterates to sum contributions 40 .

- **Matrix Unroll and Using Matrix Multiplication Instead of Convolution**

- A convolutional layer can be represented as an equivalent matrix multiplication operation (GEMM) to use highly efficient linear algebra libraries like cuBLAS 41 .
- The central idea is **unfolding and duplicating input feature map pixels** such that all elements needed to compute one output feature map pixel are stored as one sequential column in a new matrix 42 ... .
- The filter banks are represented as a matrix where each row contains all weight values needed to produce one output feature map 44 ... . This matrix has dimensions M (output feature maps) by C \* K \* K (total weights per output pixel) 44 ... . There is no duplication of weights in this matrix 45 .
- The output Y is computed by multiplying the filter bank matrix (W) by the expanded input matrix (X\_unrolled) 45 .

- **Data Layouts:**

- Input X: N x C x H x W array 46 .
- Output Y: M x (H\_out \* W\_out) array (produced by multiplication) 47 .
- Filter W: M x C x K^2 array 47 .
- Expanded Input X\_unrolled: (C \* K \* K) x (H\_out \* W\_out) matrix 48 ... . Each column contains input pixels needed for one output pixel 42 ... . Each row corresponds to a specific (c, p, q) position relative to the output pixel location 50 .
- Preparing the X\_unrolled matrix can be complex and increase the input size significantly (up to K^2 times) 47 . A sequential C function to generate X\_unrolled iterates through input channels (c), filter patch dimensions (p, q), and output dimensions (h, w) 48 ... . This process is easily parallelizable 52 .
- **CUDA Unroll Kernel:** Each thread can be responsible for gathering K\*K input elements from one input feature map for one element of an output feature map 52 . The total number of threads would be (C \* H\_out \* W\_out) 53 . Threads can be organized using a 1D block and deriving multidimensional indices 53 .

- **Unroll Kernel Code Example:**

- This kernel maps each thread to a specific (c, w\_unroll) position in the X\_unrolled matrix (equivalently, a (c, h\_out, w\_out) combination) and has it write the KK elements from the input X needed for that column segment\* 54 ... . Adjacent threads write adjacent elements in a row of X\_unrolled 50 .
- Implementing convolutions with matrix multiplication can be very efficient because it leverages highly optimized GEMM libraries 56 . However, materializing the expanded X\_unrolled matrix in global memory

can be costly in terms of space and bandwidth **57**. Optimized libraries like CUDNN avoid this by generating and loading X\_unrolled data directly into on-chip memory instead of storing it globally first **58**

... .

## Week 15: Sparse Matrix Computation (Chapter 14, excluding 14.5, 14.6)

This chapter presents sparse matrix computation as an important parallel pattern **60**. Sparse matrices have a large number of zero elements and are common in applications modeling complex phenomena **60**.

### • Sparse Matrix Vector Multiplication (SpMV)

- SpMV is a key computation involving sparse matrices.
- Due to the large number of zeros, **compaction techniques** are used to reduce storage, memory accesses, and computation on zero elements **60**.
- Different **storage formats** are used, and they impact performance considerations like storage cost, computation, memory access efficiency (especially coalescing), and load balance **61**.

### • COO Format

- COO (Coordinate List) format stores only the nonzero elements of a sparse matrix **61**.
- It typically uses three arrays: one for the nonzero values, one for their row indices, and one for their column indices **62**.
- A simple SpMV kernel using COO assigns one thread to each nonzero element **62**.
- **A simple SpMV kernel with COO:** Multi-threaded access to the output vector requires using **atomic operations** for accumulation, as multiple threads might update the same output element **62**.
- Memory access efficiency is often poor with simple COO kernels because adjacent threads, processing nonzeros that might be far apart in the matrix, access non-adjacent memory locations when writing to the output vector and sometimes reading input vectors **62**.

### • CSR Format

- CSR (Compressed Sparse Row) format is another common sparse matrix storage format **63** ... .
- It groups the nonzero elements by row **64**.
- The sources mention that a CSR representation is needed for vertex-centric push implementations in graph traversal because it provides accessibility to outgoing edges (nonzeros of a given row) **65**.
- The sources also state that code can be implemented to convert from COO to CSR using primitives like histogram and prefix sum **66**.
- The sources do *not* provide kernel code specifically for performing SpMV using the CSR format within the provided excerpts, but mention CSR as a relevant format **63** ... .

### • ELL Format

- ELL (ELLPACK) format is a sparse matrix storage format mentioned as improving memory coalescing **63**.

- The sources list it as one of the formats for representing a sparse matrix **64** .
- The sources do *not* provide kernel code specifically for performing SpMV using the ELL format within the provided excerpts, but highlight its benefit for memory coalescing **63** .

- **Memory Coalescing and Other Considerations**

- Memory access efficiency is a key design consideration for sparse matrix computations **61** .
- In the simple COO kernel, memory accesses are **not coalesced** when adjacent threads read input elements or write to the output vector, leading to poor memory bandwidth utilization **62** . For example, adjacent threads processing A, A **67** , A **67** ... in a matrix might write to widely separated locations in the output vector **62** .
- The ELL format is mentioned specifically as improving memory coalescing **63** .
- Other considerations include storage cost, the amount of computation performed on nonzero elements, and load balance **61** . Different formats compare differently on these considerations **61** .

**Week 14: Sorting and Merging (Chapters 12 excluding 12.7, 12.8; Chapter 13 excluding 13.5, 13.6, 13.8)**

- **Radix Sort (Chapter 13, excluding 13.5, 13.6, 13.8)**

- Radix sort sorts keys by distributing them across buckets based on individual digits **68** . This process is repeated for each digit, preserving order from previous digits **68** .
- The iterations (for each digit) are performed sequentially **69** .
- The opportunity for parallelization arises **within each iteration** **69** . The focus is on implementing a kernel that performs a single radix sort iteration **69** .
- A key step in a radix sort iteration is finding each key's **destination index** in the output list **70** .
- Threads can perform a boundary check, load a key, and extract the bit for the current iteration **70** .
- Threads then **collaborate to perform an exclusive scan on the extracted bits** (0s and 1s) **71** ... . This exclusive scan (prefix sum) is crucial **72** .
- The result of the exclusive scan array, at each position i, contains the number of elements with a value of 0 at the current bit position among elements 0 through i-1 **72** . This allows calculating the destination index **72** .
- The kernel code for a single radix sort iteration needs to handle potential barrier synchronization for the exclusive scan, possibly requiring sophisticated techniques or multiple kernel launches **71** ... .

- **Radix Sort Iteration Kernel Code Example:**

- *Note: The source excerpts for Chapter 13 only provide snippet 13.4 showing logic for finding the bit and calling scan 70 ... . The provided C code above is reconstructed based on the description in the source and is not directly from the source text, which assumes external functions like ExclusiveScan and GetTotalZeros.*

- **Merge Sort (Chapter 13, excluding 13.5, 13.6, 13.8)**

- Merge sort is mentioned as a parallel sort method that can be implemented using the parallel merge implementation 73 ... .
- The sources do *not* provide a detailed algorithm or kernel code for parallel merge sort itself, only indicating that it relies on a parallel merge operation 74 .

#### • Co-Rank Function and Parallel Merge (Chapter 12, excluding 12.7, 12.8)

- Merging involves combining elements from two sorted lists (A and B) into a single sorted list (C) 76 .
- A sequential merge algorithm iteratively compares the current elements of A and B, taking the smaller one 77 .
- For parallel merge, the work is divided among threads, with each thread responsible for producing a subarray of the output list C 78 .
- The **co-rank function** is essential for this parallel approach 78 . For a given rank (index k) in the output list C, the co-rank function determines how many elements come from list A (i) and how many come from list B (j) such that A[i-1] and B[j-1] are the elements that would meet just before C[k] in a sequential merge 78 . In other words, C[k] is the minimum of A[i] and B[j] 76 ... . The co-rank is essentially the pair (i, j) such that i+j=k 78 .
- The co-rank function is implemented using binary search on one of the input arrays 80 . For a target rank k in C, it finds the index i in A such that A[i] is approximately the k-th element when A[i] is merged with B[k-i] 78 . The exact index i is found by checking if A[i] is less than B[k-i-1] and greater than or equal to B[k-i] (assuming appropriate boundary checks) 76 . The corresponding j is k-i 78 .
- Each thread calls the co-rank function twice: once for its starting output index (k\_curr) to find (i\_curr, j\_curr), and once for the next thread's starting output index (k\_next) to find (i\_next, j\_next) 78 ... . This determines the subarrays of A and B that the thread needs ((i\_next - i\_curr) from A and (j\_next - j\_curr) from B) to produce its output subarray C[k\_curr] through C[k\_next-1] 79 .
- A basic parallel merge kernel (Fig 12.9 referenced) uses threads to calculate their start/end indices using the co-rank function and then calls a sequential merge function on the identified subarrays 78 ... .
- **Basic Merge Kernel Code Example (Conceptual, based on Fig 12.9 description):**
- The basic kernel has poor memory access efficiency 82 . When threads call the sequential merge function, adjacent threads access non-adjacent memory locations for input and output subarrays 82 . Co-rank function accesses (binary search) are also irregular 80 .
- A **tiled merge kernel** improves efficiency 83 ... . Blocks collectively process larger subarrays 83 . Co-rank is called at the block level to find block-level subarray boundaries 83 .
- Threads in a block **cooperatively load elements** of the block-level A and B subarrays into **shared memory** in a coalesced pattern 83 ... .
- Due to limited shared memory, processing is iterative 87 . In each iteration, threads load tiles from global to shared memory and then merge portions within shared memory 87 ... .

- The tiled kernel achieves substantial reduction in global memory accesses for the co-rank function and makes global memory accesses for loading data **coalesced** 90 .

## Week 13: Convolution on CUDA (Chapter 7)

Based on the provided sources, there is **no information available** regarding Convolution on CUDA from Chapter 7. The excerpts only include material from Chapter 10 onwards.

## Week 12: Reduction and Prefix Sum (Chapters 10 excluding 10.8; Chapter 11 excluding 11.7)

### • Reduction on CUDA (Chapter 10, excluding 10.8)

- Reduction is an important parallel pattern used in many data-processing applications 91 . It involves combining elements of an array into a single result (e.g., sum, minimum, maximum) 92 .
- Sequential reduction uses a loop to visit all elements 92 .
- Parallel reduction algorithms use the basic concept of **reduction trees** 92 >< 93 .
- A simple reduction kernel implements a reduction tree **within a single block** 93 . For N elements, it uses N/2 threads 93 .
- In each time step (iteration), threads add pairs of elements, producing partial sums 94 ... . The number of active threads halves in each step 94 .
- A **stride** variable is used for threads to locate the appropriate partial sums 96 . The stride doubles in each iteration (1, 2, 4, ...) 96 .
- Threads execute the same kernel code, but an **if**-condition based on `threadIdx.x` determines which threads are active and perform the addition 97 . Threads failing the condition are inactive 97 . Fewer threads are active as iterations progress 97 . Only thread 0 remains active at the last iteration 97 .
- `__syncthreads()` is used within the loop to ensure partial sums are written to memory before being read by active threads in the next iteration 97 ... .

#### ◦ Simple Sum Reduction Kernel Code Example (Based on Fig 10.6 description):

- The simple kernel (Fig 10.6) results in a **high degree of control divergence** 98 . Active and inactive threads are mixed within warps 98 ... . For example, in the first iteration, half the threads are inactive 98 .
- An **improved reduction kernel** (Fig 10.9 referenced) aims to minimize control divergence 100 . It uses a different access pattern where threads process elements that are further apart initially 100 . This kernel still has an **if**-statement 100 . However, the pattern ensures that whole warps become inactive together, **eliminating control divergence within warps** for certain strides (e.g., warps 0 and 1 active, warps 2 and 3 inactive for a 128-thread block, warp size 32) 99 .
- Using **shared memory** further optimizes reduction by reducing global memory accesses 101 . The kernel (Fig 10.11 referenced) first loads data into shared memory, performs reduction in shared memory, and then thread 0 writes the final sum to global memory 101 . `__syncthreads()` is used before the loop to synchronize shared memory access 101 .

- For large inputs beyond a single block's capacity, **hierarchical, segmented multiblock reduction** is used 102 . The input array is partitioned into segments, each processed by a different block 102 . Each block performs a reduction tree on its segment independently 102 . The results from each block are accumulated to the final output using an **atomic add operation** 102 ... . Partitioning is done by assigning a segment based on the block index 104 .

#### • Prefix Sum on CUDA (Chapter 11, excluding 11.7)

- Prefix sum (scan) is an important algorithm component for parallelizing many applications 105 .
- Work efficiency is a key consideration in analyzing parallel algorithms 106 .
- A sequential inclusive scan algorithm iterates through the input, adding the current element to the previous result to generate the next output element 107 . Its computational complexity is O(N) 108 .
- Parallel segmented scan algorithms partition the input into segments, with each thread block performing a scan on a segment 108 ... .
- The **Kogge-Stone algorithm** is a parallel inclusive scan algorithm 109 . It involves multiple iterations where elements are updated by adding a value from a stride distance away 110 . The stride doubles in each iteration (1, 2, 4, ...) 110 ... .
- A Kogge-Stone kernel performs local scans on segments small enough for a single block 112 . Input elements are loaded into shared memory by threads collaboratively 111 ... . Each thread is assigned to an element in the shared memory array (XY) 114 .
- The core iterative calculation in the Kogge-Stone kernel updates elements in shared memory based on elements stride away 113 . `__syncthreads()` is used to synchronize between iterations 111 .
- **Kogge-Stone Scan Kernel Code Example (Fig 11.3):**
  - This kernel loads data to shared memory 111 , performs the scan in shared memory using a loop with doubling strides 111 ... , synchronizes each step 111 , and writes results to global memory 113 .
  - An **exclusive scan kernel** can be adapted from the inclusive scan kernel with minor adjustments to how input elements are loaded 115 ... .
  - The **Brent-Kung algorithm** is another parallel scan algorithm, generally faster through the reduction tree phase but potentially slower due to SIMD inefficiencies 117 . It can also be adapted for exclusive scan 116 .
  - For higher work efficiency, a **coarsened scan** can be used, divided into three phases 118 : 1) each thread performs a sequential scan on its subsection, 2) threads collaborate to perform a scan on the last element of each section (using Kogge-Stone or Brent-Kung), and 3) results from the second phase are used to update the elements in each subsection 118 ... .
  - For arbitrary-length inputs (millions/billions), a **hierarchical scan** approach is needed to consolidate results from different sections(blocks) 121 ... . After initial block-wide scans (scan blocks), each element contains the accumulated value only within its

block 122 .

- These block scan results need to be combined by adding the sum of all preceding blocks' elements to each element of a given block 122 ... .
- This consolidation can be implemented with **three kernels** 124 ... :
  1. A kernel (like Kogge-Stone or Brent-Kung) performs the block-wide scan and writes the sum of each block to a separate array (S) 124 ... .
  2. A second kernel performs a scan (e.g., Kogge-Stone or Brent-Kung with a single block) on the S array to get the cumulative sum of block sums 125 .
  3. A third kernel takes the cumulative block sums from the scanned S array and adds the appropriate sum to each element in the Y array (which still holds the block-local scan results) 125 ... . Threads in a block add the sum of all previous scan blocks to the elements of their scan block 126 .
- Storing and reloading partially scanned results (scan blocks) to global memory between these kernels can affect performance 126 ... .

I hope this detailed explanation drawing from the provided sources is helpful!