CSC290/420 ML Systems for Efficient AI
Compound Structures / Memory

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URCS

Outline

Structures and Unions

Arrays, Matrices, and Tensors

Sparse Data Structures

Performance and Efficiency Considerations

Outline

Record Types

```
struct point {
    float x;
    float y;
};

struct point pt;
struct point pts[10];
struct point *polygon;
```

- `struct` holds multiple values
- Each *field* of struct has a name
- `struct` can be nested

Recursive structures

```
struct node {
   int value;
   struct node *left;
   struct node *right;
};
```

- This is a *recursive* structure
  - Possibly from a binary tree
- The "self-references" must be pointers

`struct` interactions with pointers

```
struct node {
   int value;
   struct node *left;
   struct node *right;
};

struct node *head;
```

Which of these accesses `head`'s right node?

- `*head.right`
- `(*head).right`

The -> operator

```
struct node {
   int value;
   struct node *left;
   struct node *right;
};

struct node *head;
```

Since field access (`.`) has higher precedence than deference, you must use (*head).right.

- Alternative: `head->right`, which has same precedence as `.`

Structure Layout

```
#include <stdio.h>

struct node {
  int value;
  struct node *left;
  struct node *right;
};

int main(void) {
  printf("%d\n", sizeof(struct node));
}
```

Output (on a LP64, i.e. long and pointers are 64-bits, system)?

- 20
- 24
- 32

Structure Memory Layout

Tight packing:

```
value left      right
[0123][01234567][01234567]
```

Packing with "holes" (also called padding)

```
value       left      right
[0123][0123][01234567][01234567]
```

- Structure layout in memory is implementation defined
- Usually:
  - Struct size is a multiple of largest field
  - Each individual field is naturally aligned

Unions

```
union intvar {
  char c;
  short s;
  int i;
  long l;
};
```

- Like `struct`, `union` contains fields
- However, all fields in a `union` *overlap* in memory
    - At most one contains valid data

Union Memory Layout

```
c|
s-|
i---|
l-------|
[01234567]
```

- This union occupies 8 bytes of memory
  - The size of its largest field
- But all fields overlap
  - Writing to one changes the others as well
- Writing to one field, and reading that data through another field is allowed
  - But it is implementation-defined

Outline

Memory Allocation

- From a program's perspective, memory is obtained using an *allocator*
  - The memory is then reserved for the program and unavailable for other programs
  - Must be de-allocated once it is no longer needed
  - Memory is allocated from the "heap"
- Manual memory management (C, C++, CUDA)
  - Programmer must explicitly deallocate memory
- Garbage collection (Java, Python, etc.)
  - Deallocation is automatic

C Runtime Allocator

The C standard library supports the following *heap* allocators, all require including `stdlib.h`:

- `malloc`: allocate memory of a certain size
- `calloc`: allocate memory and zero it
- `realloc`: change size of memory (may move data)
- `free`: free memory allocated by the above functions

- All allocators return a pointer to the newly allocated region of memory or NULL if they fail.

C memory allocation

```
 #include <stdlib.h>

void *malloc(size_t size);
void free(void *ptr);
void *calloc(size_t nmemb, size_t size);

int *p;

// allocate 1000 ints, note size is size in bytes
p = (int *) malloc(1000 * sizeof(int));

// --- OR --- //

// or allocate 1000 ints initialized to zero
p = (int *) calloc(1000, sizeof(int));

// free allocated memory
free(p);
```

Allocating an array on the heap

```
int *alloc_and_init_array(int N) {
    int *x;

    x = (int *) malloc(N * sizeof(int))

    // initialize it
    for(int i = 0; i < N; i++)  {
        x[i] = i*i;
    }

    return x;
}
```

- Note we're returning the value of `x`
  - I.e. the address *in* `x`, not the address *of* `x`
- Since the address is on the heap, it is independent of the function call
- You can treat pointers to the heap as any other pointer

Common Bugs using Dynamic Memory

- Memory leaks
  - When you lose the pointer to an allocated region of memory
  - Can't be freed until program exits
  - "harmless", program just consumes more and more memory as it runs
- Reading uninitialized memory
  - Memory from `malloc` should be initialized before reading it
- Out-of-bound accesses
  - Pointer points outside the allocated region
  - Undefined behaviour!
- Use-after-free
  - Attempt to access memory region after `free`
  - Essentially a dangling pointer pointing to the heap
  - Dangerous!
- Double-frees
  - Trying to call `free` on the same pointer twice
  - Undefined behaviour!

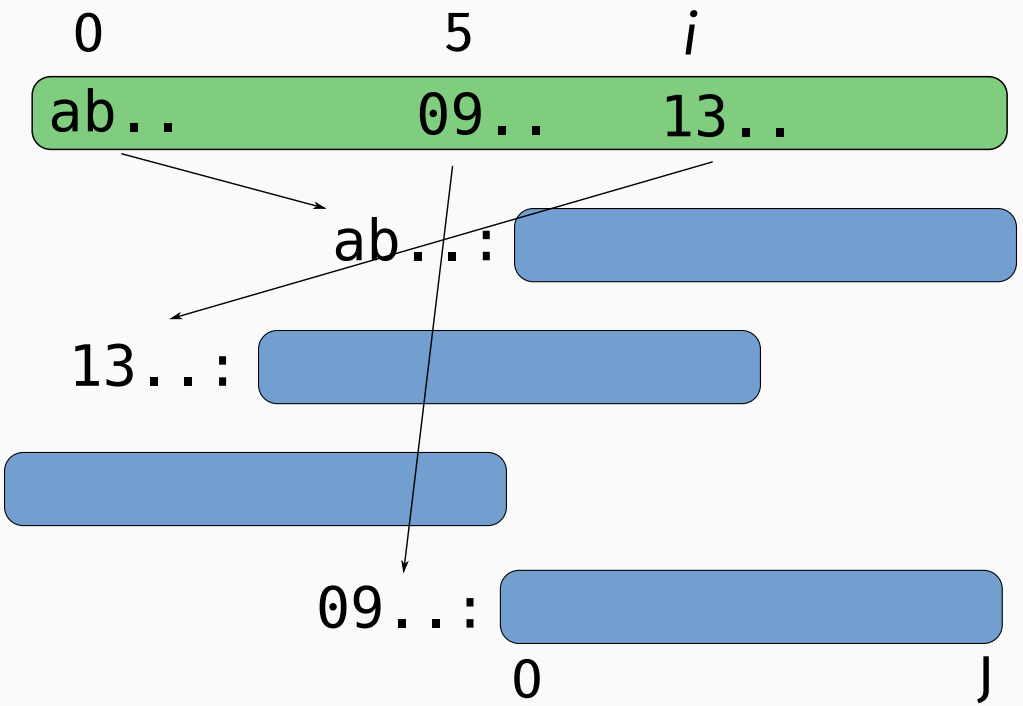
Arrays and Matrices

- Memory is 1-dimensional
  - addresses are linear ranging from 0 to some N
  - each address is a byte
- 1-D arrays are similar
  - indices range from 1 to some n, where n is the number of elements
  - i.e. arrays have a type and each index references an element
  - translation of index to address:
    $address = index * sizeof(element)$
- Most languages also support multidimensional arrays
  - `A[i][j]`
- These must be mapped to 1-D memory
  - Multiple schemes exist

Implementing Multidimensional Arrays

- Scheme 1: All data is stored contiguously in a 1-D array
  - Requires translation of a multidimensional index (i, j, k) into a 1-D index
- Scheme 2: All dimensions are 1-D arrays of *pointers*, except the last which contains data
  - Requires multiple pointer deferences `A[i][j][k]`: load `A[i]` (a 1-D array), then look up `j` (another 1-D array), and look up k-th element as data

Pointer-based Scheme



- Example of a 2-D array implemented as an 1-D array of pointers to 1-D data arrays

Contiguous Storage

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{bmatrix}$$

[0 1 2 3 4 5] *row-major*

[0 3 1 4 2 5] *column-major*

0 5

- For access `A[row][col]`
- Row major: $\text{index} = \text{row} * \text{COLS} + \text{col}$
- Column major: $\text{index} = \text{col} * \text{ROWS} + \text{row}$
- The address then multiplies the index by the size of the element.
- Extension to more than 2 dimensions?

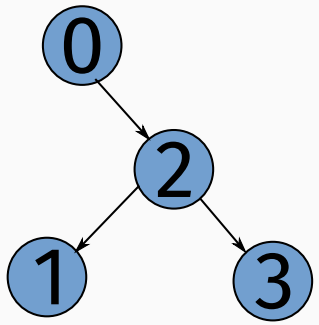
Outline

Dense and Sparse Matrices

- A sparse matrix is one in which the number of non-zeroes (NNZs) is significantly lower than the number of zeroes
- Occur commonly in large linear systems used in computational science
- Very common when storing graphs using *adjacency matrix notation*
- Most weight matrices in ML are *dense*, but increasing interest in sparse matrices

Sparse Matrices

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{bmatrix} \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



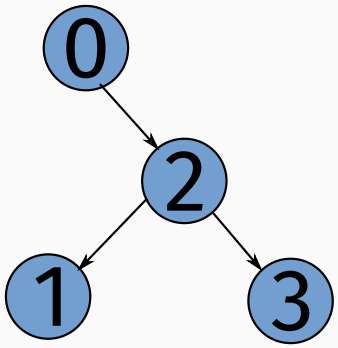
$$\begin{matrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{matrix}$$

- Dense matrix
- Sparse matrix
- Graph
- Adjacency matrix representation of graph

Storing Sparse Matrices

- Various sparse formats
- COO - coordinate format
- CSR - compressed sparse row
- CSC - compressed sparse column

COO storage

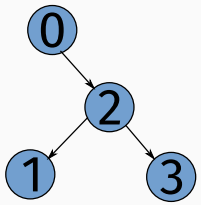


0 0 1 0
0 0 0 0
0 1 0 1
0 0 0 0

row [0 2 2]
col [2 1 3]

- Two arrays (`row` and `col`) track positions of non-zeroes
- An additional data array may be present to store the values in the cells
    - Here, all values are 1, so no data array needed

CSR storage



$$\begin{matrix}0&0&1&0\\0&0&0&0\\0&1&0&1\\0&0&0&0\end{matrix} \rightarrow \begin{matrix}0&0&2&0\\0&0&0&0\\0&1&0&3\\0&0&0&0\end{matrix} \rightarrow \begin{matrix}[\,2\,]\\[\,]\\[1\,3]\\[\,]\end{matrix}$$

$$\begin{aligned} \textit{col} &\quad [\,2\,1\,3\,] \\ \textit{row\_start} &\quad [\,0\,1\,1\,3\,3\,] \end{aligned}$$

- First, the positions of the 1s are noted
  - can be seen as replacing 1s with their index
- Second, the zeroes are dropped
  - yields variable length column arrays for each row
- Third, these column arrays are concatenated to form a 1-d array `col`
- Fourth, a `row_start` array indicates the start and end of each row
  - start: `row_start[row]`
  - end (exclusive): `row_start[row+1]`
- A data array may also be present

CSR issues

- Indirect accesses
  - Need to load multiple values to get data
  - Similar to pointer-based schemes for multidimensional arrays
- Hard to vectorize
  - hence other formats: ELLPACK (block sparse)
- Changing a zero to a non-zero requires rewriting the structure!
  - mostly used for read-only data

Outline

Considerations

- Assume byte-addressable memory
  - but data is transferred in multibyte blocks (say, 32 bytes)
- Is space usage efficient?
- Is data access efficient?
- Can data access code be vectorized?

AoS vs SoA

```
struct pt {
  float x;
  float y;
};

struct pt pts[10];  // array of structures
```

OR

```
struct pts {
  float *x;
  float *y;
};

struct pts p;   // structure of arrays

p.x = malloc(...);
p.y = malloc(...);
```

Row-major vs column-major

```
for(row=0; row < NROWS; row++)
   for(col=0; col < NCOLS; col++)
       out[row * NCOLS + col] = in[col * NROWS + row];
```

Sparse vs Dense

```
for(row = 0; row < NROWS; row++) {
  for(j = row_start[row]; j < row_start[row+1]; j++) {
      column = col[j];
    }
}
```