

Algorithms for Data Science (Part 1 - Data Structures)

Daniel Lawson — University of Bristol

Lecture 08.2.1 (v1.0.1)

Signposting

- ▶ This lecture 8.2 of Algorithms for Data Science follows 8.1 on Analysing Algorithms
 - ▶ It is about some key algorithms that make Data Science approachable, even without a Big Data Platform.
 - ▶ These ideas are building blocks for statistical and machine-learning approaches for inference.
- ▶ The lecture is in two parts:
 - ▶ Part 1 Data Structures
 - ▶ Part 2 Algorithms
- ▶ This is Part 1, covering **Dynamic Data Structures:**
 - ▶ Hashing
 - ▶ Queues/Stacks
 - ▶ Linked Lists
 - ▶ Binary Trees/Heaps
 - ▶ Hash tables

ILOs

- ▶ ILO2 Be able to **use and apply basic machine learning** tools
- ▶ ILO4 Be able to use high throughput computing infrastructure and understand appropriate algorithms
- ▶ ILO5 Be able to reason about and conceptually align problems involving real data to appropriate theoretical methods and available methodology to correctly make inferences and decisions

Hash functions

- ▶ One of the most important components in good algorithmic design is the **hash**.
- ▶ Simply, a hash h is a map for $h(x) = u$ with:

$$x \in \mathcal{X} \rightarrow u \in \mathcal{U}[0, r).$$

- ▶ i.e., we map each item in the space \mathcal{X} into the Uniform distribution on the integers $0, \dots, r - 1$.
- ▶ Each item will always map to the same integer.

Hash examples

- ▶ Some simple methods for creating keys from integers.
- ▶ Open DSA - Data Structures and Algorithms is a great reference.
- ▶ Modulo r

`x % 16 # modulo 16`

Hash examples

- ▶ Some simple methods for creating keys from integers.
- ▶ Open DSA - Data Structures and Algorithms is a great reference.
- ▶ Modulo r

```
x % 16 # modulo 16
```

- ▶ Binning (floor function or integer division)

```
x // 32 # need to know max(N) for r
```

Hash examples

- ▶ Some simple methods for creating keys from integers.
- ▶ Open DSA - Data Structures and Algorithms is a great reference.
- ▶ Modulo r

`x % 16 # modulo 16`

- ▶ Binning (floor function or integer division)

`x // 32 # need to know max(N) for r`

- ▶ Mid-Square method: square the value, use the middle digits in the hash

Hash considerations

- ▶ There are many choices for a hash function in practice. Considerations include:
- ▶ **Randomness**. For many applications (e.g. cryptography) we want no correlation between x and u .
- ▶ **Locality**. For other applications (e.g. locality sensitive hashing) we want similar x to produce similar u .
- ▶ **Collisions**. We may wish to reduce collisions on a subset of the potential input space. For example, if $x \in [0, r)$ and $u \in [0, r)$ it is possible to eliminate collisions.
- ▶ **Compute**. Hash functions vary in their compute cost.
- ▶ **Families**. It is often useful to be able to index a family of hash functions with the same computational cost that return different values.

Data Structures

- ▶ Data structures are representations of a **set** of data
- ▶ This representation is particularly important when sets are **dynamic**, i.e. grow or shrink
- ▶ We will perform **operations** on the set, which will have an associated computation cost
- ▶ The data structure has an associated space cost
- ▶ Making the right choice of data structure is an essential component of data science

Fixed size elementary data structures

- ▶ We are familiar with the concepts of:
 - ▶ **Arrays**: A segment of memory containing n data of the same type
 - ▶ **Vectors**: Arrays with additional operations defined
 - ▶ **Multi-dimensional arrays**: Arrays of length $n = n_0 \times n_1 \times \cdots \times n_k$, with entries specified according to a protocol (e.g. row-wise)
 - ▶ **Matrices/Tensors**: Multidimensional arrays with additional operations defined
- ▶ It is clear that arrays are a fundamental concept!

Elementary data structures: Stacks and Queues

5	1	5	12	3	1	7	12		
---	---	---	----	---	---	---	----	--	--

- ▶ **Stacks:** Data are stored in an array using “first in, last out”: insertions and deletions occur at the same end
 - ▶ Implemented as a pointer to the last read location
- ▶ **Queues:** Data are stored in an array using “first in, first out”: insertions occur one end, deletions the other
 - ▶ Implemented as a pointer to the end (for writing) and start (for reading) that tracks removed items

Elementary data structures: Stacks and Queues



- ▶ **Stacks:** Data are stored in an array using “first in, last out”: insertions and deletions occur at the same end
 - ▶ Implemented as a pointer to the last read location
- ▶ **Queues:** Data are stored in an array using “first in, first out”: insertions occur one end, deletions the other
 - ▶ Implemented as a pointer to the end (for writing) and start (for reading) that tracks removed items

Elementary data structures: Stacks and Queues

5	1	5	12	3	1	7	12		
---	---	---	----	---	---	---	----	--	--

- ▶ **Stacks:** Data are stored in an array using “first in, last out”:
insertions and deletions occur at the same end
 - ▶ Implemented as a pointer to the last read location
- ▶ **Queues:** Data are stored in an array using “first in, first out”:
insertions occur one end, deletions the other
 - ▶ Implemented as a pointer to the end (for writing) and start (for reading) that tracks removed items

Elementary data structures: Stacks and Queues



- ▶ **Stacks:** Data are stored in an array using “first in, last out”: insertions and deletions occur at the same end
 - ▶ Implemented as a pointer to the last read location
- ▶ **Queues:** Data are stored in an array using “first in, first out”: insertions occur one end, deletions the other
 - ▶ Implemented as a pointer to the end (for writing) and start (for reading) that tracks removed items

Elementary data structures: Stacks and Queues



- ▶ **Stacks:** Data are stored in an array using “first in, last out”: insertions and deletions occur at the same end
 - ▶ Implemented as a pointer to the last read location
- ▶ **Queues:** Data are stored in an array using “first in, first out”: insertions occur one end, deletions the other
 - ▶ Implemented as a pointer to the end (for writing) and start (for reading) that tracks removed items

Elementary data structures: Stacks and Queues

5	1	5	12	3	1	7	12		
---	---	---	----	---	---	---	----	--	--

- ▶ **Stacks:** Data are stored in an array using “first in, last out”:
insertions and deletions occur at the same end
 - ▶ Implemented as a pointer to the last read location
- ▶ **Queues:** Data are stored in an array using “first in, first out”:
insertions occur one end, deletions the other
 - ▶ Implemented as a pointer to the end (for writing) and start (for reading) that tracks removed items
- ▶ Despite implementation similarities, both have different Data Science properties!

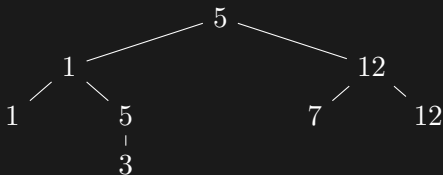
Elementary data structures: Linked List



- ▶ **Linked list:** Data are stored in a list, with a pointer to the location of the next item
 - ▶ Fast traversal, insertion and deletion
 - ▶ Slow random access
 - ▶ Can be doubly linked

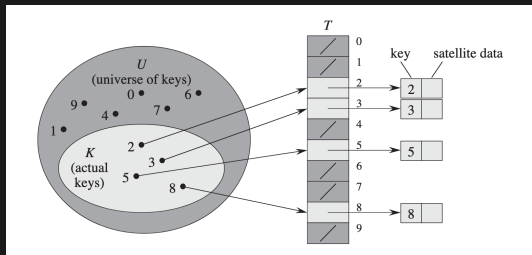
Elementary data structures: Binary Trees & Heaps

5	1	5	12	3	1	7	12		
---	---	---	----	---	---	---	----	--	--



- ▶ **Binary Trees:** Data are stored in a **binary** linked list, i.e. each node has (up to) two children
 - ▶ Data can be stored at nodes or leaves
 - ▶ **Critical** to define the left/right operation!
- ▶ Position is decided by a key, which can be related to the value
 - ▶ In the picture, values $\leq x$ go left, $> x$ go right
 - ▶ Some binary tree structures assign values to internal nodes, e.g. means/ranges
- ▶ **Heaps:** A binary tree where each node's key is (larger) than it's children

Elementary data structures: Hash Tables



- ▶ **Hash Tables:** Data location determined by the **key**
- ▶ The key is a **hash** $x = h_1$: either of an attribute (e.g. a name), or of the value
- ▶ Advantage is $O(1)$ lookup cost. Usage is:
 1. Compute $u = h_2(x)$
 2. Set $u' = u \% r$
 3. To insert: store y at this position. On collision, we use some rule to find an empty space, such as rehashing, or storing a linked list.
 4. To lookup: retrieve this value (using the same rule about collisions).

Signposting

- ▶ See 8.2 Part 2 on Algorithms for Data Science

References

- ▶ Data structures:
 - ▶ Cormen et al 2010 Introduction to Algorithms is very accessible and recommended for data structures.
 - ▶ Open DSA - Data Structures and Algorithms.