Scientific Computation

Spring 2019

Lecture 4

Imperial College
London

22 January, 2019

Today

- Constant-time search

- Lecture 2: Binary search applied to sorted array requires $\log_2 N$ operations
- Can we do better?

- **Lecture 2: Binary search applied to sorted array requires $\log_2 N$ operations**

- **Can we do better?**

- **Proposal: Set the value of an integer as index in an array**

6	8	23	32

  - **Then for the example above we would have an array (or list),** X, **where** X[6] = X[8] = X[23] = X[32] = 1

  - **Speed for search would be constant time** (O(1))

  - **But many weaknesses:**
    - **What about more general data (not just non-negative integers)**
    - **Inserting and deleting entries would require** O(N) **time**

Searching

- Lecture 1: Binary search applied to sorted array requires $\log_2 N$ operations
- Can we do better?
- Real-world problem:
  - A startup is keeping track of unique visitors to its website each month
  - Each visitor must be assessed as “new” or “repeat”
  - Visitors who have not visited in 30+ days must be removed
  - Everything must be fast and accurate!

Searching

- **Lecture 1: Binary search applied to sorted array requires $\log_2 N$ operations**

- **Can we do better?**

Searching

- Visitors are identified by IP addresses
  - IP addresses are 4 8-bit numbers which (in base-10) take the form: 251.31.241.80 and identify a user's location on the internet
  - There are 256^4 possible addresses so it's not feasible to maintain an array for all possible addresses
  - Could maintain a sorted list but inserting new addresses would require O(N) operations (in Python)

Searching

- **Visitors are identified by IP addresses**
  - **IP addresses are 4 8-bit numbers which (in base-10) take the form: 251.31.241.80 and identify a user's location on the internet**
  - **There are 256^4 possible addresses so it's not feasible to maintain an array for all possible addresses**
  - **Could maintain a sorted list but inserting new addresses would require O(N) operations (in Python)**

- **Alternate approach: IP addresses are assigned indices based on their values**
  - **A *hash function* takes an address as input and provides and index as output**
  - **The design of hash functions is an important and active subject**
  - **What are the "desirable" properties of a hash function?**

Hash function

- **Consider a hash function** $i = H(a)$
  - i **is a non-negative integer**
  - a **is a numeric representation of an IP address**
  - **Let's say we expect about** 1e3 **unique visitors each month**

- **Then,** H **should distribute these visitors to about** 1e3 **indices**
  - **Desirable property 1: It should always assign a particular IP to the same index on repeat visits**

Hash function

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- **Then,** H **should distribute these visitors to about** 1e3 **indices**
  - **Desirable property 1: It should always assign a particular IP to the same index on repeat visits**

- **Since there are** 256^4 **possible IPs, it is impossible to design H so that unique visitors are always assigned unique indices**
  - **When two or more different IPs are assigned the same index, we have a *hash collision***
  - **Say** $0<=i<=N$**. Desirable property 2: *Probability of 2 distinct visitors being assigned same index,*** i ***should be*** $1/N$

Hash function

An example:

- **The IP address is four integers,** a_1,a_2,a_3,a_4
- **Choose four arbitrary integer weights,** w_1,w_2,w_3,w_4

- **Is:** $i = \Sigma w_j a_j$ **a suitable hash function?**

Hash function

An example:

- **The IP address is four integers,** a_1,a_2,a_3,a_4
- **Randomly choose four arbitrary integer weights,** w_1,w_2,w_3,w_4

- **Is:** $i = \Sigma w_j a_j$ **a suitable hash function?**

- **Not quite:**
  - **This can generate** 256^4 **indices, we only want about** 1e3

- **What about** $i = (\Sigma w_j a_j) \bmod 1000$**?**
  - **We'll now have the right number of indices**
  - **But if there are patterns in the IPs, could have large number of visitors assigned the same index**

- **Better to use a prime number,** $i = \Sigma w_j a_j \bmod 997$

Hash function

Better to use a prime number, $i = h(a_j) = \Sigma w_j a_j \bmod 997$

- **How well does this function work?**
- **Given two different addresses** a **and** b**, what is the probability that** $h(a) = h(b)$**?**

Let's assume that $a_4 \neq b_4$ **and that the weights are 4 random integers** mod 997

- **There will be a hash collision if:** $\sum_{j=1}^{4} w_j a_j \equiv \sum_{j=1}^{4} w_j b_j \pmod{997}$

where $x \equiv y \pmod{\mathrm{n}}$ if n divides $x - y$

- **Rearranging:** $\sum_{j=1}^{3} w_j (a_j - b_j) \equiv w_4 (b_4 - a_4) \pmod{997}$
- **The LHS is just some, integer,** c**, and we need to "solve" the following congruence for** w_4: $w_4(b_4 - a_4) \equiv c \pmod{997}$

Hash function

$$w_4(b_4 - a_4) \equiv c \pmod{997}$$

To solve this for w_4, need a result from modular arithmetic:

Let p *be a prime. If* k *is not a multiple of* p*, then there exists an integer* $k^{-1} \in \{1, 2, \ldots, p-1\}$ *such that:* $k \cdot k^{-1} \equiv 1 \pmod{p}$

Hash function

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In our example, $p=997$, $k = (b_4-a_4)$
so, $w_4 \equiv c(b_4 - a_4)^{-1} \pmod{997}$

We *choose:* $w_4 = c(b_4-a_4)^{-1} \bmod 997$
and more generally, require: $w_i \in \{0, 1, ..., p-1\}$

This allow us to state that there is only one w_4 in the range [1 p-1] for which a and b will be assigned the same index.
So, probability(h(a)=h(b)) = 1/p.

Hash table

- **We now have a hash function that will assign indices to IP addresses**

- **What is the general workflow?**

  0. Initialize a dictionary or list (a *hash table)* where you will store addresses
  1. **Given an IP, compute an index**
  2. **And store the IP in the corresponding location in the hash table**
  3. **Append the IP if there is already an address in the computed list**

Hash table

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  0. Initialize a dictionary or list (a *hash table)* where you will store addresses
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- Let's assume that we have M IP addresses and N indices with M>N

- On average, each index will be assigned M/N IPs

- Should choose M to be a prime number close to N (in practice, maybe close to 2N)

Hash table

We started looking for something faster than binary search

What is the cost of using a hash table?

- ***Search* (lookup): Given an IP, find it in the table**
  - **Evaluate the hash function and obtain an index**
  - **Check the number of items stored at index, i.**
  - **If $i > 1$, iterate through items**
  - **Overall, $O(\max(1,M/N))$**
  - **For well-designed hash table and function, will be close to $O(1)$!**

- ***Insert*: Add an IP to table**
  - **Search**
  - **Then append at computed index if IP is not already present**
  - **Overall, close to $O(1)$ – for a careful implementation**

- ***Delete*: Remove an IP**
  - **Same as Insert, just replace "append" with "delete"**

Hash table

Summary:

- **Binary search:** $O(\log_2 N)$ **but requires the maintenance of a sorted list/array**

- **Hash table:** $O(1)$ **for search as well as maintenance**
  - **Provided that the hash function and table are both well-designed!**

Hash table

Summary:

- **Binary search: $O(\log_2 N)$ but requires the maintenance of a sorted list/array**

- **Hash table: O(1) for search as well as maintenance**
  - **Provided that the hash function and table are both well-designed!**

- **What does this look like in Python?**

  - **Let’s move away from the IP problem to a more general task**

  - **Consider input that may be real numbers or even non-numeric**

Python hash function

Python provides a hash function that returns an integer for (almost) any input

- **For an integer,** i, hash(i) = i
- **For two inputs if** a==b **then** hash(a)=hash(b)
  - hash(3.0) = hash(3) = 3
- **For non-integers, the function is less predictable:**

```
In [1]: hash('m3sc')
Out[1]: 5237192937700339269

In [2]: hash('m3c')
Out[2]: 1091467703030128764
```

Python hash table

Can use list of lists to build hash table

- **Compute hash for each item of interest**
- **Store item using hash value as index for list**
- **For hash collisions, append item at index**
- **Lookup:**
  - **Compute hash value**
  - **Search through sub-list at index for item**
- **Not too difficult – try it!**

Python dictionaries

- **But we don't have to build our own hash table!**

- **Python dictionaries *are* hash tables**
  (technically, they are "associative arrays")

- **Dictionaries are containers where each element is a key-value pair**
  - **A key can be considered a label or id**
  - **Example:**

```
In [6]: key = "123.45.241.12"

In [7]: value=[14,1,2019,20]

In [8]: d = {key:value}

In [9]: d
Out[9]: {'123.45.241.12': [14, 1, 2019, 20]}

In [10]: d["123.45.241.12"]
Out[10]: [14, 1, 2019, 20]
```

Python dictionaries

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  - Example:

```
In [6]: key = "123.45.241.12"

In [7]: value=[14,1,2019,20]

In [8]: d = {key:value} #or d[key]=value

In [9]: d
Out[9]: {'123.45.241.12': [14, 1, 2019, 20]}

In [10]: d["123.45.241.12"]
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```

  - Python applies a hash function to keys to know where to store them and where to look for them

Python dictionaries

- **Important dictionary operations**

***Constant time* O(1):**

```
In [36]: d = dict()     #initialize a new dictionary

In [37]: d[key] = value #associate key with value and store in d

In [38]: d[key]  #value associated with key in d, raises KeyError if key has not been added to d
Out[38]: [14, 1, 2019, 20]

In [39]: x=1

In [40]: d.get(key,x) #value associated with key if key is present, otherwise x
```

Python dictionaries

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In [40]: d.get(key,x) #value associated with key if key is present,
otherwise x

In [42]: key in d   #is key in d?
Out[42]: True

In [43]: len(d)   #number of key-value pairs in d
Out[43]: 1

In [44]: del d[key]  #remove key (and its associated value) from d
```

Python dictionaries

- **Important dictionary operations**

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```
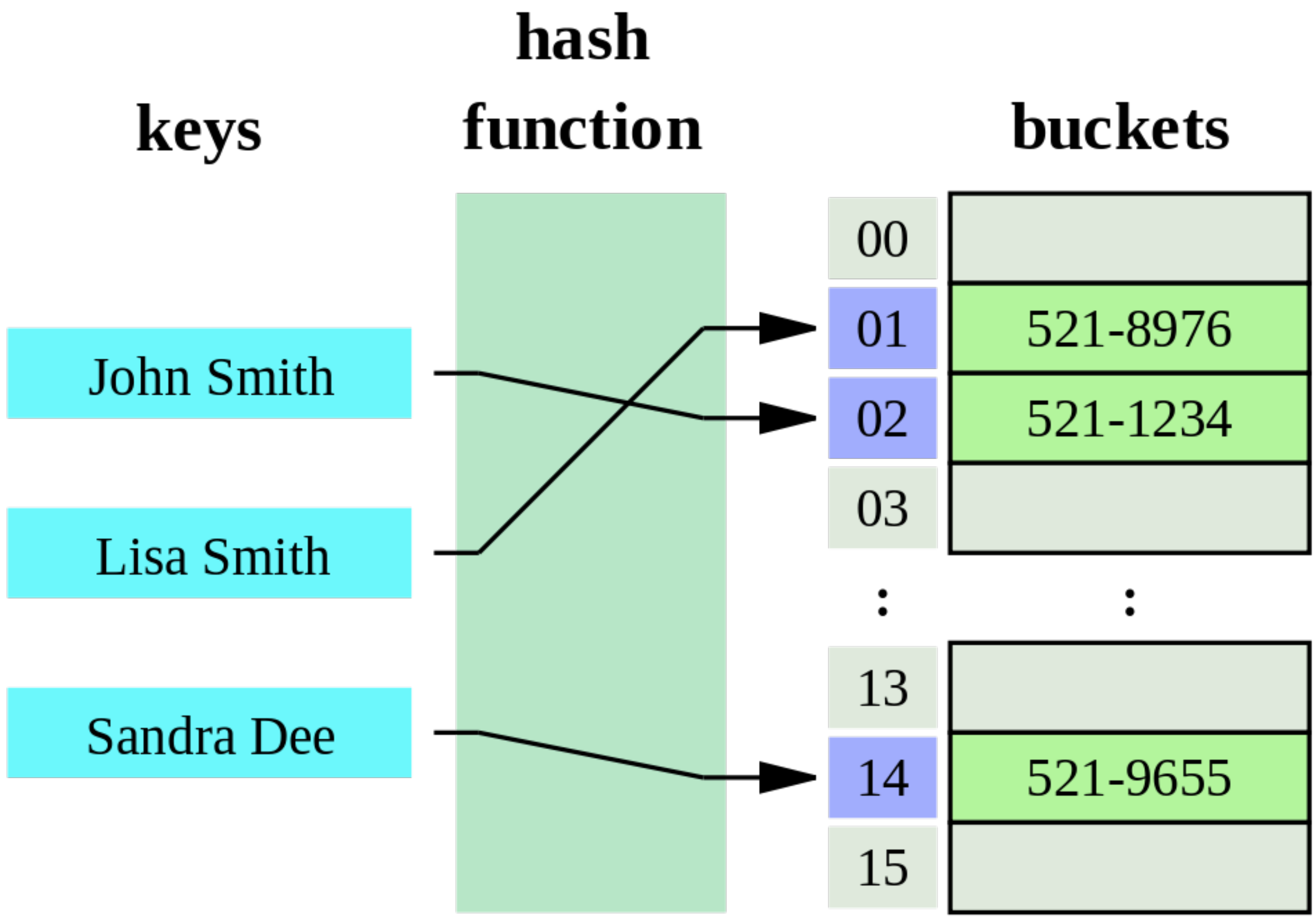

***linear time* O(N):** `In [45]: for key in d:   # iterate over keys in d`

This is exactly what we need to build and maintain a hash table.

Python hash table



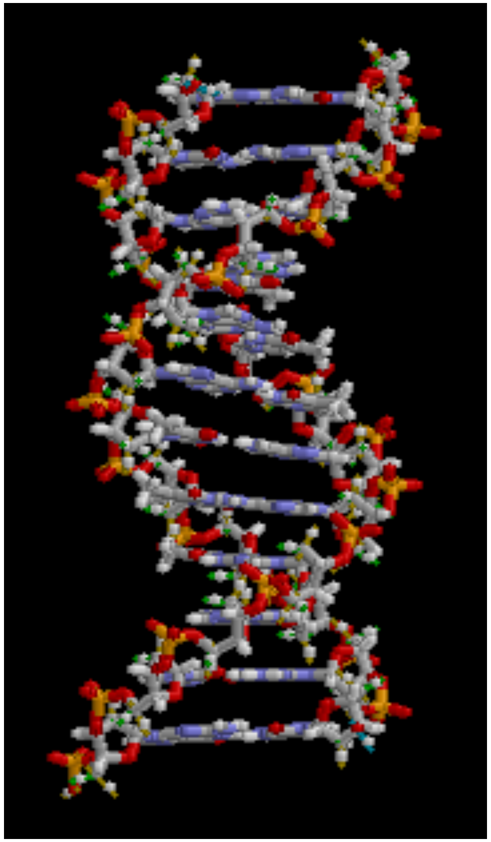
Genetic code

- DNA (and RNA) consists of two “strands” arranged in a double helix and connected with covalent bonds

- Each strand contains a sequence of nucleotides

- DNA is constructed from 4 nucleotides:
  - Adenine
  - Cytosine
  - Guanine
  - Thymine

  (RNA has Uracil in place of Thymine)



from wikipedia

Genetic code

- DNA is constructed from 4 nucleotides (or *bases*):
  - Adenine
  - Cytosine
  - Guanine
  - Thymine

  (RNA has Uracil in place of Thymine)

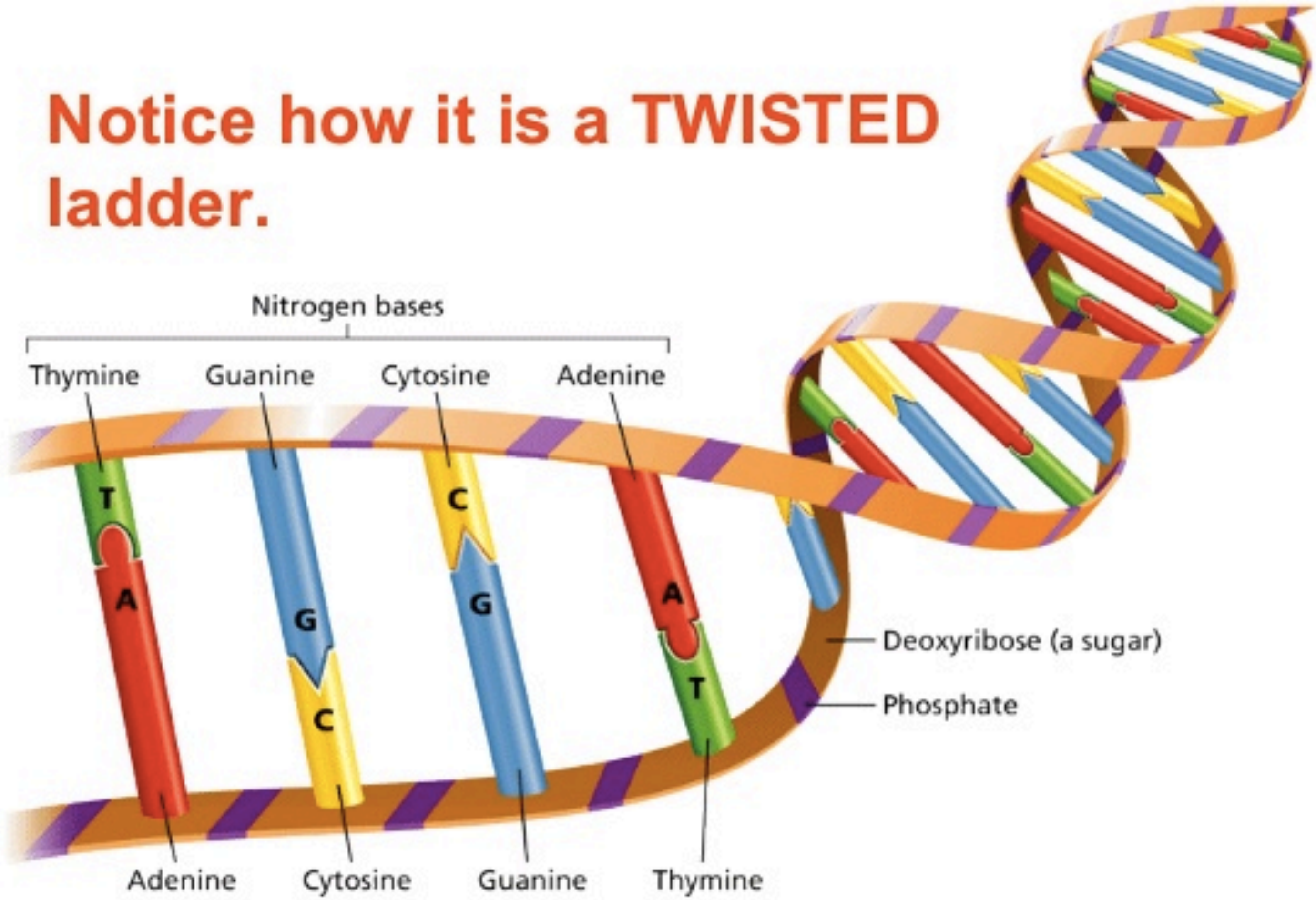
- Adenine bonds with Thymine and Guanine bonds with Cytosine

- So if one strand contains the sequence GCTTCA the other strand will contain CGAAGT in the corresponding location

- During cell division, each daughter cell gets one strand
  - And then the needed 2nd strand can be constructed so A's pair with T's and C's pair with G's

Here is a DNA Molecule

Notice how it is a TWISTED ladder.



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  - Adenine
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  (RNA has Uracil in place of Thymine)

- *Codons* consist of three DNA bases and contain code for synthesizing amino acids
  - Proteins are built from amino acids
  - 64 possible codons, but there are only 20 essential amino acids specified by DNA

- Gene sequencing involves:
  - Extracting the sequence of bases from DNA samples
  - Investigating the proteins or functions associated with codons and their sequences

Pattern finding

- A fundamental computational problem:
  - Given a DNA sequence, search for a pattern
  - Both the sequence and the pattern can be extremely long
  - The number of patterns can also be large
- Fruit fly genome: 139.5 million base pairs

- Humans: 3 billion or 6 billion pairs (depending on the cell type)

- How can we *efficiently* search for patterns?

Pattern search

- **Problem setup:**
  Specify a N-character sequence, *S*, and a M-character pattern, *P*
  Find all locations in *S* where *P* occurs

- **Example:**

  ***S* = ATGTTGTACCGTATCGG**
  ***P* = GTA**

  N=16, M=3