Introduction to Theoretical Computer Science

Introduction to Theoretical CS

Fundamental questions:

Q. What can a computer do?

Q. What can a computer do with limited resources?

General approach.

- Don't talk about specific machines or problems.
- Consider minimal abstract machines.
- Consider general classes of problems.

Why Learn Theory?

In theory …

- Deeper understanding of what is a computer and computing.
- Foundation of all modern computers.
- Pure science.
- Philosophical implications.

In practice …

- Web search: theory of pattern matching.
- Sequential circuits: theory of finite state automata.
- Compilers: theory of context free grammars.
- Cryptography: theory of computational complexity.
- Data compression: theory of information.

Regular Expressions

Pattern Matching

Pattern matching problem. Is a given string in a specified set of strings?

Ex. [genomics]

- Fragile X syndrome is a common cause of intellectual disability.
- Human genome contains triplet repeats of CGG or AGG, bracketed by GCG at the beginning and CTG at the end.
- Number of repeats is variable, and correlated with syndrome.

Specified set of strings: "all strings of G, C, T, A having some occurrence of GCG followed by any number of CGG or AGG triplets, followed by CTG"

Q: "Is this string in the set?"

`GCGGCGTGTGTGCGAGAGAGTGGGTTTAAAGCTGGCGCGGAGGCGGCTGGCGCGGAGGCTG`

A: Yes GCG|CGG|AGG|CGG|CTG

First step:

Regular expression. A formal notation for specifying a set of strings.

Pattern Matching Application

PROSITE. Huge database of protein families and domains.

Q. How to describe a protein motif?

Ex. [signature of the C_2H_2-type zinc finger domain]

1. C
2. Between 2 and 4 amino acids.
3. C
4. 3 more amino acids.
5. One of the following amino acids: LIVMFYWCX.
6. 8 more amino acids.
7. H
8. Between 3 and 5 more amino acids.
9. H

A. Use a regular expression.

CAASCGGPYACGGWAGYHAGWH

Pattern Matching Applications

Test if a string matches some pattern.

- Process natural language.
- Scan for virus signatures.
- Access information in digital libraries.
- Search-and-replace in a word processors.
- Filter text (spam, NetNanny, ads, Carnivore, malware).
- Validate data-entry fields (dates, email, URL, credit card).
- Search for markers in human genome using PROSITE patterns.

Parse text files.

- Compile a Java program.
- Crawl and index the Web.
- Read in data stored in TOY input file format.
- Automatically create Java documentation from Javadoc comments.

Regular Expressions: Basic Operations

Regular expression. Notation to specify a set of strings.

"in specified set" → matches; "not in specified set" → does not match

operation	regular expression	matches	does not match
concatenation	aabaab	aabaab	*every other string*
wildcard	.u.u.u.	cumulus jugulum	succubus tumultuous
union	aa | baab	aa baab	*every other string*
closure	ab*a	aa abbba	ab ababa
parentheses	a(a|b)aab	aaaab abaab	*every other string*
parentheses	(ab)*a	a ababababa	aa abbba

Regular Expressions: Examples

Regular expression. Notation is surprisingly expressive.

regular expression	matches	does not match
`.*spb.*` *contains the trigraph* **spb**	raspberry crispbread	subspace subspecies
`a* | (a*ba*ba*ba*)*` *multiple of three* **b**'s	bbb aaa bbbaababbaa	b bb baabbbaa
`.*0....` *fifth to last digit is* **0**	1000234 98701234	111111111 403982772
`gcg(cgg|agg)*ctg` *fragile X syndrome indicator*	gcgctg gcgcggctg gcgcggaggctg	gcgcgg cggcggcggctg gcgcaggctg

Generalized Regular Expressions

Regular expressions are a standard programmer's tool.

- Built in to Java, Perl, Unix, Python, ...
- Additional operations typically added for convenience.
  - Ex 1: `[a-e]+` is shorthand for `(a|b|c|d|e)(a|b|c|d|e)*`.
  - Ex 2: `\s` is shorthand for "any whitespace character" (space, tab, ...).

operation	regular expression	matches	does not match
one or more	`a(bc)+de`	abcde abcbcde	ade bcde
character class	`[A-Za-z][a-z]*`	lowercase Capitalized	camelCase 4illegal
exactly k	`[0-9]{5}-[0-9]{4}`	08540-1321 19072-5541	111111111 166-54-1111
negation	`[^aeiou]{6}`	rhythm	decade
whitespace	`\s`	space, tab, newline, . . .	anything else

Regular Expression Challenge 1

Q. Consider the RE

a*bb(ab|ba)*

Which of the following strings match (is in the set described)?

a. **abb**
b. **abba**
c. **aaba**
d. **bbbaab**
e. **cbb**
f. **bbababbab**

Regular Expression Challenge 2

Q. Give an RE that describes the following set of strings:

- characters are **A**, **C**, **T** or **G**
- starts with **ATG**
- length is a multiple of 3
- ends with **TAG**, **TAA**, or **TTG**

Pattern Matching Application

PROSITE. Huge database of protein families and domains.

Q. How to describe a protein motif?

Ex. [signature of the C_2H_2-type zinc finger domain]

1. C
2. Between 2 and 4 amino acids.
3. C
4. 3 more amino acids.
5. One of the following amino acids: LIVMFYWCX.
6. 8 more amino acids.
7. H
8. Between 3 and 5 more amino acids.
9. H

A. `C.{2,4}C...[LIVMFYWC].{8}H.{3,5}H`

CAASCGGPYACGGWAGYHAGWH

REs in Java

public class String (*Java's String library*)

`boolean matches(String re)`	*does this string match the given regular expression?*
`String replaceAll(String re, String str)`	*replace all occurrences of regular expression with the replacement string*
`int indexOf(String r, int from)`	*return the index of the first occurrence of the string r after the index from*
`String[] split(String re)`	*split the string around matches of the given regular expression*

```
String re = "C.{2,4}C...[LIVMFYWC].{8}H.{3,5}H ";
String input = "CAASCGGPYACGGAAGYHAGAH";
boolean test = input.matches(re);
```

is the input string in the set described by the RE?

REs in Java

Validity checking. Is `input` in the set described by the `re`?

```
public class Validate
{
   public static void main(String[] args) {
      String re    = args[0];
      String input = args[1];
      StdOut.println(input.matches(re));
   }
}
```

powerful string library method

```
% java Validate "C.{2,4}C...[LIVMFYWC].{8}H.{3,5}H" CAASCGGPYACGGAAGYHAGAH
true

% java Validate "[$_A-Za-z][$_A-Za-z0-9]*" ident123
true

% java Validate "[a-z]+@([a-z]+\.)+(edu|com)" doug@cs.princeton.edu
true
```

C_2H_2 type zinc finger domain

legal Java identifier

valid email address (simplified)

need quotes to "escape" the shell

REs in Java

public class String (*Java's String library*)

`boolean matches(String re)`	*does this string match the given regular expression?*
`String replaceAll(String re, String str)`	*replace all occurrences of regular expression with the replacement string*
`int indexOf(String r, int from)`	*return the index of the first occurrence of the string r after the index from*
`String[] split(String re)`	*split the string around matches of the given regular expression*

```
String s = StdIn.readAll();
s = s.replaceAll("\\s+", " ");
```

RE that matches any sequence of whitespace characters (at least 1).

Extra \ distinguishes from the string \s+

replace each sequence of at least one whitespace character with a single space

REs in Java

`public class String` (*Java's String library*)	
`boolean matches(String re)`	*does this string match the given regular expression?*
`String replaceAll(String re, String str)`	*replace all occurrences of regular expression with the replacement string*
`int indexOf(String r, int from)`	*return the index of the first occurrence of the string r after the index from*
`String[] split(String re)`	*split the string around matches of the given regular expression*

```
String s = StdIn.readAll();
String[] words = s.split("\\s+");
```

create an array of the words in StdIn

DFAs

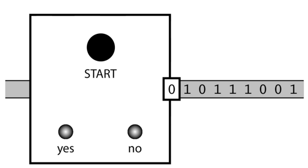
Solving the Pattern Match Problem

Regular expressions are a concise way to describe patterns.

- How would you implement the method `matches()` ?
- Hardware: build a deterministic finite state automaton (DFA).
- Software: simulate a DFA.

DFA: simple machine that solves a pattern match problem.

- Different machine for each pattern.
- Accepts or rejects string specified on input tape.
- Focus on `true` or `false` questions for simplicity.

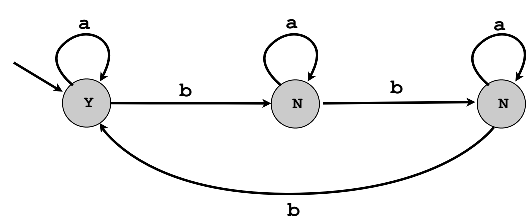


Deterministic Finite State Automaton (DFA)

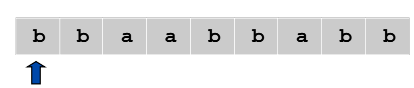
Simple machine with N states.

- Begin in start state.
- Read first input symbol.
- Move to new state, depending on current state and input symbol.
- Repeat until last input symbol read.
- Accept input string if last state is labeled Y.

DFA



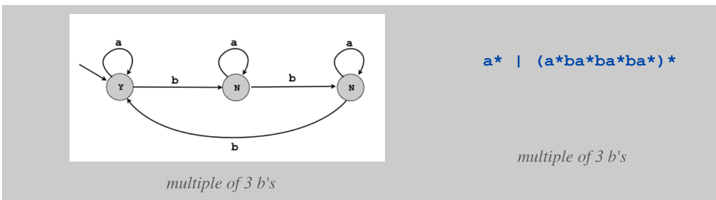
Input



DFA and RE Duality

RE. Concise way to describe a set of strings.
DFA. Machine to recognize whether a given string is in a given set.

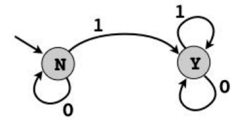
Duality (Kleene).
- For any DFA, there exists a RE that describes the same set of strings.
- For any RE, there exists a DFA that recognizes the same set.



Practical consequence of duality proof: to match RE,
- build corresponding DFA, then
- simulate DFA on input string.

DFA Challenge 1

Q. Consider this DFA:



Which of the following sets of strings does it recognize?

a. Bitstrings with at least one 1

b. Bitstrings with an equal number of occurrences of 01 and 10

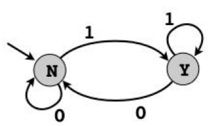
c. Bitstrings with more 1s than 0s

d. Bitstrings with an equal number of occurrences of 0 and 1

e. Bitstrings that end in 1

DFA Challenge 2

Q. Consider this DFA:



Which of the following sets of strings does it recognize?

a. Bitstrings with at least one 1

b. Bitstrings with an equal number of occurrences of 01 and 10

c. Bitstrings with more 1s than 0s

d. Bitstrings with an equal number of occurrences of 0 and 1

e. Bitstrings that end in 1

Implementing a Pattern Matcher

Problem. Given a RE, create program that tests whether given input is in set of strings described.

Step 1. Build the DFA.
- A compiler!
- See COS 226 or COS 320.

It is actually better to use an NFA, an equivalent (but more efficient) representation of a DFA. We ignore that distinction in this lecture.

Step 2. Simulate it with given input.

```
State state = start;
while (!StdIn.isEmpty())
{
   char c = StdIn.readChar();
   state = state.next(c);
}
StdOut.println(state.accept());
```

Direct Application: Harvester

Harvest information from input stream.

- Harvest patterns from DNA.

```
% java Harvester "gcg(cgg|agg)*ctg" chromosomeX.txt
gcgcggcggcggcggcggctg
gcgctg
gcgctg
gcgcggcggcggaggcggaggcggctg
```

- Harvest email addresses from web for spam campaign.

```
% java Harvester "[a-z]+@([a-z]+\.)+(edu|com)" http://www.princeton.edu/~cos126
rs@cs.princeton.edu
dgabai@cs.princeton.edu
doug@cs.princeton.edu
wayne@cs.princeton.edu
```


Direct Application: Harvester

Harvest information from input stream.

- Use `Pattern` data type to compile regular expression to NFA.
- Use `Matcher` data type to simulate NFA.

```
import java.util.regex.Pattern;
import java.util.regex.Matcher;

public class Harvester
{
   public static void main(String[] args)
   {
      String re       = args[0];
      In in           = new In(args[1]);
      String input    = in.readAll();
      Pattern pattern = Pattern.compile(re);
      Matcher matcher = pattern.matcher(input);

      while (matcher.find())
         StdOut.println(matcher.group());

   }
}
```

create NFA from RE

create NFA simulator

look for next match

the match most recently found


```
% java Harvester "gcg(cgg|agg)*ctg" chromosomeX.txt
gcgcggcggcggcggcggctg
gcgctg
gcgctg
gcgcggcggcggaggcggaggcggctg
```


Real-World Application: Parsing a Data File

Java's `Pattern` and `Matcher` classes

- use REs for pattern matching (previous slide)
- extend REs to facilitate processing string-based data

Ex: parsing an NCBI genome data file.

header info

```
LOCUS AC146846 128142 bp DNA linear HTG 13-NOV-2003
DEFINITION Ornithorhynchus anatinus clone CLM1-393H9,
ACCESSION AC146846
VERSION AC146846.2 GI:38304214
KEYWORDS HTG; HTGS_PHASE2; HTGS_DRAFT.
SOURCE Ornithorhynchus anatinus
ORIGIN
     1 tgtatttcat ttgaccgtgc tgtttttcc cggtttttca gtacggtgtt agggagccac
    61 gtgattctgt ttgttttatg ctgccgaata gctgctcgat gaatctctgc atagacagct  // a comment
   121 gccgcaggga gaaatgacca gtttgtgatg acaaaatgta ggaaagctgt ttcttcataa
   ...
128101 ggaaatgcga cccccacgct aatgtacagc ttctttagat tg
//
```

line numbers

spaces

comments

Goal. Extract the data as a single **actg** string.

Real-World Application: Parsing a Data File

```
import java.util.regex.Pattern;
import java.util.regex.Matcher;

public class ParseNCBI
{
   public static void main(String[] args)
   {
      String re = "[ ]*[0-9]+([actg ]*).*";
      Pattern pattern = Pattern.compile(re);
      In in = new In(args[0]);
      String data = "";
      while (!in.isEmpty())
      {
         String line = in.readLine();
         Matcher matcher = pattern.matcher(line);
         if (matcher.find())
            data += matcher.group(1).replaceAll(" ", "");
      }
      System.out.println(data);
   }
}
```

identify a "group" in any match

extract the part of match in () [just a, c, t, g and spaces, not line numbers or comments]

remove spaces


```
LOCUS AC146846 128142 bp DNA linear HTG 13-NOV-2003
DEFINITION Ornithorhynchus anatinus clone CLM1-393H9,
ACCESSION AC146846
VERSION AC146846.2 GI:38304214
KEYWORDS HTG; HTGS_PHASE2; HTGS_DRAFT.
SOURCE Ornithorhynchus anatinus
ORIGIN
     1 tgtatttcat ttgaccgtgc tgtttttcc cggtttttca gtacggtgtt agggagccac
    61 gtgattctgt ttgttttatg ctgccgaata gctgctcgat gaatctctgc atagacagct  // a comment
   121 gccgcaggga gaaatgacca gtttgtgatg acaaaatgta ggaaagctgt ttcttcataa
   ...
128101 ggaaatgcga cccccacgct aatgtacagc ttctttagat tg
//
```

Limitations of DFA

No DFA can recognize the language of all bit strings with an equal number of 0's and 1's.

- Suppose some N-state DFA can recognize this language.
- Consider following input: 0000000011111111

  N+1 0's   N+1 1's
- Our DFA must accept this string.
- Some state x is revisited during first N+1 0's since only N states.

0000000011111111

x   x

- Machine would accept same string without intervening 0's.

  000011111111

  x
- This string doesn't have an equal number of 0's and 1's.

Summary

Programmer.
- Regular expressions are a powerful pattern matching tool.
- Implement regular expressions with finite state machines.

Theoretician.
- Regular expression is a compact description of a set of strings.
- DFA is an abstract machine that solves pattern match problem for regular expressions.
- DFAs and regular expressions have limitations.

Variations
- Yes (accept) and No (reject) states sometimes drawn differently
- Terminology: Deterministic Finite State Automaton (DFA), Finite State Machine (FSM), Finite State Automaton (FSA) are the same
- DFA's can have output, specified on the arcs or in the states
  - These may not have explicit Yes and No states

Fundamental Questions

Q. Are there patterns that cannot be described by any RE/DFA?

A. Yes.
- Bit strings with equal number of 0s and 1s.
- Decimal strings that represent prime numbers.
- DNA strings that are Watson-Crick complemented palindromes.
- and many, many more . . .

Q. Can we extend RE/DFA to describe richer patterns?

A. Yes.
- Context free grammar (e.g., Java).
- Turing machines.

7.4 Turing Machines

Alan Turing (1912-1954)

Turing Machine

Desiderata. Simple model of computation that is "as powerful" as conventional computers.

Intuition. Simulate how humans calculate.

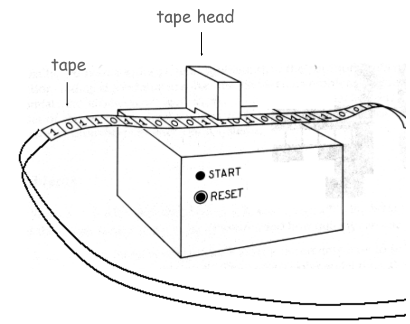
Ex. Addition.

			1	2	3	4	5	6		
		+	3	1	4	1	5	9		

Turing Machine: Tape

Tape.
- Stores input, output, and intermediate results.
- One arbitrarily long strip, divided into cells.
- Finite alphabet of symbols.

Tape head.
- Points to one cell of tape.
- Reads a symbol from active cell.
- Writes a symbol to active cell.
- Moves left or right one cell at a time.



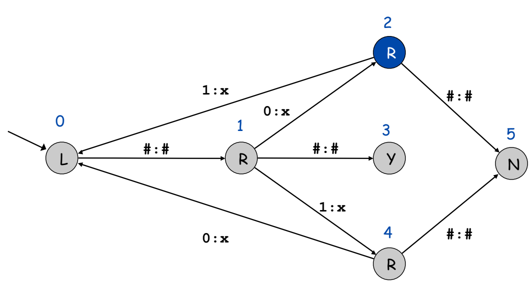
tape head ↓

tape	...	#	1	1	**0**	0	+	1	0	1	1	#	...

Turing Machine: Execution

States.
- Finite number of possible machine configurations.
- Determines what machine does and which way tape head moves.

State transition diagram.
- Ex. if in state 2 and input symbol is 1 then: overwrite the 1 with x, move to state 0, move tape head to left.

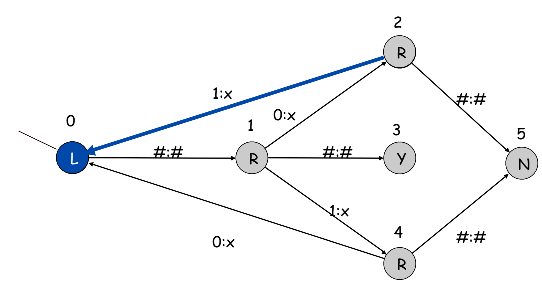


Before	...	#	#	x	x	x	**1**	1	0	#	#	...

Turing Machine: Execution

States.
- Finite number of possible machine configurations.
- Determines what machine does and which way tape head moves.

State transition diagram.
- Ex. if in state 2 and input symbol is 1 then: overwrite the 1 with x, move to state 0, move tape head to left.



After	...	#	#	x	x	**x**	x	1	0	#	#	...

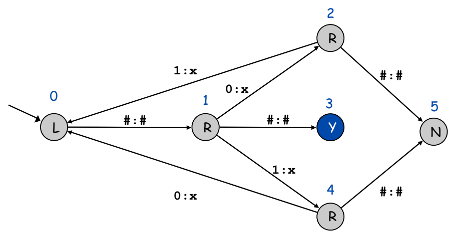
Turing Machine: Initialization and Termination

Initialization.

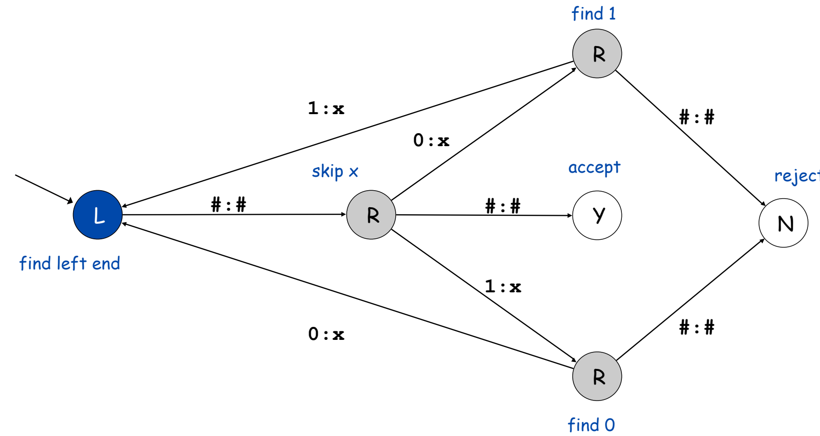
- Set input on some portion of tape.
- Set tape head position.
- Set initial state.

Termination.

- Stop if enter yes, no, or halt state.
- Infinite loop possible.
  - (definitely stay tuned !)



Example: Equal Number of 0's and 1's



Turing Machine Summary

Goal: simplest machine that is "as powerful" as conventional computers.

Surprising Fact 1. Such machines are very simple: TM is enough!
Surprising Fact 2. Some problems cannot be solved by ANY computer.

next lecture

Consequences.

- Precursor to general purpose programmable machines.
- Exposes fundamental limitations of all computers.
- Enables us to study the physics and universality of computation.
- No need to seek more powerful machines!

Variations

- Instead of just recognizing strings, TM's can produce output: the contents of the tape.
- Instead of Y and N states, TM's can have a plain Halt state.