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*
	`(ab)*a`	`a` `abababababa`	`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

C_2H_2 type zinc finger domain

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

legal Java identifier

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

valid email address (simplified)

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

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*

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

Extra \ distinguishes from the string \s+

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

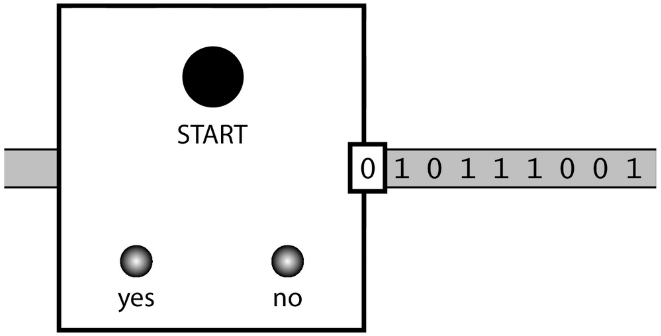
Solving the Pattern Match Problem

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.

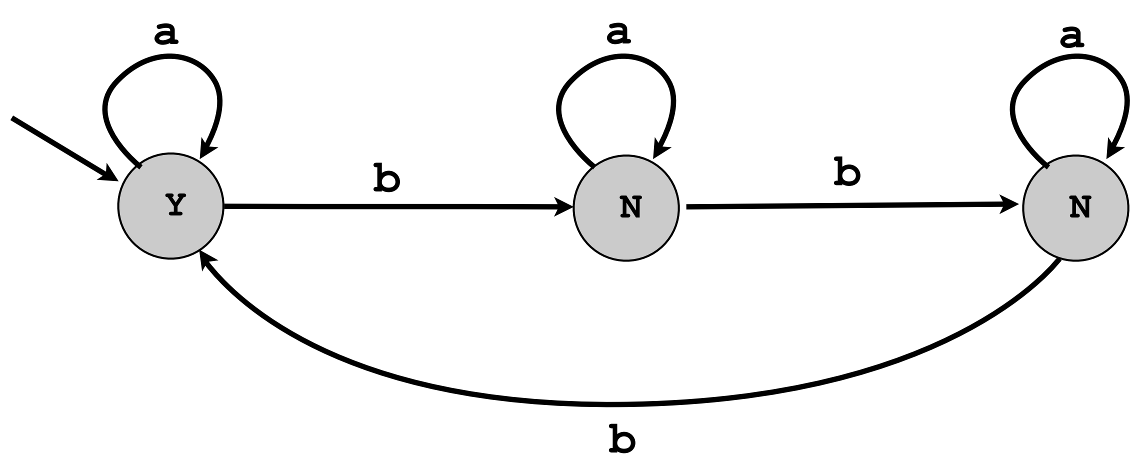


Deterministic Finite State Automaton (DFA)

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

b	b	a	a	b	b	a	b	b

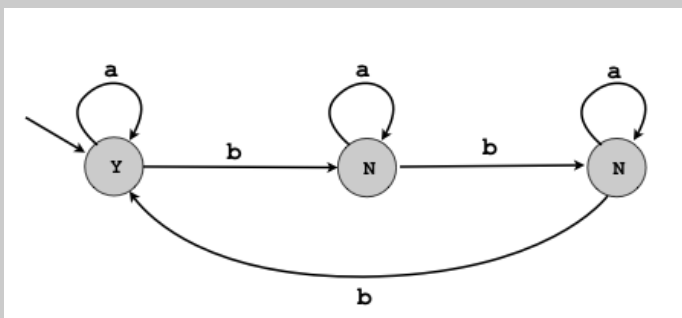
DFA and RE Duality

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.



multiple of 3 b's

`a* | (a*ba*ba*ba*)*`

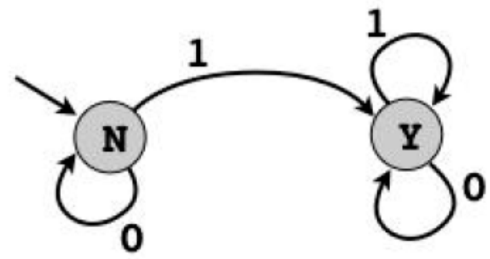
multiple of 3 b's

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

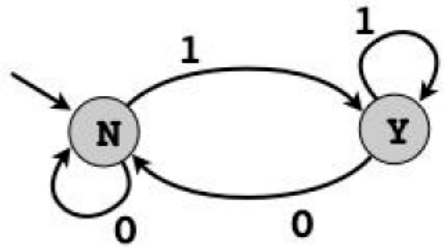
c. Bitstrings with more 1s than 0s

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 tgttttttcc 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 tgttttttcc 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: $\underbrace{00000000}_{N+1\ \ 0's}\underbrace{11111111}_{N+1\ \ 1's}$
- 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.

0000011111111
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		

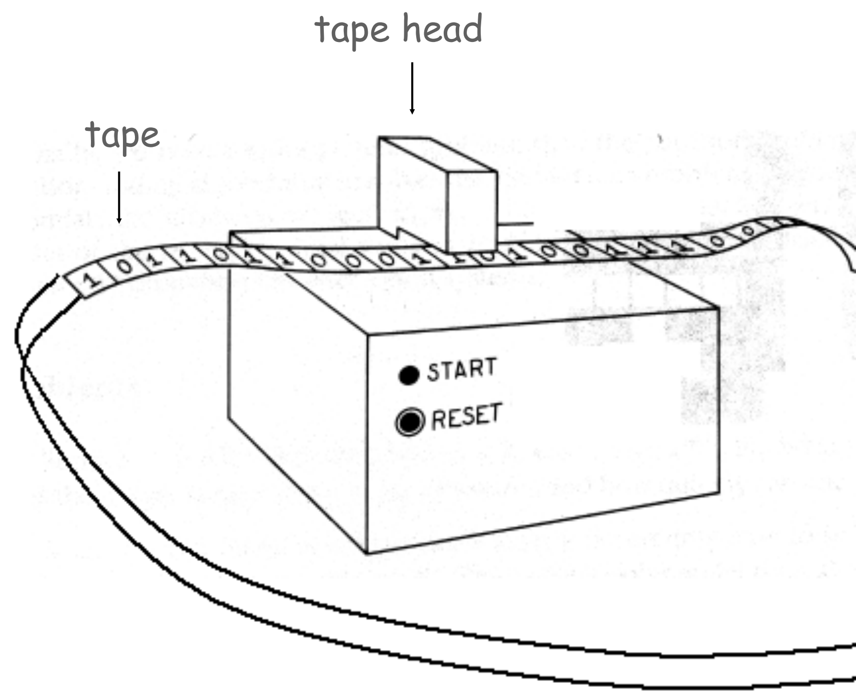
Turing Machine: Tape

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.



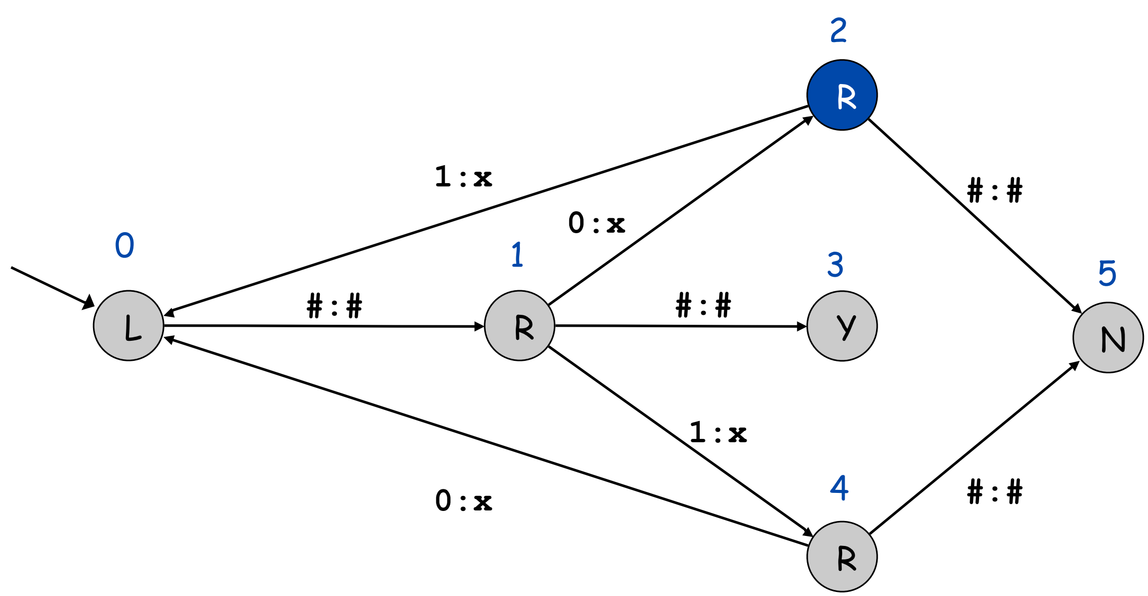
tape head ↓ (at the fifth cell)

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.



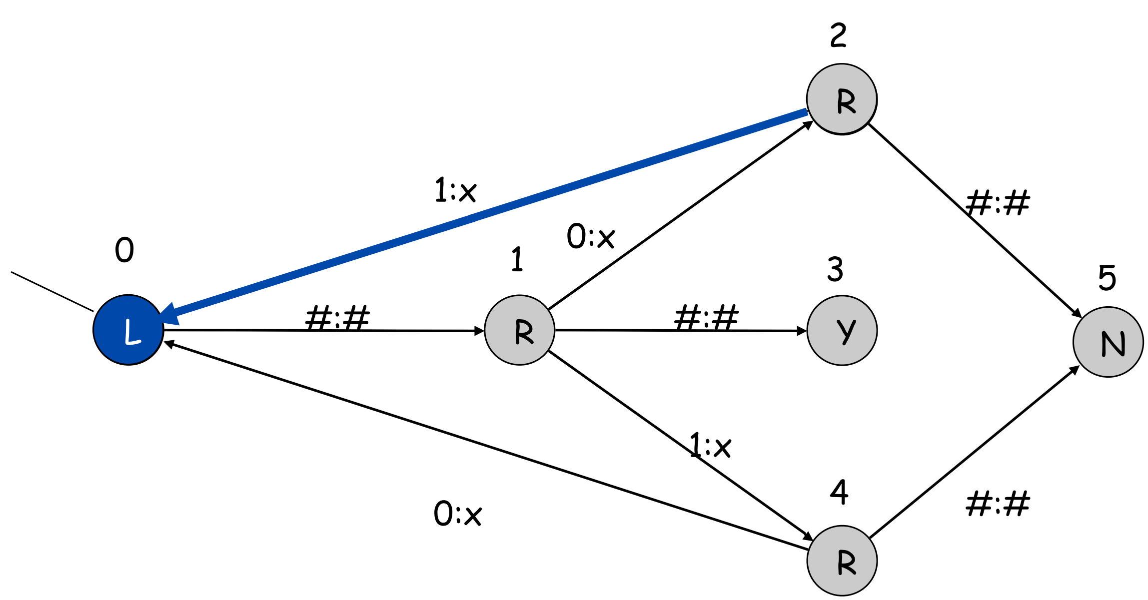
Before

...	#	#	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

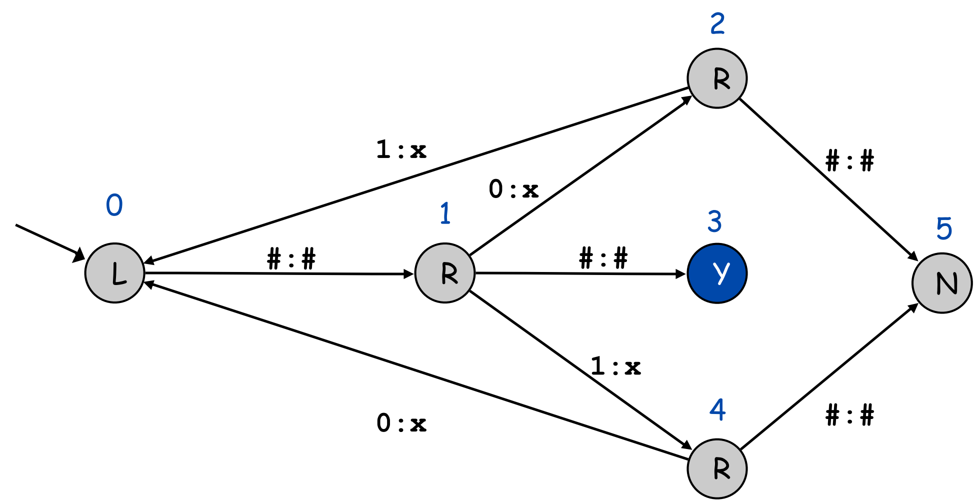
Initialization.

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

...	#	#	0	0	1	1	1	0	#	#	...

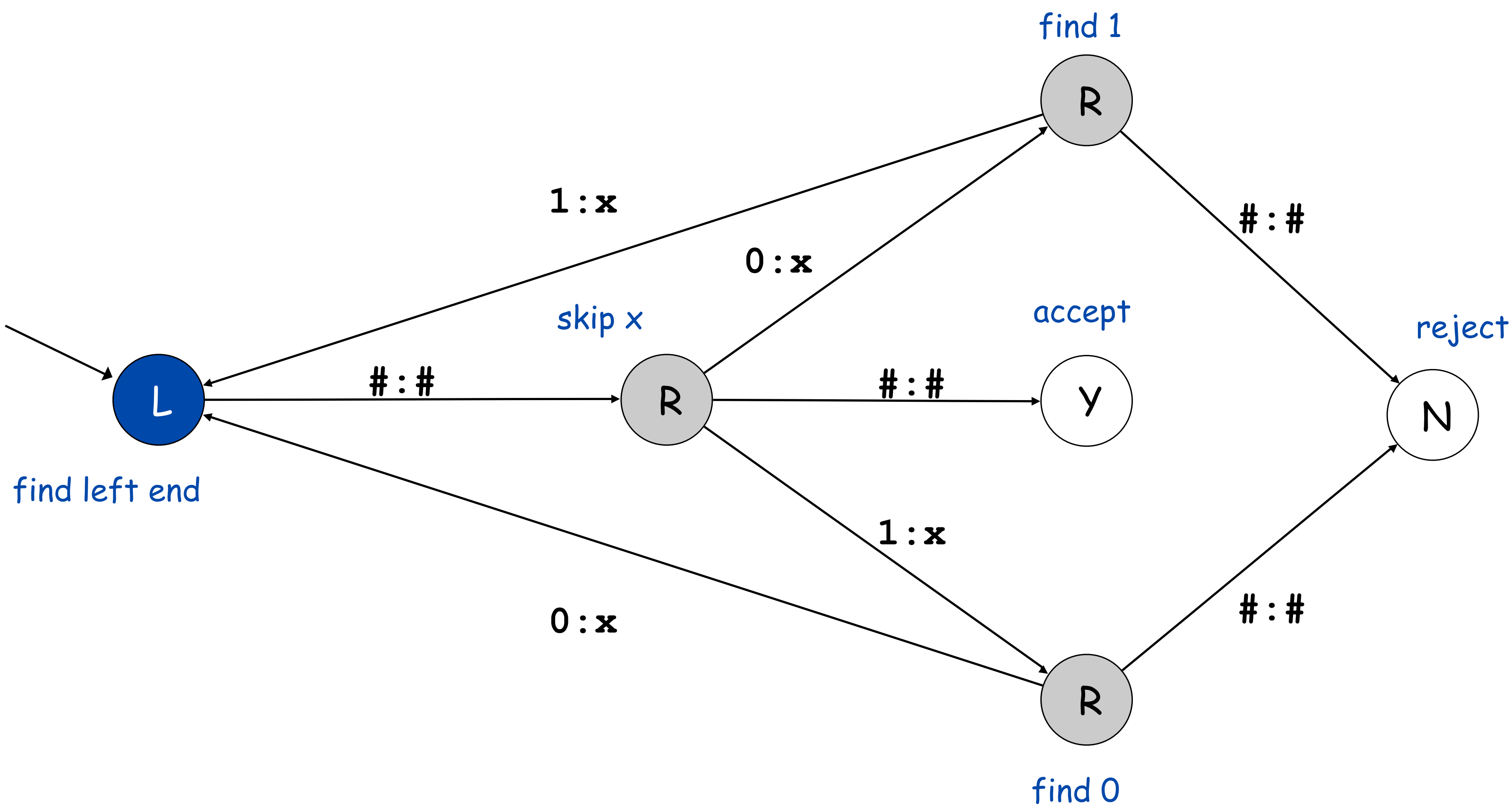
Termination.

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



...	#	#	x	x	x	x	x	x	#	#	...

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



...	#	#	0	0	1	1	1	0	#	#	...

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.