Scientific Computing with MATLAB

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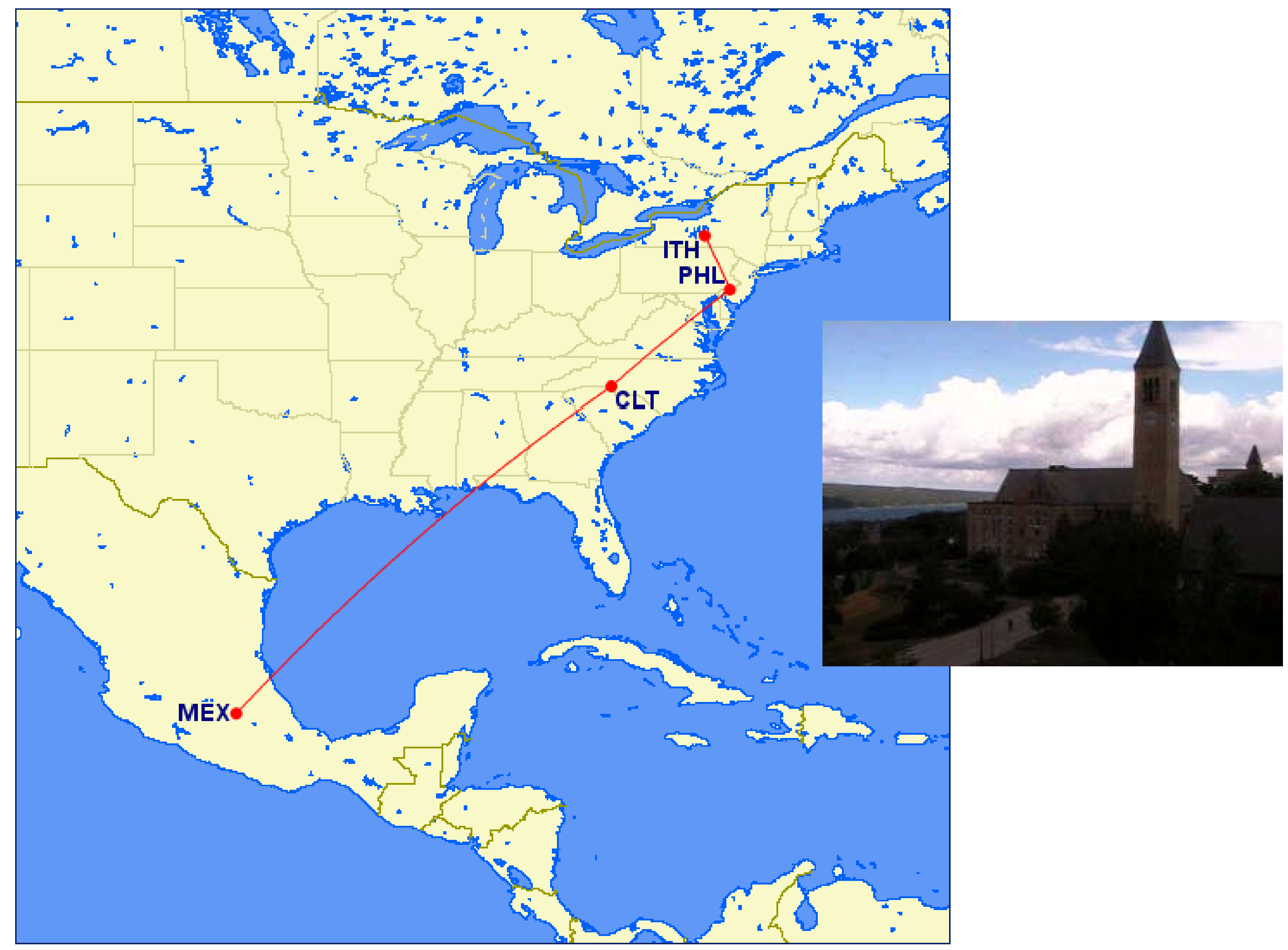
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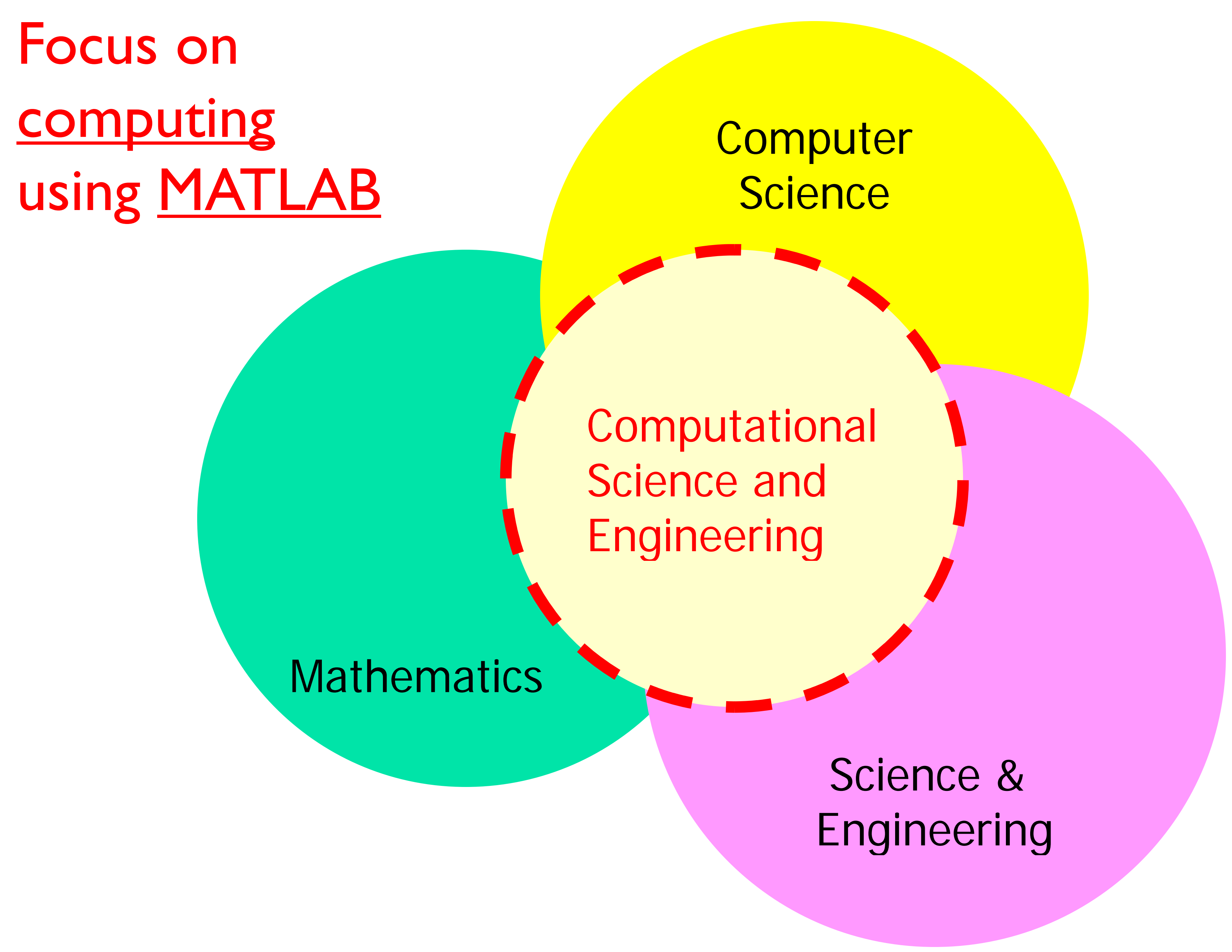
Focus on computing using MATLAB

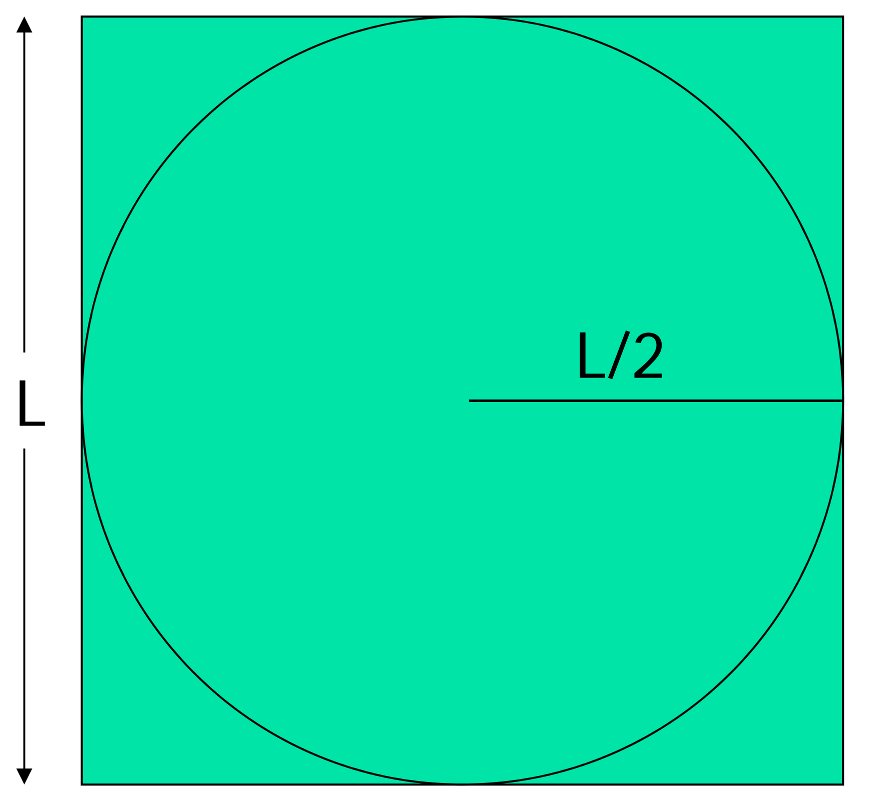


Scientific Computing with MATLAB

1. Programming Fundamentals
   - Functions, control flow, arrays and vectorized computation
2. Graphics for Research and Publication
3. Manipulating Data Sets
   - Working with external data files, including numeric, image, and text
4. Numerical Simulation
   - Fundamental ideas, probability, and numerical methods
5. Specialized Topics
   - Advanced data objects in MATLAB, …

MATLAB desktop environment

Monte Carlo Approximation of π



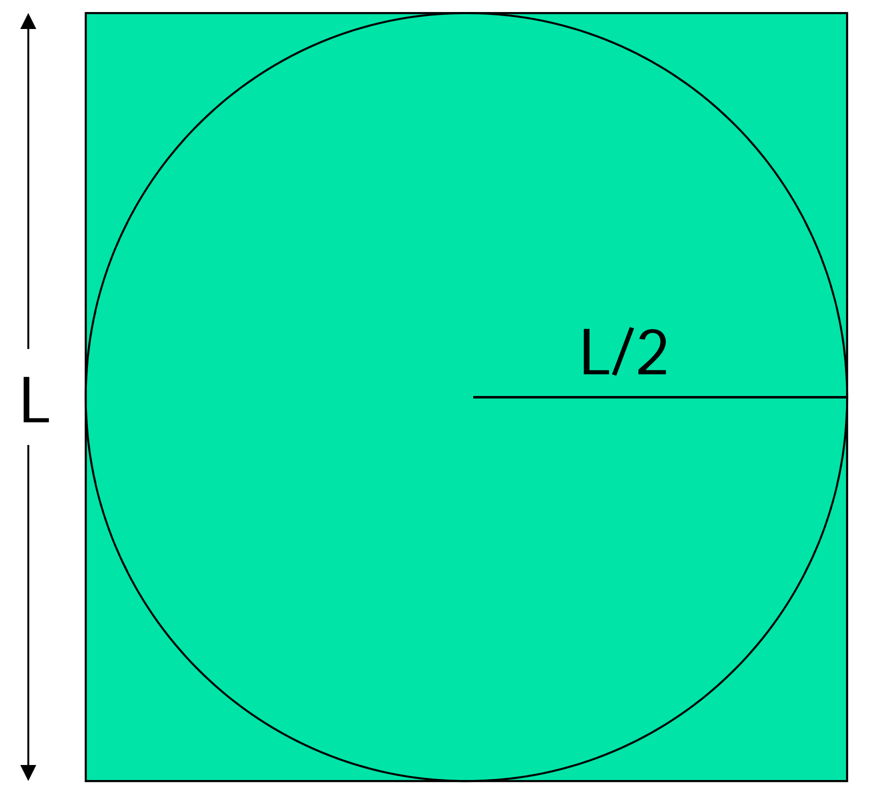
Throw N darts

Sq. area $= \boldsymbol{N} = \boldsymbol{L} \times \boldsymbol{L}$

Circle area $= \boldsymbol{N_{in}}$

$= \pi \boldsymbol{L^2/4}$

Monte Carlo Approximation of π



Throw N darts

Sq. area = $\boldsymbol{N} = \boldsymbol{L} \times \boldsymbol{L}$

Circle area = $\boldsymbol{N_{in}}$

$= \pi \boldsymbol{L^2/4}$

$\pi = \mathbf{4}\ \boldsymbol{N_{in} / N}$

Monte Carlo Approximation of π

For each of N trials

Throw a dart

If it lands in circle

add 1 to total # of hits

Pi is 4*hits/N

Monte Carlo π with N darts on L-by-L board

```
N= ____;
for k = 1:N




end
myPi = 4*hits/N;
```

Monte Carlo π with N darts on L-by-L board

```
N= ____;
for k = 1:N
    % Throw kth dart



    % Count it if it is in the circle




end
myPi = 4*hits/N;
```

Monte Carlo π with N darts on L-by-L board

```
N= ____;  L= ____;
for k = 1:N
    % Throw kth dart
    x = rand(1)*L - L/2;
    y = rand(1)*L - L/2;
    % Count it if it is in the circle



end
myPi = 4*hits/N;
```

Monte Carlo π with N darts on L-by-L board

```
N= ___;  L= ___;  hits= 0;
for k = 1:N
   % Throw kth dart
   x = rand(1)*L - L/2;
   y = rand(1)*L - L/2;
   % Count it if it is in the circle
   if sqrt(x^2+y^2) <= L/2
      hits = hits + 1;
   end
end
myPi = 4*hits/N;
```

Input & output

- *variable* = **input** ('*prompt* ')

```
N= input('How many darts? ')
```

- **fprintf** ('*message to print* ')

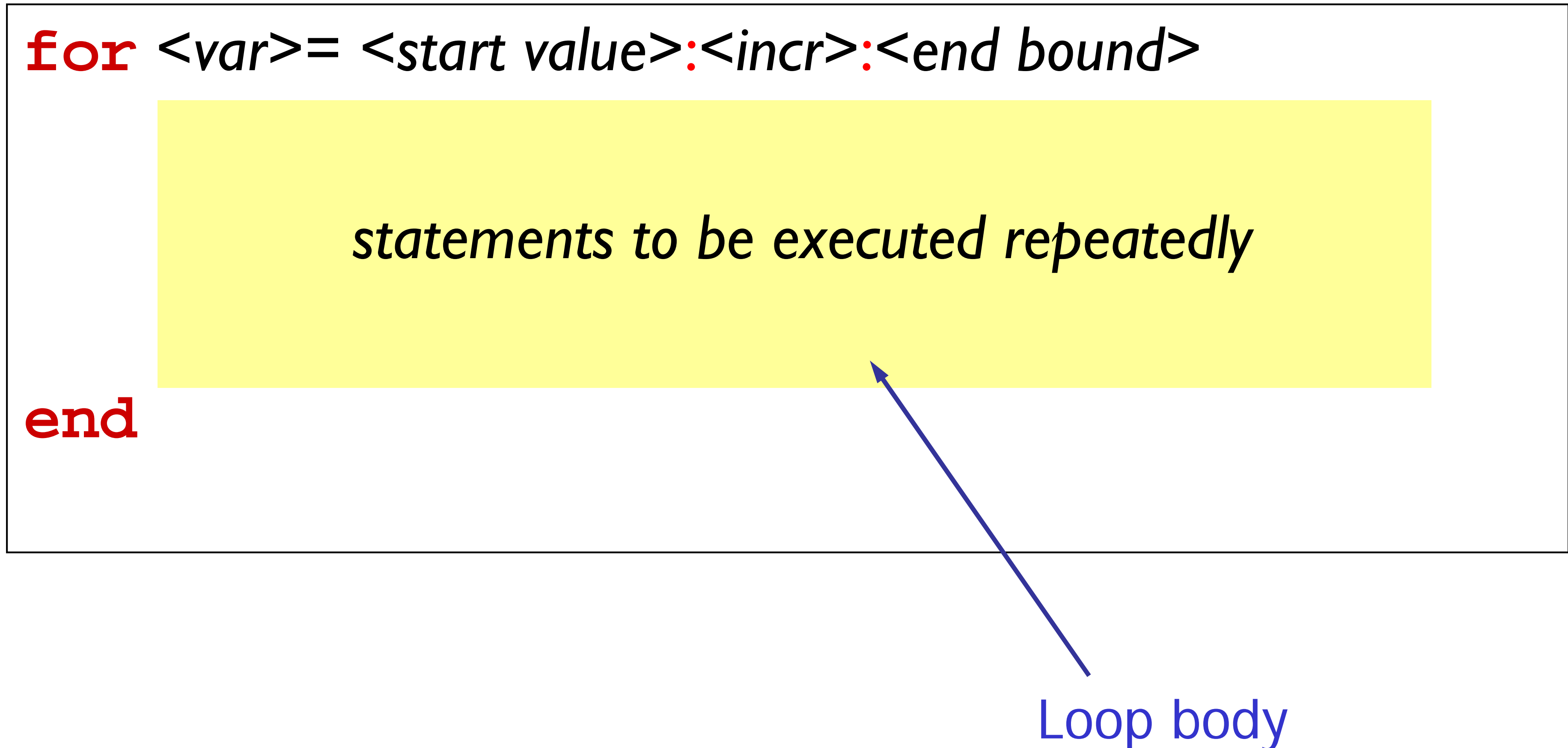
```
fprintf('My pi ')
fprintf('is %f\n', p)
fprintf('Error is %f, %d darts\n', e,N)
```

Substitution sequences (conversion specifications)

`%f`	fixed point (or floating point)
`%d`	decimal—whole number
`%e`	exponential
`%g`	general—Matlab chooses a format
`%c`	character
`%s`	string

Examples: `%f` `%15.2f`

Syntax of the `for` loop



Syntax of the `for` loop

```
for <var>= <start value>:<incr>:<end bound>

        statements to be executed repeatedly

end
```

Loop header specifies all the values that the index variable will take on, one for each pass of the loop.

E.g, `k= 3:1:7` means `k` will take on the values 3, 4, 5, 6, 7, one at a time.

`for` loop examples

```
for k= 2:0.5:3
     disp(k)
end
```

`k` takes on the values ____________

Non-integer increment is OK

```
for k= 1:4
     disp(k)
end
```

`k` takes on the values ____________

Default increment is 1

```
for k= 0:-2:-6
     disp(k)
end
```

`k` takes on the values ____________

"Increment" may be negative

```
for k= 0:-2:-7
     disp(k)
end
```

`k` takes on the values ____________

Colon expression specifies a *bound*

```
for k= 5:2:1
     disp(k)
end
```

`for` loop examples

```
for k= 2:0.5:3
     disp(k)
end
```

`k` takes on the values 2,2.5,3

Non-integer increment is OK

```
for k= 1:4
     disp(k)
end
```

`k` takes on the values 1,2,3,4

Default increment is 1

```
for k= 0:-2:-6
     disp(k)
end
```

`k` takes on the values 0,-2,-4,-6

"Increment" may be negative

```
for k= 0:-2:-7
     disp(k)
end
```

`k` takes on the values 0,-2,-4,-6

Colon expression specifies a *bound*

```
for k= 5:2:1
     disp(k)
end
```

The set of values for k is the empty set: the loop body won't execute

The **if** construct

if *boolean expression1*

statements to execute if *expression1* *is true*

elseif *boolean expression2*

statements to execute if *expression1* *is false*

but *expression2* *is true*

:

else

statements to execute if all previous conditions

are false

end

Can have any number of elseif branches but at most one else branch

Relational operators

Operator	Meaning
`<`	Less than
`>`	Greater than
`<=`	Less than or equal to
`>=`	Greater than or equal to
`==`	Equal to
`~=`	Not equal to

“Truth table”

X, Y represent boolean expressions.
E.g., d>3.14

X	Y	X && Y “and”	X || Y “or”	~y “not”
F	F	F	F	T
F	T	F	T	F
T	F	F	T	T
T	T	T	T	F

"Truth table"

Matlab uses **0** to represent false,
1 to represent true

X	Y	X && Y "and"	X || Y "or"	~y "not"
0	0	0	0	1
0	1	0	1	0
1	0	0	1	1
1	1	1	1	0

Logical operators “short-circuit”

a > b && c > d

true

Go on

a > b && c > d

false

Stop

Entire expression is false since the first part is false

A **&&** condition short-circuits to false if the left operand evaluates to *false*.

A **||** condition short-circuits to true if the left operand evaluates to *true*.

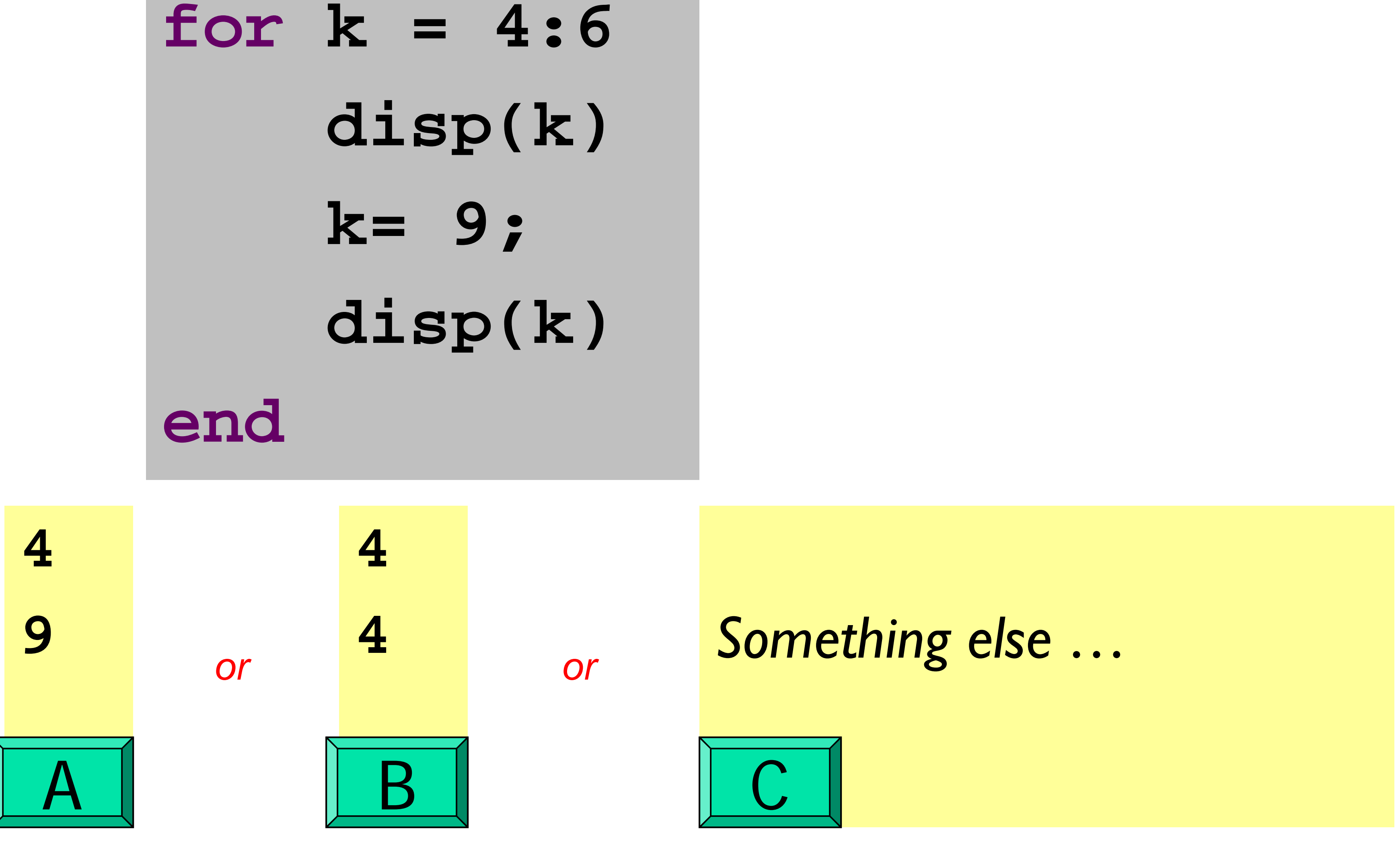
Exercise: Print a table of function values

$$f(x) = \begin{cases} \sin(x) & x < 0 \\ x^2 - 2x & 0 \leq x < 2 \\ x^3/4 - x & x \geq 2 \end{cases}$$

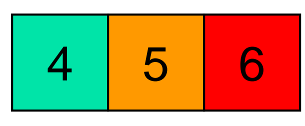
Solicit a range of x values and the step size from the user and print the values of $f(x)$. Example run:

```
Enter smallest value of x: -1
Enter largest value of x: 4
Enter the step size:
```

What will be displayed when you run the following script?

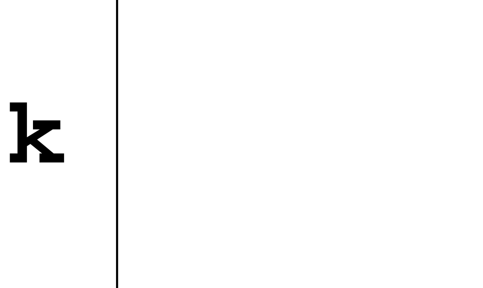


```
for k = 4:6
    disp(k)
    k= 9;
    disp(k)
end
```



With this loop header, **k** "promises" to be these values, one at a time

Output in Command Window



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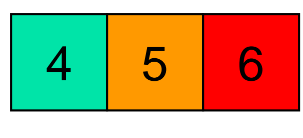

With this loop header, **k** "promises" to be these values, one at a time

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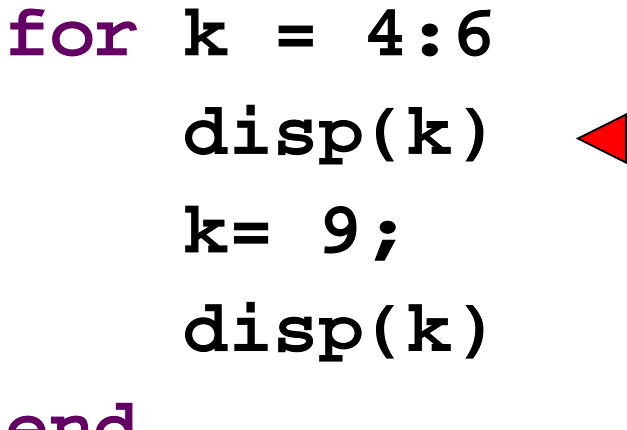
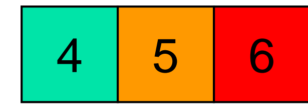
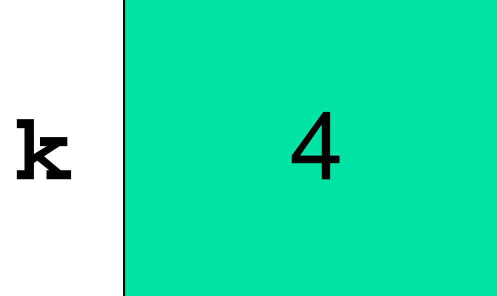
k 4







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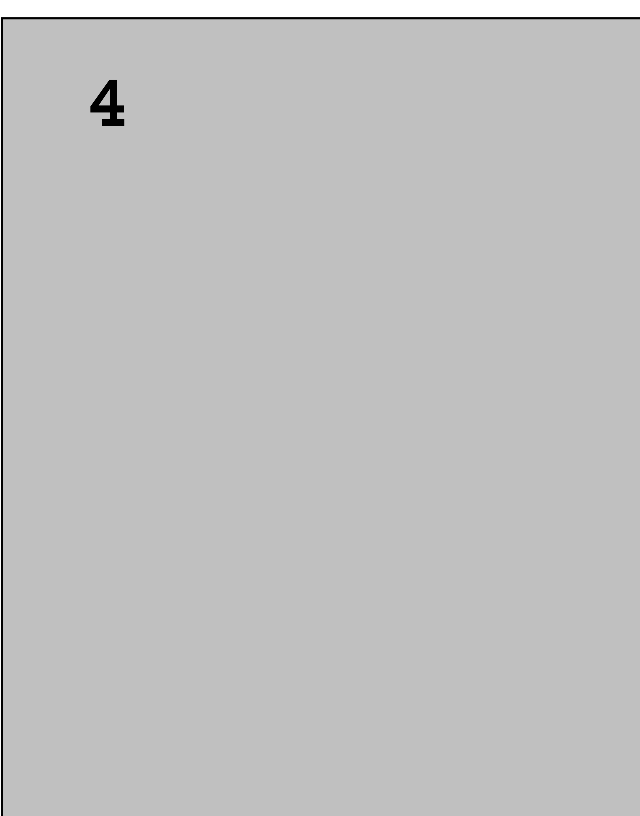

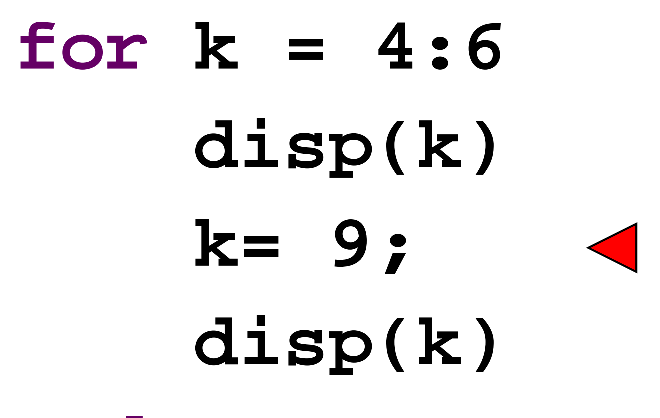

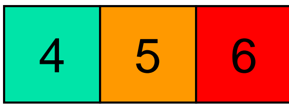

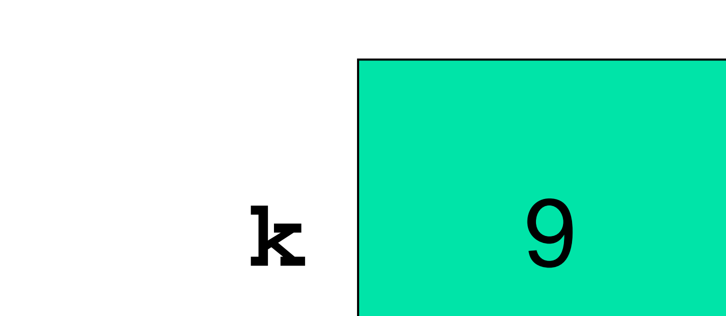

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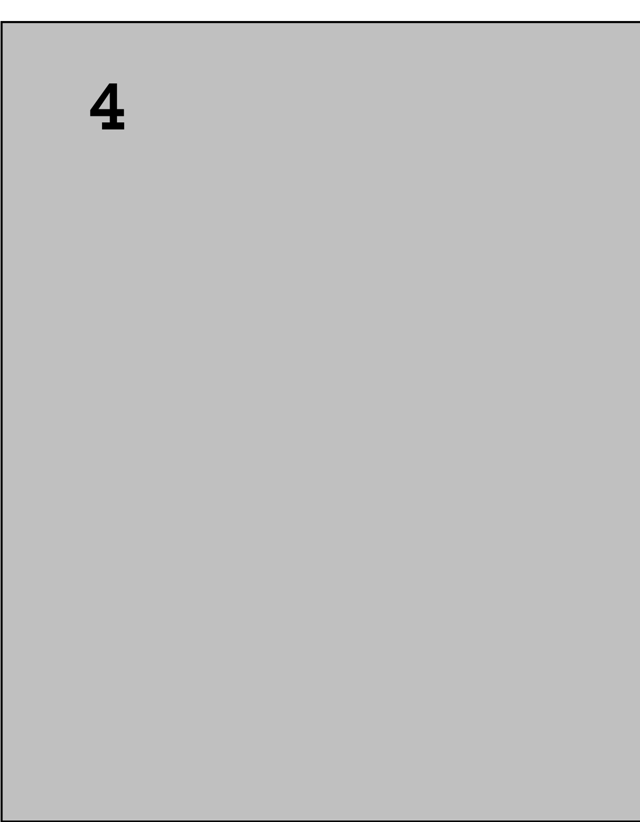

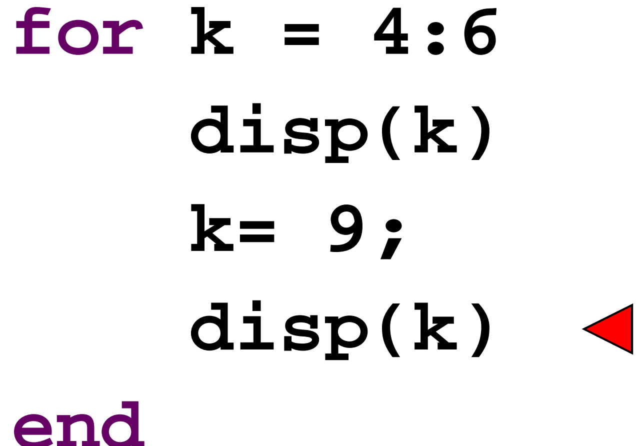

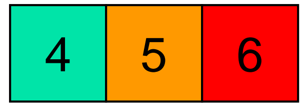

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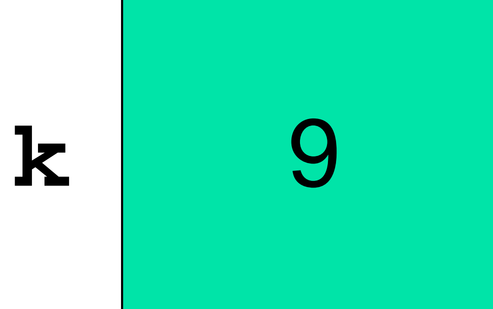

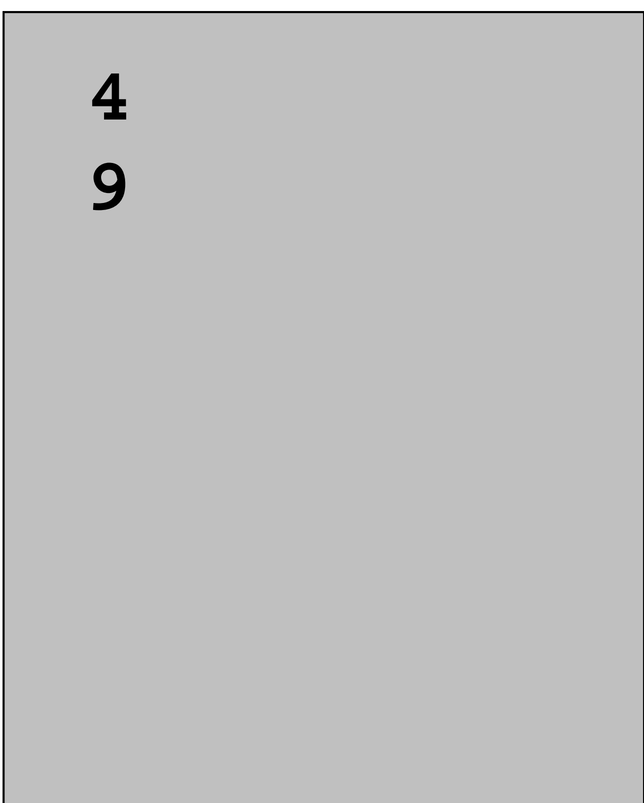

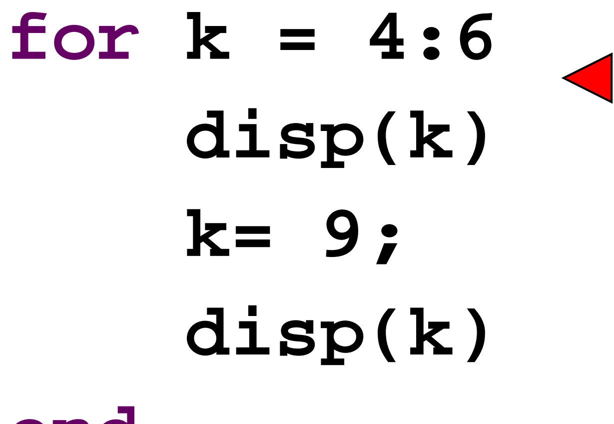

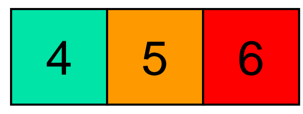

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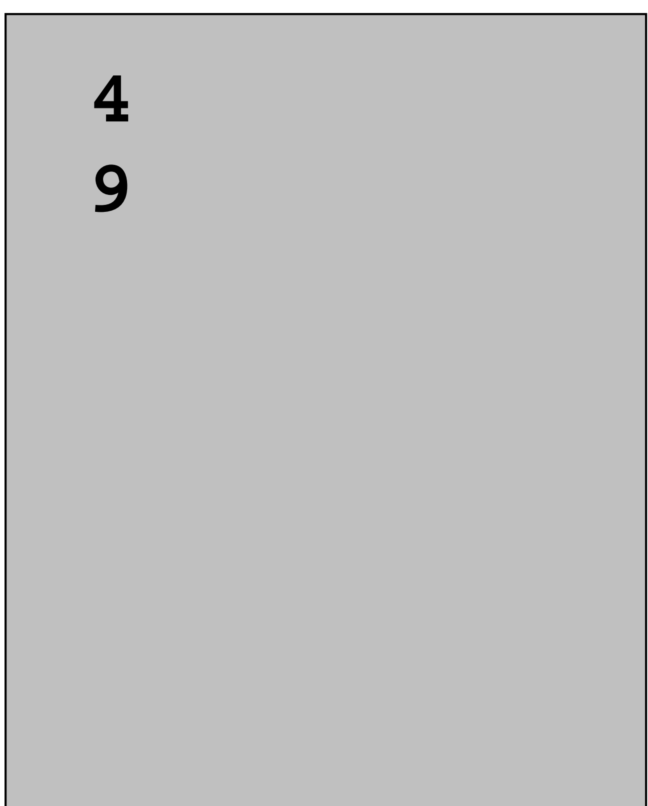

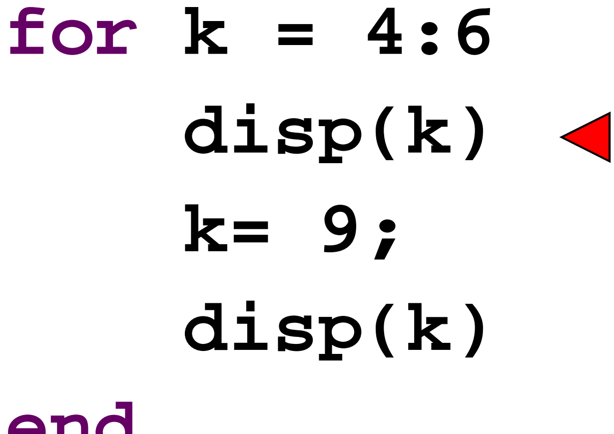

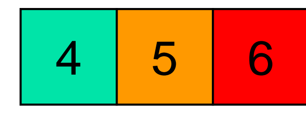

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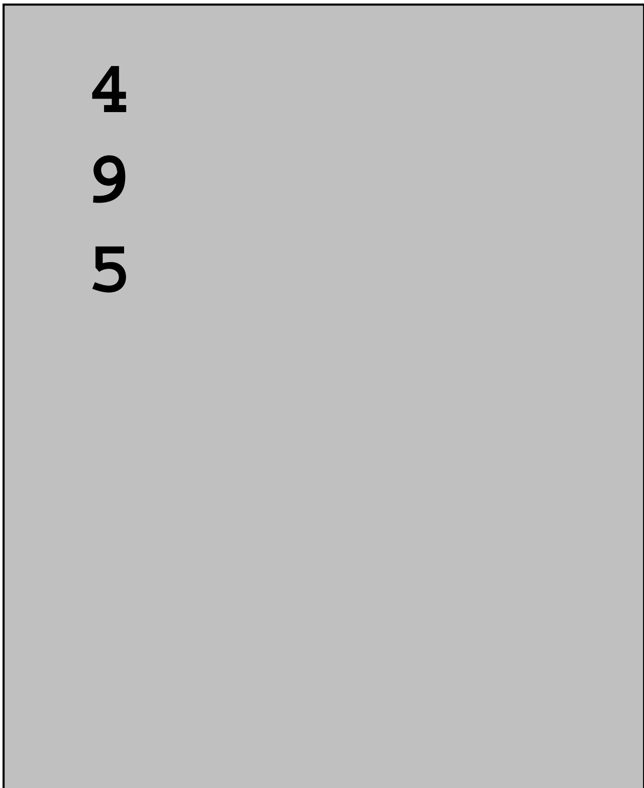

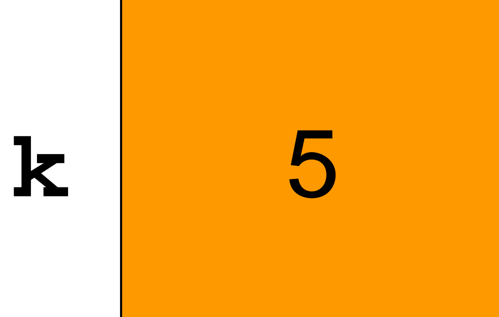

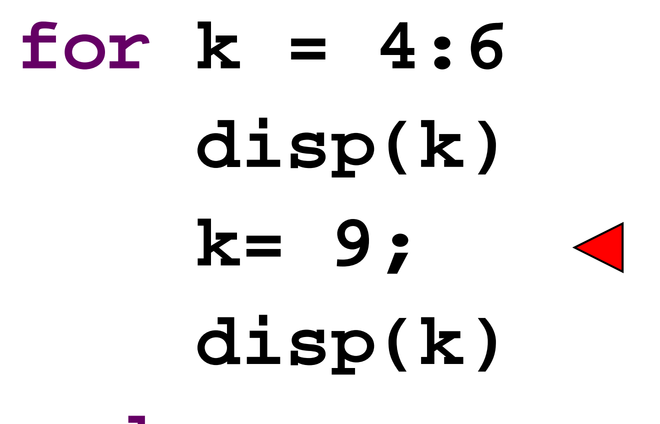

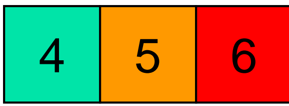

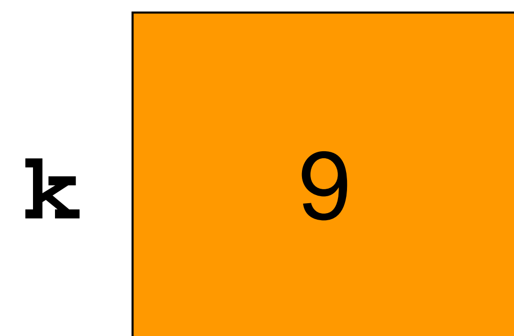

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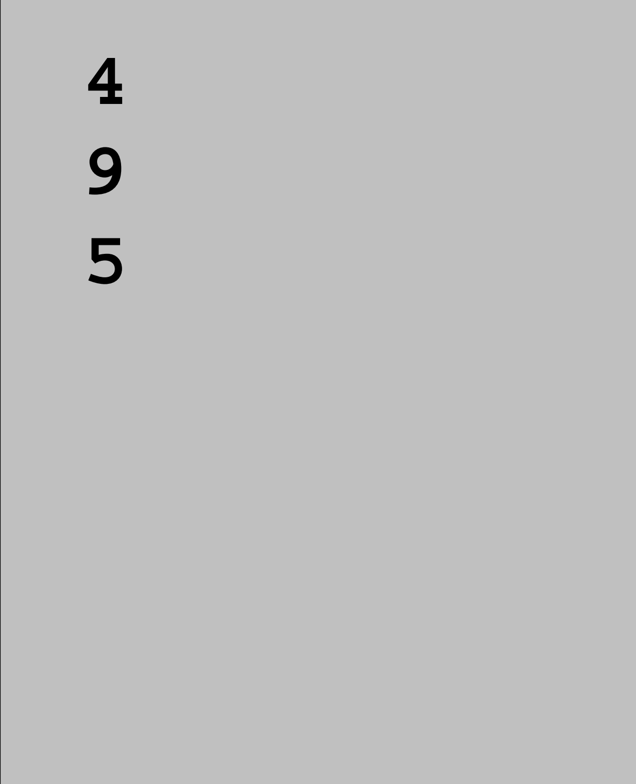

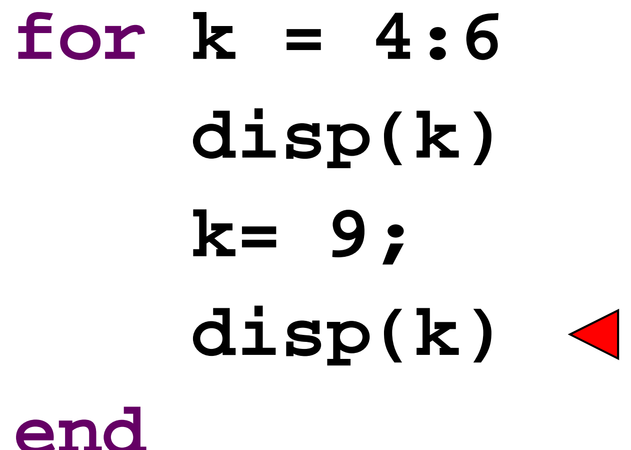

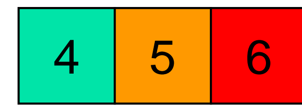

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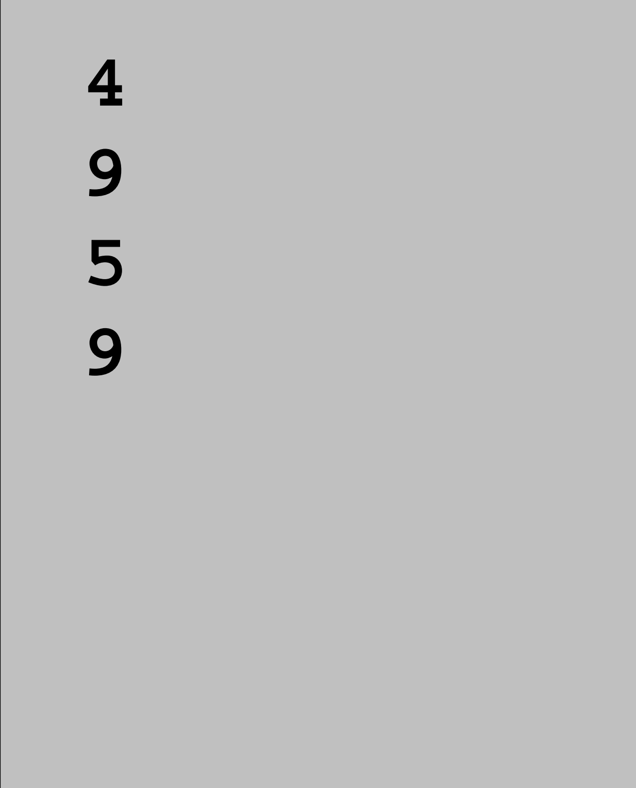

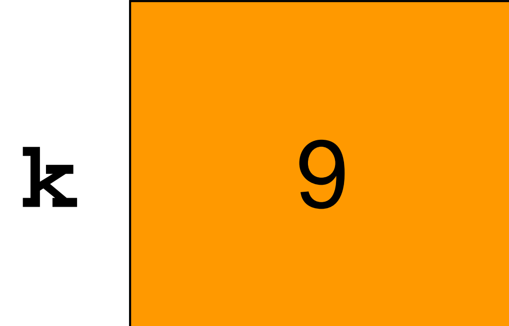

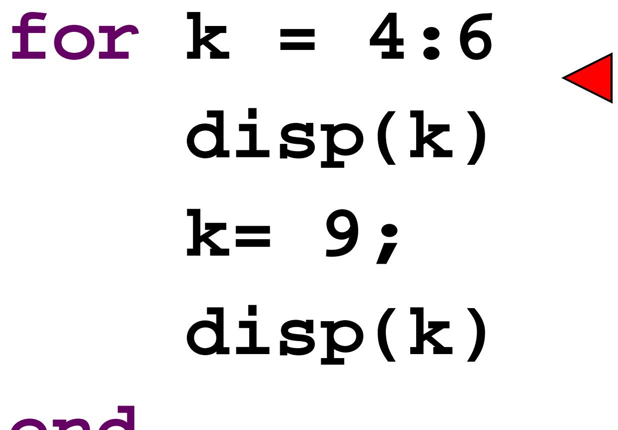

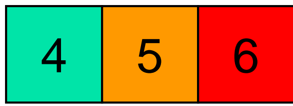

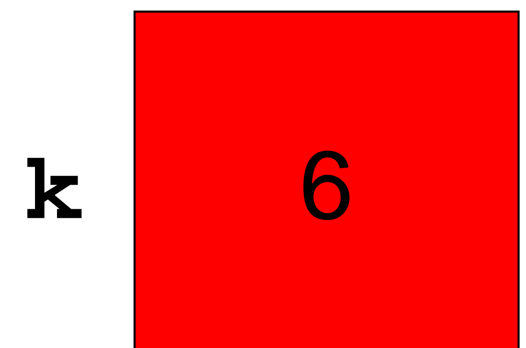

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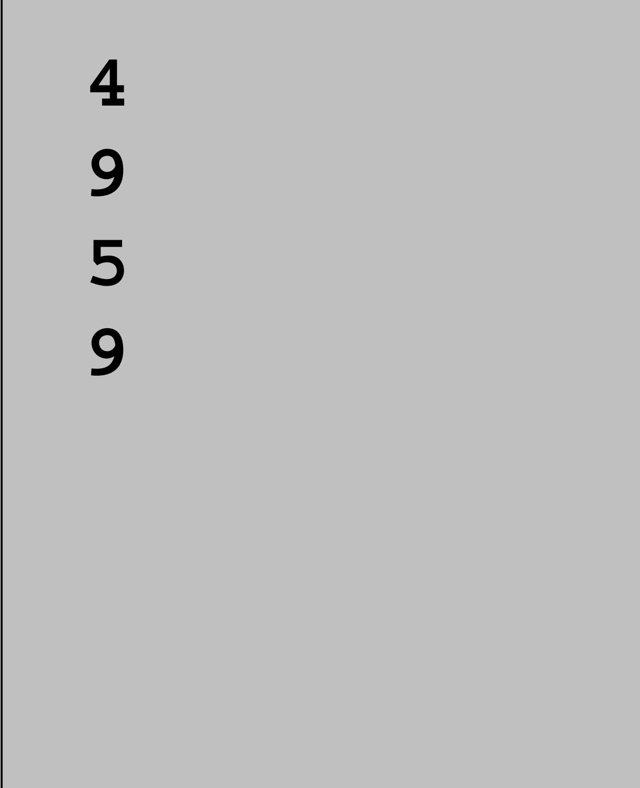

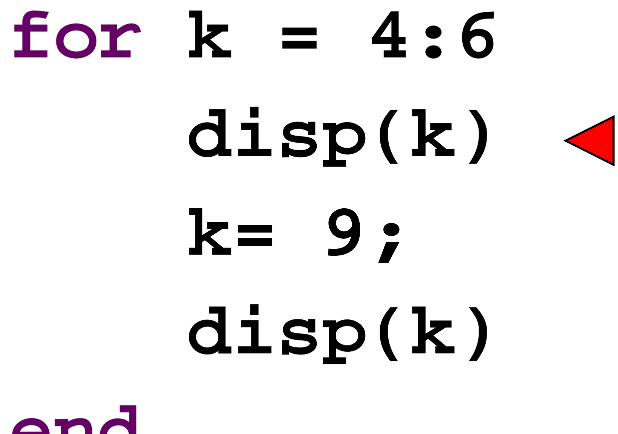

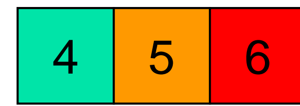

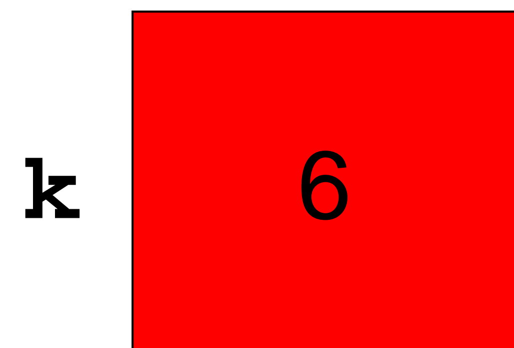

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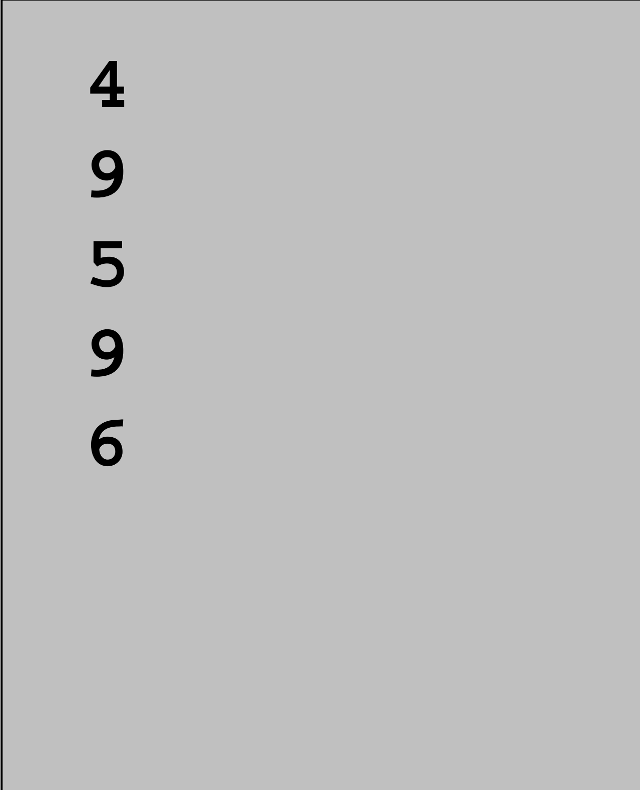

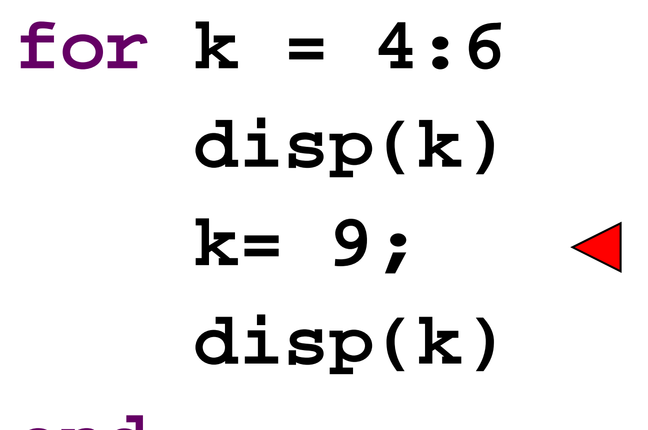

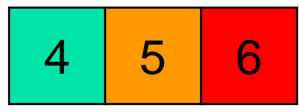

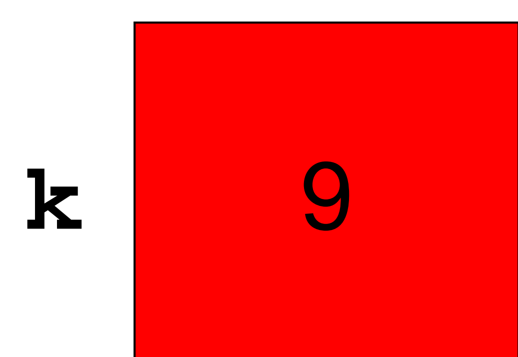

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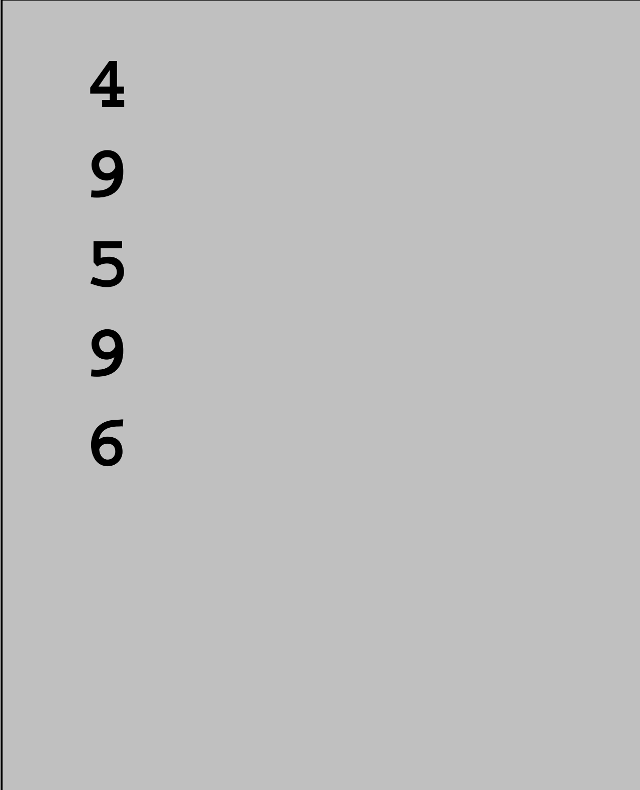

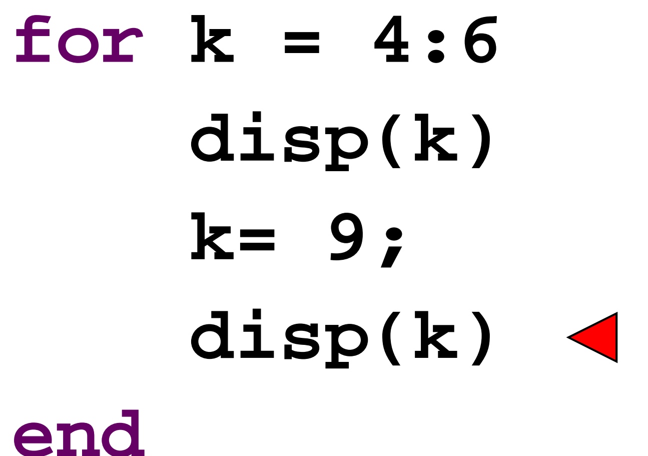

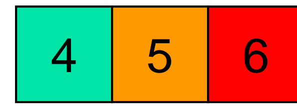

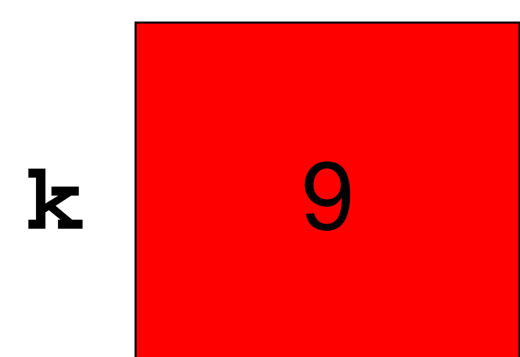

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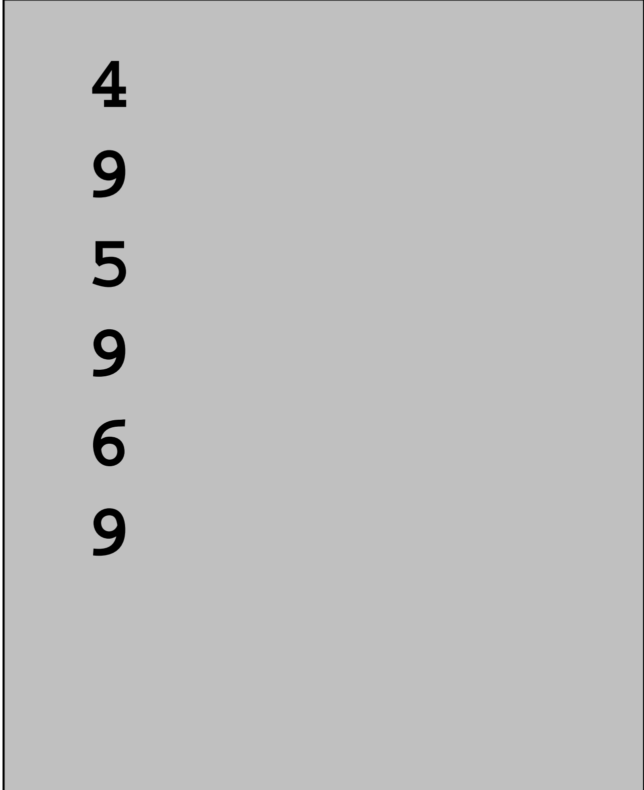

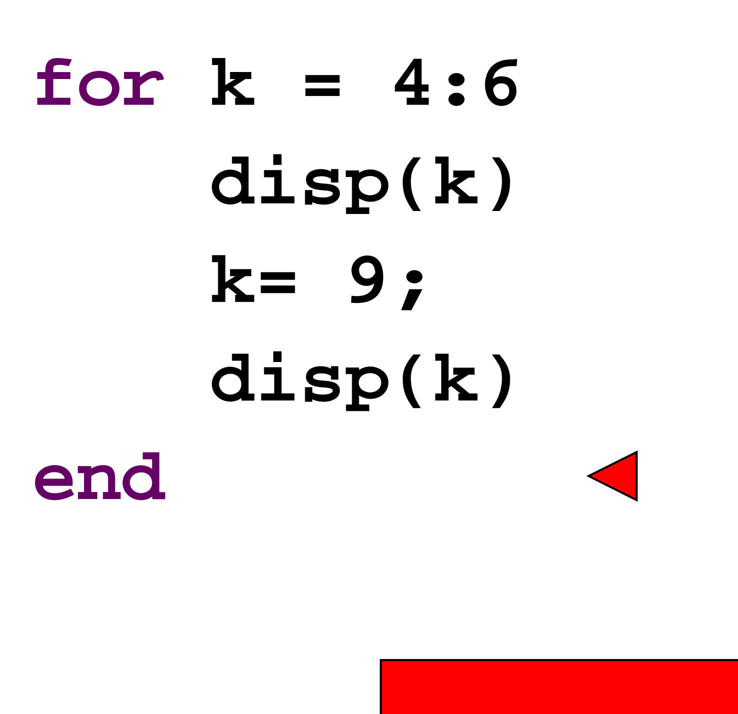
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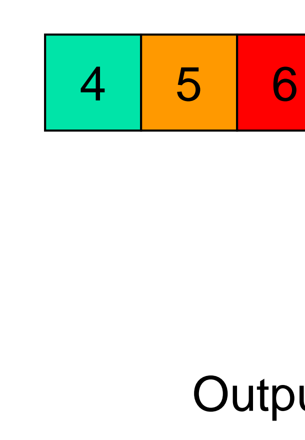
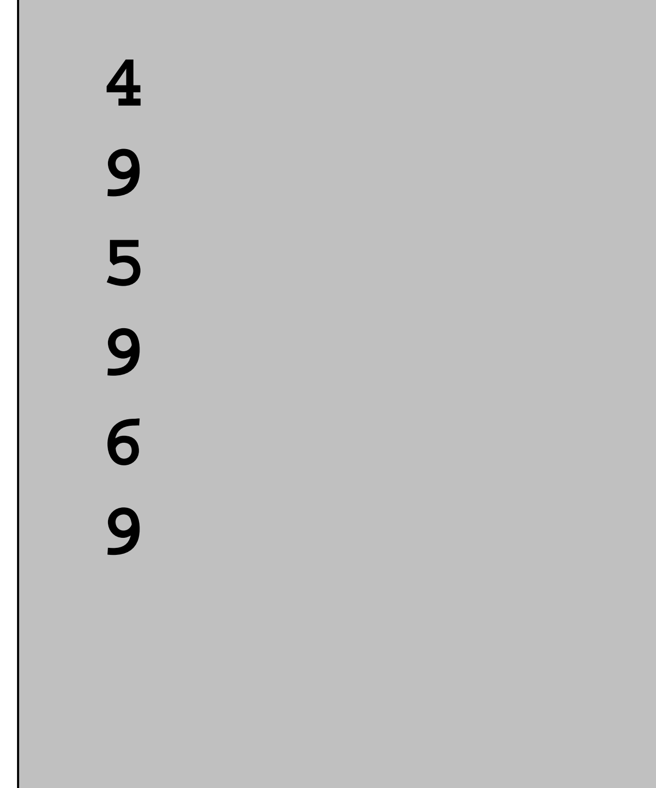
k= 9;
disp(k)
end
k
9


4
5
6

Output in Command Window


4
9
5
9
6
9

```
for k = 4:6
    disp(k)
    k= 9;
    disp(k)
end
```

Not a condition (boolean expression) that checks whether k<=6.

It is an expression that specifies values:

Monte Carlo π with N darts on L-by-L board

```
N= ___;  L= ___;  hits= 0;
for k = 1:N
   % Throw kth dart
   x = rand(1)*L - L/2;
   y = rand(1)*L - L/2;
   % Count it if it is in the circle
   if sqrt(x^2+y^2) <= L/2
      hits = hits + 1;
   end
end
myPi = 4*hits/N;
```

Using a while-loop

```
N= ___;  L= ___;  hits= 0;  k= 1;
while k <= N
   % Throw kth dart
   x = rand(1)*L - L/2;
   y = rand(1)*L - L/2;
   % Count it if it is in the circle
   if sqrt(x^2+y^2) <= L/2
      hits = hits + 1;
   end
   k = k+1;
end
myPi = 4*hits/N;
```

Common loop patterns

Do something *n* times

```
for k= 1:1:n
    % Do something

end
```

Do something an indefinite number of times

```
%Initialize loop variables

while ( not stopping signal )
    % Do something

    % Update loop variables

end
```

Patterns to do something n times

```
for k= 1:1:n
    % Do something

end
```

```
%Initialize loop variables
k= 1;
while ( k <= n )
    % Do something


    % Update loop variables
    k= k+1;
end
```

General form of a user-defined function

```
function [out1, out2, …]= functionName (in1, in2, …)
% 1-line comment to describe the function
% Additional description of function

    Executable code that at some point assigns
    values to output parameters out1, out2, …
```

- *in1*, *in2*, … are defined when the function begins execution. Variables *in1*, *in2*, … are called function *parameters* and they hold the function *arguments* used when the function is invoked (called).
- *out1*, *out2*, … are not defined until the executable code in the function assigns values to them.

```
function myPi = mcPiFun(N)
% myPi is Monte Carlo estimate of pi by
% throwing N darts

N= ___;  L= ___;  hits= 0;
for k = 1:N
    % Throw kth dart
    x = rand(1)*L - L/2;
    y = rand(1)*L - L/2;
    % Count it if it is in the circle
    if sqrt(x^2+y^2) <= L/2
        hits = hits + 1;
    end
end
myPi = 4*hits/N;
```

(The "N= ___;" assignment is struck through on the slide.)

```
function [x, y] = polar2xy(r,theta)
% Convert polar coordinates (r,theta) to
% Cartesian coordinates (x,y).
% theta is in degrees.

rads= theta*pi/180;  % radian
x= r*cos(rads);
y= r*sin(rads);
```

A function file
`polar2xy.m`

Function header is the “contract” for how the function will be used (called)

You have this function:

```
function  [x, y] = polar2xy(r, theta)
% Convert polar coordinates (r, theta) to
% Cartesian coordinates (x,y).  Theta in degrees.
…
```

Code to call the above function:

```
% Convert polar (r1,t1) to Cartesian (x1,y1)
r1= 1;  t1= 30;
[x1, y1]= polar2xy(r1, t1);
plot(x1, y1, 'b*')
…
```

Given this function:

```
function m = convertLength(ft,in)
% Convert length from feet (ft) and inches (in)
% to meters (m).

   . . .
```

How many proper calls to convertLength are shown below?

```
% Given f and n
d= convertLength(f,n);
d= convertLength(f*12+n);
d= convertLength(f+n/12);
x= min(convertLength(f,n), 1);
y= convertLength(pi*(f+n/12)^2);
```

A: 1

B: 2

C: 3

D: 4

E: 5 or 0

Comments in functions

- Block of comments after the function header is printed whenever a user types

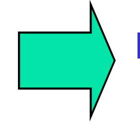
  help <*functionName*>

  at the Command Window

- 1st line of this comment block is searched whenever a user types

  lookfor <*someWord*>

  at the Command Window



- Every function should have a comment block after the function header that says what the function does concisely

Subfunction

- There can be more than one function in an M-file
- top function is the main function and has the name of the file
- remaining functions are subfunctions, accessible only by the functions in the same m-file
- Each (sub)function in the file begins with a function header
- Keyword `end` is not necessary at the end of a (sub)function

Arrays

The basic variable in Matlab is a matrix:

- Scalar → 1 x 1 matrix

- 1-d array of length 4 →
  1 x 4 matrix   or   4 x 1 matrix

- 2-d array → a matrix, naturally

Array index starts at 1

x	5	.4	.91	-4	-1	7
	1	2	3	4	5	6

Let k be the index of vector x, then

- k must be a positive integer
- 1<= k <= length(x)
- To access the kth element: x(k)

Here are a few different ways to create a vector

```
count= zeros(1,6)
```

Similar functions: `ones`, `rand`

```
a= linspace(10,30,5)

b= 7:-2:0

c= [3 7 2 1]

d= [3; 7; 2]
```

count

0	0	0	0	0	0

a

10	15	20	25	30

b

7	5	3	1

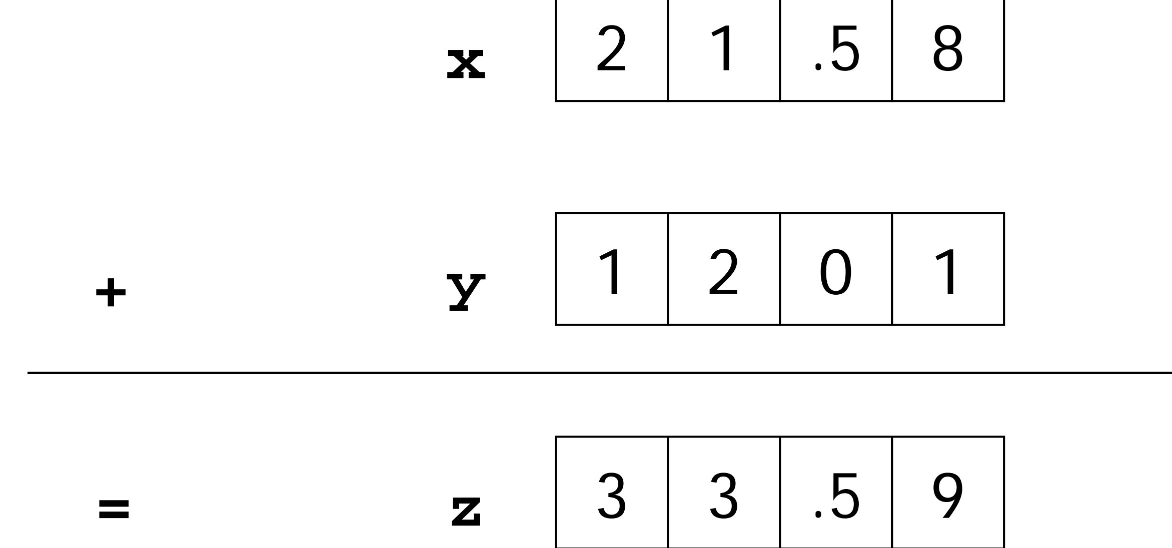
c

3	7	2	1

d

3
7
2

Vectorized addition



Matlab code: `z= x + y`

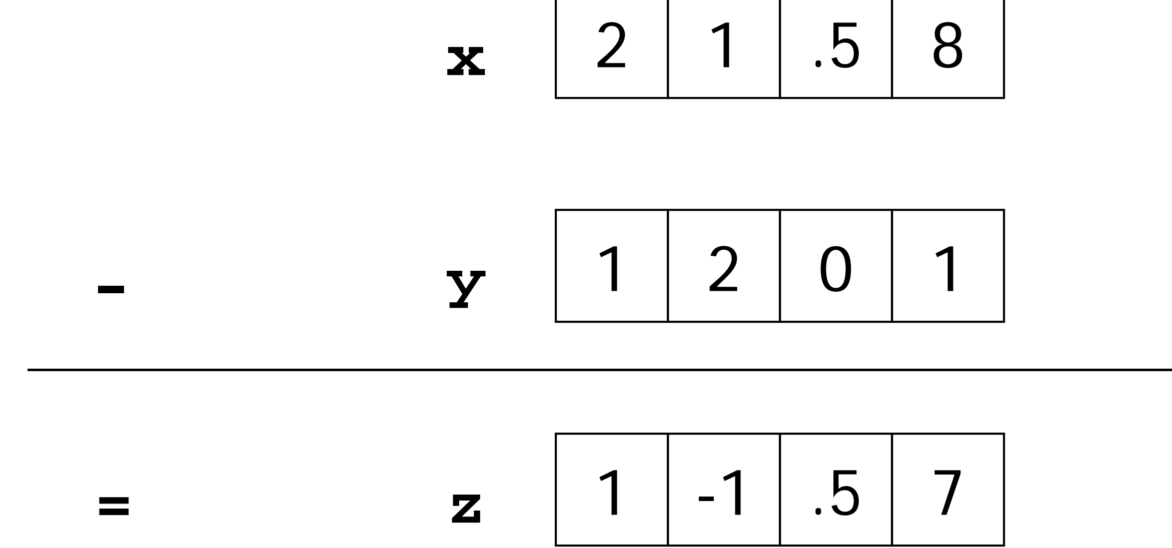
Vectorized code
—a Matlab-specific feature

- Code that performs element-by-element arithmetic/relational/logical operations on array operands in one step

- Scalar operation: x + y
  where x, y are scalar variables

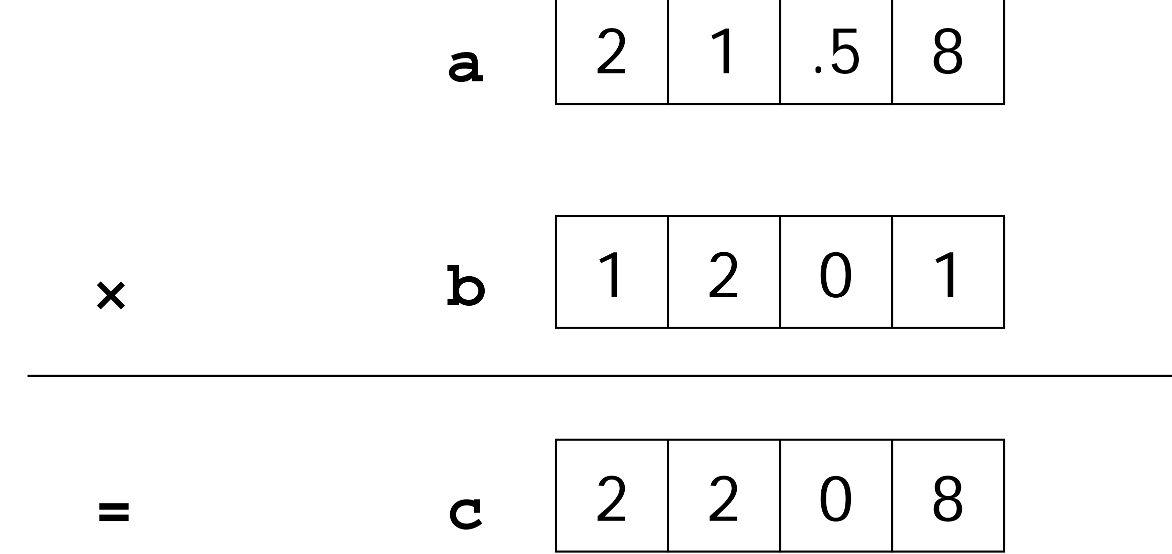
- Vectorized code: x + y
  where x and/or y are vectors. If x and y are both vectors, they must be of the same shape and length

Vectorized subtraction



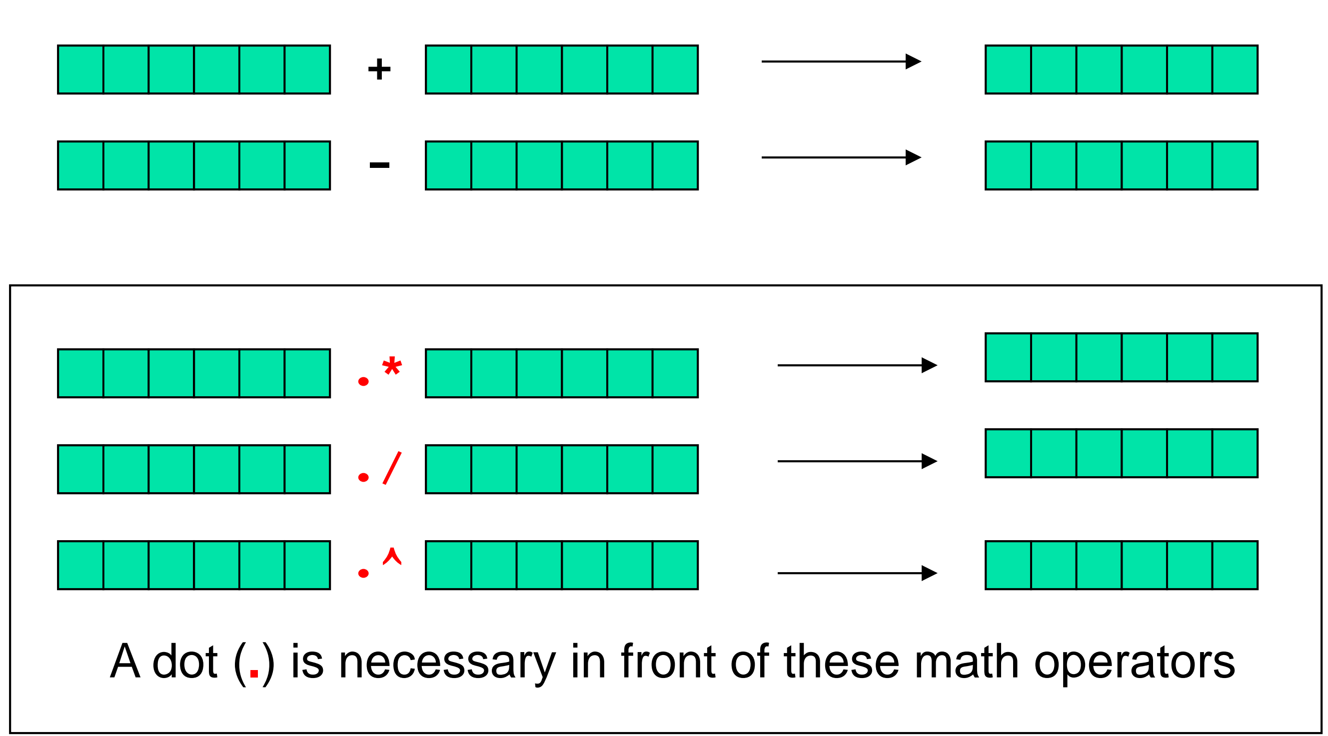
Matlab code: `z= x - y`

Vectorized multiplication

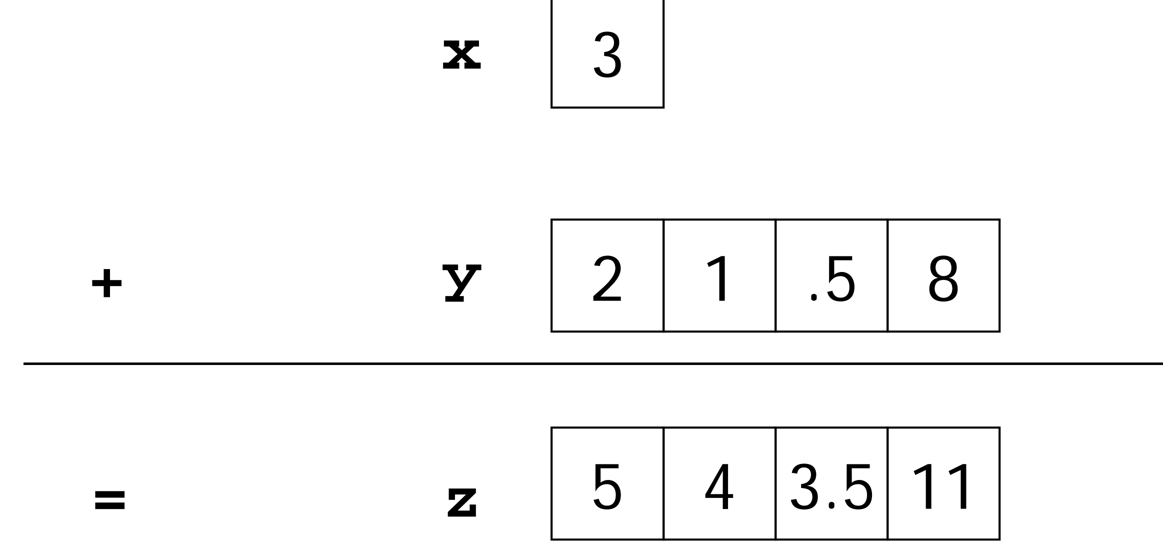


Matlab code: `c= a .* b`

Vectorized
element-by-element arithmetic operations on arrays

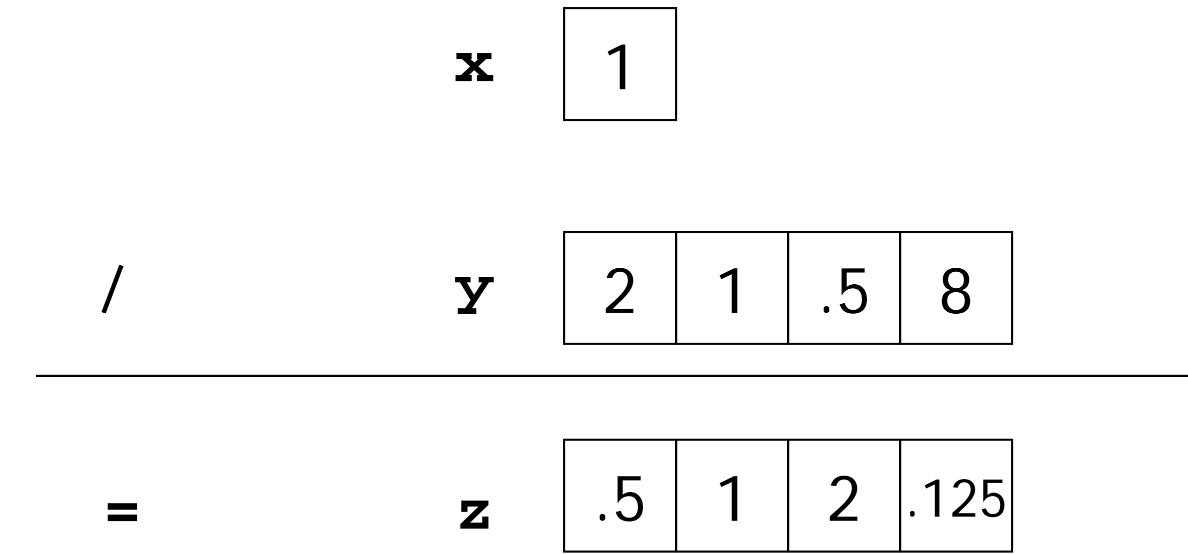


Shift



Matlab code: `z= x + y`

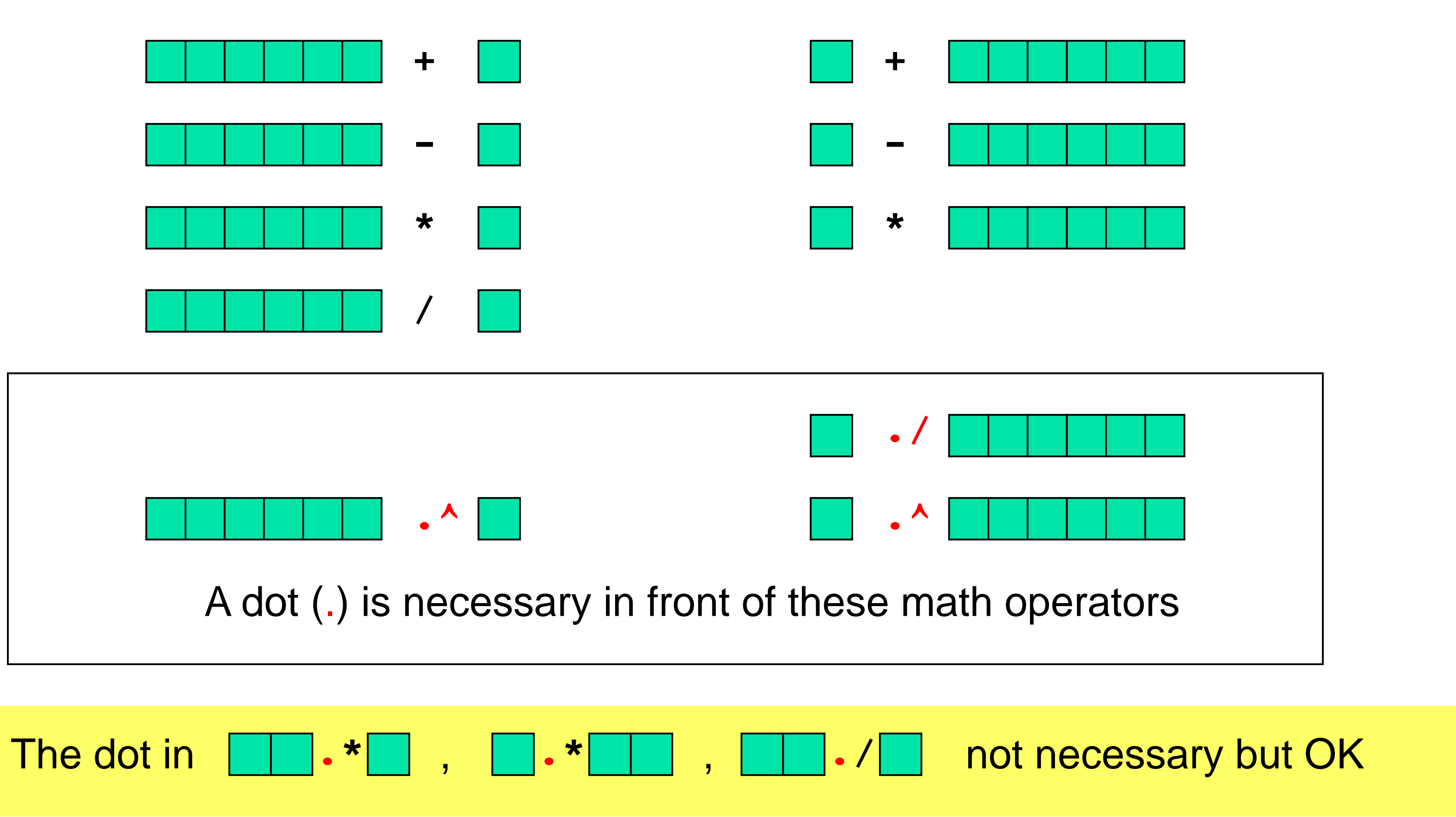
Reciprocate



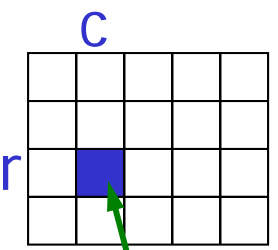
Matlab code:

```
z= x ./ y
```

Vectorized
element-by-element arithmetic operations between an array and a scalar



2-d array: **matrix**



- An array is a named collection of like data organized into rows and columns
- A 2-d array is a table, called a *matrix*
- Two *indices* identify the position of a value in a matrix, e.g.,

  `mat(r,c)`

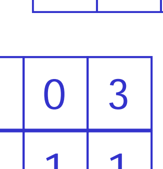
  refers to component in row r, column c of matrix mat
- Array index starts at 1
- Rectangular: all rows have the same #of columns

Creating a matrix

- Built-in functions: ones, zeros, rand
  - E.g., zeros(2,3) gives a 2-by-3 matrix of 0s
- "Build" a matrix using square brackets, [ ], but the dimension must match up:
  - [x y] puts y to the right of x
  - [x; y] puts y below x
  - [4 0 3; 5 1 9] creates the matrix

4	0	3
5	1	9

  - [4 0 3; ones(1,3)] gives
  - [4 0 3; ones(3,1)] doesn't work



What will **A** be?

```
A= [0  0]
A= [A'  ones(2,1)]
A= [0  0  0  0;  A  A]
```

```
% Given an nr-by-nc matrix M.
% What is A?
for  r= 1: nr
    for c= 1: nc
        A(c,r)= M(r,c);
    end
end
```