

Computing with MATLAB™

Part 2



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Outline

Using MATLAB for data manipulation and analysis

An example of MATLAB array arithmetic

plotting results

programming logic

array manipulations

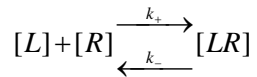
for loops

Strategies for using for loops

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Example of array arithmetic

Equation for bound receptor as function of [ligand]



In the steady-state, bound receptor can be calculated as:

$$[LR] = \frac{R_{TOT} [L]}{K_D + [L]} \quad K_D = \frac{k_-}{k_+}$$

We want to plot [LR] versus [L] for range of different K_D s

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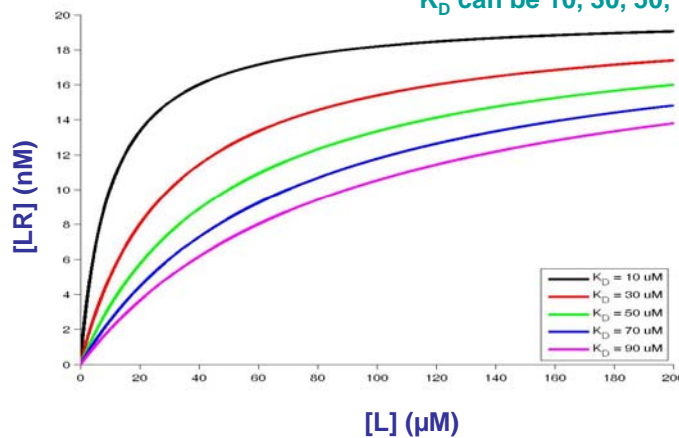
Example of array arithmetic

$$[LR] = \frac{R_{TOT} [L]}{K_D + [L]}$$

$R_{TOT} = 20 \text{ nM}$

[L] varies from 0 to 200 μM

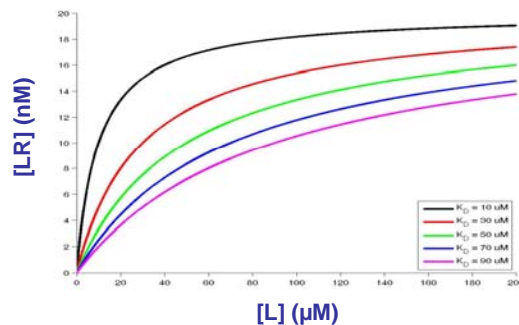
K_D can be 10, 30, 50, 70, 90 μM



We want to exploit MATLAB's functionality to generate such a plot

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MATLAB-generated plot of [LR] versus [L]



Principles illustrated by this example:

Plotting: plot colors, figure, hold on, legend, xlabel, ylabel

Array arithmetic: $LR = L * R_{tot} ./ (L + K_D)$;

Programming logic: command line vs. copy-paste vs. script

Programming logic: for loops

Array manipulations: accessing one row, $LR_all(i,:) = LR$;

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for loops

One of the most commonly-used and powerful programming tactics

Used to repeat certain calculations several times

Typical generic structure

```
for (variable) = (sequence)
    (MATLAB commands to be repeated)
end
```

Example:

```
for i=1:5
    output = 4*i^2 + 13
end
```

this will calculate and display 5 values of the variable output according to the formula

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Notes/hints on using for loops

All commands between `for` and `end` will be repeated

Each time through the loop, the “index variable” will be different

This can be exploited to make each trip through the loop slightly different

Example:

```
for i=1:5
    parameter = 2*i ;      [this will take on values 2, 4, 6, 8, 10]

    (run model with different values of the parameter)
end
```

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Notes/hints on using for loops

All commands between `for` and `end` will be repeated

Each time through the loop, the “index variable” will be different

This can be exploited to make each trip through the loop slightly different

A second example:

```
values_to_test = [1,13,22,300] ;
for i=1:length(values_to_test)
    parameter = values_to_test(i) ;      [this way your values do not have to be
                                         evenly spaced]

    (run model with different values of the parameter)
end
```

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Summary

MATLAB can be used for calculating, plotting, etc.

for loops are the most convenient way to repeat calculations

Perform calculations using the index variable so that each iteration through the for loop is slightly different

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Self-assessment question

You are working with an array **A**, dimensions 100 x 4. You also have a vector **time**, dimensions 100 x 1. Each column in **A** represents a different variable measured in your experiment. Each row represents the corresponding time point in the vector **time**. You wish to write a **for** loop to plot 4 time courses in different colors. You paste the following lines into your command window:

```
colors = 'krgb' ;  
for i=1:4  
    plot(time,A(i))  
end
```

This does not produce the desired result for 3 reasons. Why not?

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