Mathematica Introduction

Week 1 of Introduction to Computational Biology Labs

At this point you should inform your teaching assistant if you lack algebra or calculus knowledge. Don’t wait until the end of the course when you get a bad grade. When that happens, you are stuck with that grade :-(.
Additionally, don’t forget that google can be a good friend :-).

Background

The basics in *Mathematica*

Using Mathematica

Programming in Mathematica

Examples

Here are some examples that use multiple things learned in the previous sections. For further details about specific functions you can consult the documentation.
The first example creates a parameter and function list. We solve for where the functions are equal and plot the functions to check.

```
paramsA = {k1 → 1, k2 → 0.5, k3 → 0.1}(*parameter list*)
functA = {f1 → k1 + k2 x, f2 → k3 x}(*function list*)
solA = Solve[0 == f1 - f2 /. functA /. paramsA, x]
(*solving the function1 for f1=f2*)
p1 = {solA[[1]][[1]][[2]], f1 /. functA /. paramsA /. solA[[1]]}
(*point where f1=f2*)
Show[
 Plot[{
   f1 /. functA /. paramsA,
   f2 /. functA /. paramsA},
  {x, -10, 10},
  AxesLabel → {"x", "f1 & f2"},
  PlotLegends → {"f1", "f2"}],
 Graphics[{PointSize[Large], Point[p1]}]]
```

Simple parametric plot with and without animation.

```
ParametricPlot[{2 Cos[t], 2 Sin[t]},
 {t, 0, 2 π}, AspectRatio → Automatic, AxesLabel → {x, y}]
```

```
x[t_] := Cos[2 t]
y[t_, a_] := Cos[5 (t + a)]
Animate[ParametricPlot[{x[t], y[t, a]}, {t, 0, 2 π}, AspectRatio → Automatic],
 {a, 0, π/5 - π/120, π/120}]
```

Plotting a 3D shell shape that can be rotated interactively:

```
ParametricPlot3D[
 RotationTransform[2 π v, {0, 0, 1}][.5^v {Cos[u 2 π], 0, Sin[u 2 π]}] +
  .5^v {Cos[2 π v], Sin[2 π v], 1}, {u, 0, 1}, {v, 0, 4}, PlotRange → All,
 PlotPoints → {20, 40}, Axes → None, Boxed → False, Mesh → None]
```

Exercises

We will use some general biological problems to practice with *Mathematica*.

1. Bacterial Growth

Bacteria are inoculated in a petri dish at a density of 10/ml. The bacterial density doubles in twenty hours. Assume that this situation is described by the differential equation:

$$\frac{dx}{dt} = C\,x$$

where x is the bacterial density and C is a constant.

a. Integrate this equation giving x as a function of time and find the value of C.
b. How long does it take for the density to increase to eight times its original value? And to ten times its original value?

2. Fitting linear or exponential to growth data

We have a dataset that we need to fit.

a. What better describes, i.e. linear or exponential growth, the following data. The data is given in the form {{x,y},...,....}.

myData =
{{0.5,1.27},{0.6,6.58},{0.7,7.00},{0.8,8.83},{0.9,8.66},{1.0,5.53},{1.1,9.33},{1.2,14.57},{1.3,8.51},{1.4,17.61},{1.5,12.94},{1.6,18.45},{1.7,19.85},{1.8,25.03},{1.9,28.14},{2.0,28.31},{2.1,33.41},{2.2,41.43},{2.3,40.87},{2.4,56.71},{2.5,59.32}};

Find out by fittings functions, plotting them with the data and finding the error of both fits.

b. What is the differential equation for the fitted function? Also give the numerical values for the parameters.

3. The SIR model - Seasonal epidemics

With the SIR model you can study how the probability of getting a disease varies with the seasons of the year. SIR stands for Susceptibility - Infection - Recovery and is a set of nonlinear differential equations with periodically varying parameters. The periodically forced SIR model is:

$$\frac{dS}{dt} = \mu - \mu S - \beta(t) I S$$
$$\frac{dI}{dt} = \beta(t) I S - (\gamma + \mu) I$$
$$\frac{dR}{dt} = \gamma I - \mu R$$

Here S, I, and R are the fractions of susceptible, infective, and recovered individuals in the population; μ is the birth and death rate; $\beta(t)$ is the seasonally dependent infection rate; and γ is the recovery rate. We take $\beta(t)$ to be periodic; $\beta(t) = \beta_0\left[1 + \sin\left(\frac{2\pi t}{T}\right)\right]$, where T is the length of the infection season and β_0 is a

constant. The reproduction number for this system is $\frac{1}{T}\int_0^T \frac{\beta(t)}{\mu+\gamma}\,dt$; if the integral is greater than one, the disease will not disappear and may undergo interesting and complex phenomena of nonlinear parametric resonance .
More info can be found here.

a. We want to see how S, I and R change over time with varying parameters. Make a plot (or plots) to analyze how the dynamics change by varying the death rate($\mu = 0 - 1$), recovery rate($\gamma = 0 - 1$), season length ($T = 0 - 30$), initial infections rate ($\beta_0 = 0 - 1$) and the amount of initially infected (I_0).

References

Information for this notebook was taken from

1. “*Mathematica* programming: an advanced introduction. Part I: The core language” by Leonid Shifrin.
2. *Mathematica* main website and documentation.