Mean-field modeling using ordinary differential equations.

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Terminology

Types

There are a few types of ordinary differential equations (ODE), including:

- Separable;
- Linear/non-linear;
- First-order, second-order.

Solutions

Regarding the solutions of ODEs, there are, among others:

- Explicit/implicit solutions;
- Fixed point(s);
- Locally/globally stable fixed points; unstable fixed points

Notes

- In the first part you are asked to do some analytical work. In the second part you will implement a simple numerical solution (approximation) scheme.
- You will check your own analytical solutions by also performing the numerical solution, so if you are not sure about your own mathematical derivations you can continue and check back later using the numerical solution.
- When you are asked for a derivation or a solution then always show clearly the steps which you made to arrive at it. You can work it out on a notepad first, then write or type a clean version in your answer sheet.
- Please submit a PDF or textfile to Canvas and a Python or Jupyter Notebook file containing your code. Do not compress the files, but hand them in separately. Try to write concisely and limit your submission to 10 pages.
- If you are asked to draw a figure, you may either print a figure from any program or you may (roughly) sketch a figure by hand. In both cases, identify the important features.

Analytical skills needed

To solve all ODEs in this assignment you only need the following 4 skills.

1. Solve an ODE by 'separation of variables', which you already learned in the first part of the course in the *CA Analytics* slide deck. The basic steps of this technique are:

   (a) *Separate the variables.* All $x(t)$ (or just x for short) on one side, all t on the other side. E.g.:

   $$\frac{dx}{dt} = x,$$
   $$\frac{1}{x}dx = 1 \cdot dt.$$

   (b) *Integrate both sides.* This simply means: put an integration symbol on both side. E.g.:

   $$\int \frac{1}{x}dx = \int 1 \cdot dt.$$

   Then use high-school calculus and/or a list of known integral solutions[1] to solve the integrals. The solution of the example (collecting all integration constants into one constant C):

   $$\ln x = t + C$$

   (c) *Solve for $x(t)$.* Find a (nice) formula for $x(t)$. That is, use basic algebra to get $x(t)$ on one side and everything else on the other side. In the example, exponentiate both sides and done! I also rearrange a bit for aesthetics:

   $$x = e^{t+C},$$
   $$x = e^t e^C,$$
   $$x = C_0 \cdot e^t$$

   In the last step I collected the constant term e^C and made (redefined) a new constant C_0, just for simplicity. You can also leave the original form if you wish. As long as the result of this step is an equation of the form $x = ...$ and no x appears on the right side.

[1] To solve an integral you may use find and use the appropriate equation in e.g. `http://www.wikiwand.com/en/List_of_integrals_of_rational_functions`.

(d) *Specialize to a specific initial condition.* We cannot plot the above solution yet because we do not know the initial conditions of the ODE. That is, we know that $x(t)$ grows exponentially as function of t, but we do not know yet where this growth starts – i.e., we do not know the value for $x(0)$ (so $t = 0$). But suppose we are given the initial condition $x(0) = 2$. Then we can find the value for the unknown C_0, and then we are ready to plot the solution.

$$x(0) = C_0 \cdot e^0,$$
$$2 = C_0 \cdot 1,$$
$$C_0 = 2.$$

And thus the final solution (for the given initial condition $x(0) = 2$) that can be plotted using any software:

$$x(t) = 2 \cdot e^t.$$

One straightforward way to plot is to make an array of values for t in, for this example, the range $[0, 3]$, say with step size 0.1. Then compute the array of corresponding x values using the solution above. Then use `matplotlib` as usual to plot the x array versus the t array, like `plt.plot(t_array, x_array, '-o')`. For other ODEs, play around with the range for t and the step size to see what looks nice and shows the important features.

2. Find fixed point(s) of an ODE. A fixed point is a value for x such that x does not change anymore (remains 'fixed'). This means that the first derivative of x equals zero. Easy! The first derivative is precisely the given ODE to begin with! So all we need to do is set the ODE equal to 0 and then solve it, meaning, find values for x which satisfy this equation. Using the above simple example:

$$\frac{dx}{dt} = x = 0.$$

This is particularly simple: only $x = 0$ satisfies this equation. Thus we found that there is only one fixed point for this ODE, namely $x = 0$.

3. Determine stability of the fixed points. A fixed point $x(t) = F$ is called 'locally stable' iff $x(t) = F \pm \epsilon$ (where $\epsilon \neq 0$) moves towards F whenever it is (very) close to F already (so 'small enough' but still non-zero ϵ). It is called 'globally stable' if $x(t)$ will always converge to F no matter the initial condition, so for any value of ϵ. Finally, a fixed point is called 'unstable' if $x(t)$ moves away from the fixed point, no matter how close $x(t)$ is to F – with the single exception of exactly $x(t) = F$ of course.

   Local stability of a fixed point can be determined in the following two different ways. You may use either one.

   (a) *Use the second derivative (exact option).* Observe that local stability means the following two things. If $x(t) < F$ then the first derivative dx/dt should be positive (to increase $x(t)$ toward F). Conversely, if $x(t) > F$ then the first derivative dx/dt should be negative (to decrease $x(t)$ toward F). This means that the second derivative (derivative of first derivative, which we write as d^2x/dt^2) must be negative, i.e., $d^2x/dt^2 < 0$. That's it! So, using the same reasoning you can verify easily that a positive second derivative implies that the fixed point is unstable.[2]

   Let's do it for the running example $dx/dt = x$. The second derivative is $d^2x/dt^2 = 1$, which is positive, so this fixed point is unstable. This implies that *only* if we set exactly $x(0) = 0$ then we reach the fixed point; any other initial condition, no matter how close to zero, will move away from 0.

   (b) *Graph nearby initial conditions (approximate option).* In the running example, simply plot two solutions for two 'nearby' initial conditions, say $x(0) = 0.1$ and $x(0) = -0.1$. You will see that both curves move away from 0, no matter how close to 0 you set the initial conditions. This means that the fixed point is unstable. Just to be sure you did your math right you can also plot a third curve with initial condition $x(0) = 0$, just to verify that this curve will stay perfectly horizontal. If the solution were stable then both curves would converge to the fixed point 0.

4. *Numerical approximation of a solution.* Plotting a solution means putting t on the horizontal axis and $x(t)$ on the vertical axis. You can find this curve analytically as described above, but more often than not computational scientists use so-called numerical approximations.[3] By this we mean that we use an algorithm that results in an approximate curve for $x(t)$, which we can plot and should look very similar to the analytical solution (if any). 'Numerical' just means that we use the (finite) floating-point operations of the computer to get our result, instead of (exact) mathematical derivation like above.

   There is a very simple algorithm to plot an approximate solution, with any desired accuracy (at the cost of more computation). It is called the Euler algorithm. Most instructive is to watch the 10-minute video:
   `https://www.khanacademy.org/math/differential-equations/first-order-differential-equa`
   `eulers-method-tutorial/v/eulers-method`. There is also reading material mentioned below on the subject.

[2] You may wonder: what if the second derivative equals 0? Well then you usually have a semi-stable fixed point, which is stable on one side but unstable on the other side. But not necessarily! It can also be e.g. that any initial condition simply remains fixed, in which case there are infinitely many fixed points but none of them are considered stable.

[3] This is because most ODEs encountered in realistic applications cannot be (easily) analytically solved.

Background material

These videos and reading material give you a basic introduction of ODEs and how they are solved. You should be able to just start with the exercises below, but it is of course instructive to review this material at any time, or to use it as reference.

Short video lectures

- First 3 videos of `https://youtu.be/-_POEWfygmU?list=PL96AE8D9C68FEB902`
- `https://www.khanacademy.org/math/differential-equations/first-order-differential-equa` `logistic-differential-equation/v/logistic-differential-equation-intuition`
- `https://www.khanacademy.org/math/differential-equations/first-order-differential-equa` `eulers-method-tutorial/v/eulers-method`

Reading material

- `http://mathinsight.org/ordinary_differential_equation_introduction`
- `http://www.stewartcalculus.com/data/CALCULUS%20Concepts%20and%20Contexts/upfiles/3c3-LinearDiffEqns_Stu.pdf`. It is only needed to understand the definition of what a 'linear' ODE[4] is (first two equations); the way to solve such ODEs (using 'integrating factors') is optional to read (or to use).
- `http://tutorial.math.lamar.edu/Classes/DE/Modeling.aspx`. This is a general introduction to how modeling is done and how ODEs are created to model things; this page does not explain (well) how to actually solve ODEs. Perhaps needless to say, but you do not need to study hard on the example problems that are listed; just make sure you understand the main point.
- `http://tutorial.math.lamar.edu/Classes/DE/EulersMethod.aspx`
- `http://tutorial.math.lamar.edu/Classes/DE/EquilibriumSolutions.aspx`[5]

[4] Remind yourself of what linear and non-linear functions are, then you'll see a parallel.

[5] Here they use the term 'equilibrium point' where I use 'fixed point', but it is the same thing.

Problems

This section contains a mix of problems that you must solve analytically and problems to tackle numerically.

1. (Terminology) Explain briefly each type of ODE from the Terminology section above.
2. (Terminology) Explain briefly each type of solution from the Terminology section above.
3. (Numerical) Implement the simple Euler algorithm for estimating the solution $x(t)$ of a given single ODE $dx/dt = f(x,t)$. For each of the following three ODEs, derive an analytical solution and validate your Euler implementation against it by integrating from $t = 0$ to $t = 3$:
   - $dx/dt = 1$, with $x(0) = 0$,
   - $dx/dt = 2t$, with $x(0) = -4$
   - $dx/dt = -x$, with $x(0) = 4$

   Experiment with different values for the time step, $\Delta t = 1$, $\Delta t = 0.1$ and $\Delta t = 0.01$. Do this by plotting both the analytical solution and the numerical approximation in the same figure. For which equation(s) does your result improve? *For bonus: do the same for the second order Runge-Kutta method.*

   You now have a (crude) tool with which you can later check your analytical results.
4. (Analytical) Consider the concentration of a specific protein over time in a biological cell, denoted $x(t)$. Assume that these protein molecules are generated at a constant rate (increasing the concentration). Each protein also has a constant rate at which it degrades (decreasing the concentration). Thus we can model this simple system by the ODE

$$\frac{dx}{dt} = g - k \cdot x$$

   (a) (Analytical) Mention briefly the role of g and the role of k in this model.

   (b) (Analytical) Find an explicit solution for $x(t)$ in the general case.

   (c) Your solution should include an additional constant that is currently unknown. What is the role of this constant?

   (d) (Analytical) Now solve this ODE assuming the initial condition: $x(0) = 0$. In the remaining questions we will assume this solution.

   (e) (Analytical) Plot the following four curves of $x(t)$ versus t in the same figure, over the range $0 \leq t \leq 5$. (Can you already guess how g and k determine the long-term behavior?)
   - $g = 2, k = 3$
   - $g = 1, k = 1.5$
   - $g = 2, k = 2$
   - $g = 1, k = 1$

(f) (Numerical) Check the above results by numerical integration. Use a time step less than $0.1/k$.

(g) (Analytical) Derive the expression for the fixed point(s) to which $x(t)$ settles in general, so in terms of g and k.

(h) (Analytical) Plot dx/dt versus $x(t)$ for the values $g = 2$ and $k = 3$. Try a few other parameter values yourself. Use this figure to explain whether this ODE is unstable, locally stable, or globally stable.

(i) (Thought experiment) Suppose that g can now change over time, that is, $g(t)$ is now a function of time t. Suppose that at time $t = t_0$ the stable concentration of the protein is too low for the purpose of the cell. Biological cells can adapt to such situations. In this example, the cell can do nothing to change k since the decay rate depends on the chemistry of the protein molecule. But it *can* change the rate at which it produces new protein molecules, g. Assume that the cell can freely change g over time in order to make the new stable concentration, say, 100% higher. Sketch manually a possible graph of g over time of how the cell could achieve its goal, and explain its features. (Can you find a second possible shape, depending on how 'opportunistic' the cell changes g?)

(j) (Explain) Explain briefly why you think this model is called a 'mean-field' or 'mean-field approximation' model.

5. (a) Consider a population of rabbits and assume unlimited resources and space. Let us assume that each rabbit has a constant rate k of dying at any given time.

Consider the case where each rabbit can always easily find another rabbit, so that the reproduction only depends on the population of rabbits $x(t)$ itself (i.e., the more rabbits, the more new rabbits). Consider that each rabbit has a constant reproduction rate r. A simple ODE that models this situation can be:

$$\frac{dx}{dt} = r \cdot x - k \cdot x.$$

Explain briefly why.

(b) (Analytical) Solve this ODE for the general case. (Tip: remember that logarithms do not operate on negative arguments, be mindful when integrating.)

(c) (Analytical) Sketch the three typical behaviors of $x(t)$ in one figure. What are the fixed points, if any? If there are fixed points, are they stable (mathematically speaking)?

(d) (Numerical) Check your results numerically. Negative numbers of rabbits are not possible.

(e) (Analytical) In biology it is impossible to fix a rate accurately up to an infinite number of digits. There is just too much fluctuation and environmental influence for that. So consider that k and r are both very slightly (infinitesimally) changed during a simulation. Which fixed points of the three typical cases are affected by this and which remain unchanged (stable)?

(f) (Analytical) Now assume that the reproduction also depends on the concentration of rabbits, meaning that rabbits find a mate more easily if there are more rabbits. This means that if the density is low, then reproduction should be low, and if the density is high, then reproduction is high. We'll assume that there is no limit to the number of partners that a rabbit can have in a given time-frame. We can then change the ODE to include this effect in the simplest manner as follows:

$$\frac{dx}{dt} = r \cdot x \cdot x - k \cdot x.$$

Explain briefly why.

(g) (Analytical, bonus) Solve this ODE for the general case (i.e., not assuming any values already for the rates). Use also the constraint $x(0) = x_0$ in the solution, in order to see clearly how the initial condition alters the solution. Thus there should be no integration constant C in your solution. Hint: I suggest you use `http://www.wikiwand.com/en/List_of_integrals_of_rational_functions` to find the solution of difficult integrals (unless you feel confident: then use the substitution rule).

(h) (Numerical) Now study the equation numerically for $k = 1$, $r = 1$ and $x_0 = 0.5$, $x_0 = 1.0$ and $x_0 = 1.5$. Plot the results in a single figure. Note that your numerical integrator may not be able to compute all results due to overflow. Stop such an integration if x exceeds a limit of your own choosing.

(i) (Numerical) Above, you have studied some simple population models for rabbits with infinite food and space. A more realistic model that takes these constraints into account is the famous logistic differential equation, which is essentially obtained by flipping the sign of dx/dt in the previous equation and renaming the constants:

$$\frac{dx}{dt} = x(1 - x/x_{max}).$$

The analytic solution for this equation is actually given in the lecture slides on ODEs. Let's study it numerically. Plot a few curves ('numerical approximations') for two different initial conditions and two different values for x_{max} in a single figure. What is the biological meaning of x_{max}?

(j) (Analysis) Now explain briefly in your own words how this ODE implements the notion of population dynamics with bounded resources. For instance, in the previous assignment about rabbits you first had a positive term in the ODE which results in exponential growth. Then you added a factor that models the 'difficulty' of finding mates if the density is low. Compare this to the factor that is added now.

(k) (Analytical) Show analytically what the fixed point(s) of this model are, and whether they are stable.

(l) Plot dx/dt versus x in a figure with x ranging from -1 to $x_{max} + 1$, for an arbitrary value for x_{max}. Explain how this figure shows visually the same as the previous, analytical answer.

(m) (Numerical) Now suppose that rabbits also die at a constant rate r. Incorporate this term into the ODE and explain your change briefly.

(n) Determine analytically for what values of r and x_{max} the population will reach a stable fixed point of 0, i.e., the rabbits cannot reproduce fast enough and die out. Do the value(s) make sense?

(o) (Numerical) Suppose you pick a value of r that is, say, twice as high as needed to let the population die out. Make a numerical approximation of the solution with a (way too) coarse step size in t. What happens if you pick the step size too large? Show an example.