Physical Modeling in Octave®

Geoffrey Pleiss

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Ordinary differential equations

1.1 A Note on Syntax

Up until now, if you have followed the syntax that I've been using, especially the guidelines that were layed out in Section **??**, the code you've written has been compatible with MATLAB. This means that someone who is creating models in MATLAB can run your code and get the same results. In general, Octave and MATLAB share vary similar syntax and function names.

However, starting with this chapter, we are going to introduce functions that aren't compatible with MATLAB. Most of the syntax will be similar, so it won't be difficult to modify your code so it works with MATLAB. Nevertheless, don't expect the code you are about to write to work with any program besides Octave. You will get many strange errors if you try running it in MATLAB or any other scientific computing program.

1.2 Differential equations

A **differential equation** (DE) is an equation that describes the derivatives of an unknown function. "Solving a DE" means finding a function whose derivatives satisfy the equation.

For example, when bacteria grow in particularly bacteria-friendly conditions, the rate of growth at any point in time is proportional to the current population. What we might like to know is the population as a function of time. Toward that end, let's define f to be a function that maps from time, t, to population y. We don't know what it is, but we can write a differential equation that describes it:

$$\frac{df}{dt} = af$$

where a is a constant that characterizes how quickly the population increases.

Notice that both sides of the equation are functions. To say that two functions are equal is to say that their values are equal at all times. In other words:

$$\forall t : \frac{df}{dt}(t) = af(t)$$

This is an **ordinary** differential equation (ODE) because all the derivatives involved are taken with respect to the same variable. If the equation related derivatives with respect to different variables (partial derivatives), it would be a **partial** differential equation.

This equation is **first order** because it involves only first derivatives. If it involved second derivatives, it would be second order, and so on.

This equation is **linear** because each term involves t, f or df/dt raised to the first power; if any of the terms involved products or powers of t, f and df/dt it would be nonlinear.

Linear, first order ODEs can be solved analytically; that is, we can express the solution as a function of t. This particular ODE has an infinite number of solutions, but they all have this form:

$$t \to be^{at}$$

For any value of b, this function satisfies the ODE. If you don't believe me, take its derivative and check.

If we know the population of bacteria at a particular point in time, we can use that additional information to determine which of the infinite solutions is the (unique) one that describes a particular population over time.

For example, if we know that $f(0) = 5$ billion cells, then we can write

$$f(0) = 5 = be^{a0}$$

and solve for b, which is 5. That determines what we wanted to know:

$$f : t \to 5e^{at}$$

The extra bit of information that determines b is called the **initial condition** (although it isn't always specified at $t = 0$).

Unfortunately, most interesting physical systems are described by nonlinear DEs, most of which can't be solved analytically. The alternative is to solve them numerically.

1.3 Euler's method

The simplest numerical method for ODEs is Euler's method. Here's a test to see if you are as smart as Euler. Let's say that you arrive at time t and measure the current population, y, and the rate of change, r. What do you think the population will be after some period of time h has elapsed?

If you said $y + rh$, congratulations! You just invented Euler's method (but you're still not as smart as Euler).

This estimate is based on the assumption that r is constant, but in general it's not, so we only expect the estimate to be good if r changes slowly and h is small.

But let's assume (for now) that the ODE we are interested in can be written so that

$$\forall t, y : \frac{df}{dt}(t) = g(t, y)$$

where $y = f(t)$ and g is some function that maps (t, y) onto r; that is, given the time and current population, it computes the rate of change. Then we can advance from one point in time to the next using these equations:

$$T_{n+1} = T_n + h \tag{1.1}$$
$$F_{n+1} = F_n + g(t, y)h \tag{1.2}$$

where T is a sequence of times where we estimate the value of f, and F is the sequence of estimates. For each index i, F_i is an estimate of $f(T_i)$. The interval h is called the **time step**.

Assuming that we start at $t = 0$ and we have an initial condition $f(0) = y_0$ (where y_0 denotes a particular, known value), we would set $T_1 = 0$ and $F_1 = y_0$, and then use Equation 1.1 and Equation 1.2 to compute values of T_i and F_i until T_i gets to the value of t we are interested in.

If the rate doesn't change too fast and the time step isn't too big, Euler's method is accurate enough for most purposes. One way to check is to run it once with time step h and then run it again with time step $h/2$. If the results are the same, they are probably accurate; otherwise, cut the time step again.

Euler's method is **first order**, which means that each time you cut the time step in half, you expect the estimation error to drop by half. With a second-order method, you expect the error to drop by a factor of 4; third-order drops by 8, etc. The price of higher order methods is that they have to evaluate g more times per time step.

1.4 Another note on notation

There's a lot of math notation in this chapter, and some of it is non-standard, so I want to pause to review what we have so far. Here are the variables, their meanings, and their types:

Name	Meaning	Type
f	The unknown function specified, implicitly, by an ODE.	function $t \to y$
df/dt	The first time derivative of f	function $t \to r$
f_t	Alternative notation for the first time derivative of f	function $t \to r$
g	A "rate function," derived from the ODE, that computes rate of change for any t, y.	function $t, y \to r$
t	time	scalar variable
y	population	scalar variable
r	rate of change	scalar variable
h	time step	scalar constant
T	a sequence of times, t, where we estimate $f(t)$	sequence
F	a sequence of estimates for $f(t)$	sequence

So f is a function that computes the population as a function of time, $f(t)$ is the function evaluated at a particular time, and if we assign $f(t)$ to a variable, we usually call that variable y. Similarly, g is a "rate function" that computes the rate of change as a function of time and population. If we assign $g(t, y)$ to a variable, we call it r.

df/dt is the most common notation for the first derivative of f, but I have never liked it because it looks like a fraction. I prefer f_t, which has the benefit of looking like a function.

It is easy to get f_t confused with g, but notice that they are not even the same type. g is more general: it can compute the rate of change for any (hypothetical) population at any time; f_t is more specific: it is the actual rate of change at time t, given that the population is $f(t)$.

1.5 `lsode`

Euler's method is an example of a **fixed-step** differential equation solver. It is a fixed-step solver because the time step is pre-determined and constant. In other words, all points that the DE solver calculates the function at will be equally spaced. The alternative to a fixed-step solver is a **variable-step** solver, which – like the name implies – has a step size that changes as the function value changes. We will examine some variable-step solvers in another section. Right now we will learn how to use Octave's built-in fixed-step solver, `lsode`.

You could take time to write out a function for Euler's method, but using `lsode` is a much better choice. First of all, `lsode` is already written for you. There's no point writing your own fixed-step solver when Octave already has one! More importantly, `lsode` combines a number of fixed-step solvers, many of which are much more powerful than Euler's method. Using `lsode` will make your code faster and more accurate.

To use `lsode`, you will first have to write a Octave function that evaluates g as a function of t and y. As an example, suppose that the rate of population growth for rats depends on the current population, y, and the availability of food, which varies over the course of the year. The governing equation might be something like

$$f_t = af\left[1 + \sin(\omega t)\right]$$

where a is a **parameter*** that characterizes the reproductive rate, and ω is the frequency of a periodic function that characterizes the effect of varying food supply on reproduction.

This is an equation that specifies a relationship between a function and its derivative. In order to estimate values of f numerically, we have to transform it into a rate function. The first step is to write the equation more explicitly; to say that two function are equal means that they are equal all all times. In other words

$$\forall t : f_t(t) = af(t)\left[1 + \sin(\omega t)\right]$$

where t is time in days. The next step is to introduce a variable, y, as another name for $f(t)$

$$\forall t : f_t(t) = ay\left[1 + \sin(\omega t)\right]$$

This equation means that if we are given t and y, we can compute $f_t(t)$, which is the slope, or rate of change, of f. The last step is to express that computation as a function called g:

$$g : y, t \to ay\left[1 + \sin(\omega t)\right]$$

We have now written out the differential equation as a function, which we can use with `lsode` to estimate values of f. Here's what the function looks like using the values $a = 0.01$ and $\omega = 2\pi/365$ (one cycle per year):

*A parameter is a value that appears in a model to quantify some physical aspect of the scenario being modeled. For example, in Exercise **??** we used parameters `rho` and `r` to quantify the density and radius of a duck. Parameters are often constants, but in some models they might vary in time.

```
function res = rats(y, t)
  a = 0.01;
  omega = 2 * pi / 365;
  res = a * y * (1 + sin(omega * t));
end
```

You can test this function from the Command Window by calling it with different values of `t` and `y`; the result is the rate of change (in units of rats per day):

```
octave:1> r = rats(2, 0)
r = 0.020000
```

So if there are two rats on January 1, we expect them to reproduce at a rate that would produce 2 more rats per hundred days. But if we come back in April, the rate has almost doubled:

```
octave:2> r = rats(2, 120)
r = 0.037600
```

Since the rate is constantly changing, it is not easy to predict the future rat population, but that is exactly what `ode45` does. Here's how you would use it:

```
octave:3> T = 0:5:365;
octave:4> Y = lsode(@rats, 2, T);
```

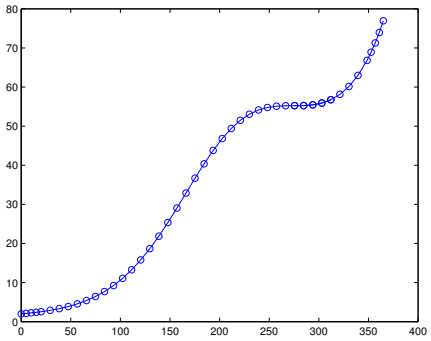
With the first command, we are creating a vector for all the times that we want to find values of f at. In this example, we want to know the rat population every 5 days for an entire year. Another way of saying this: we want our ODE solver to find the population for an entire year with a step-size of 5 days.

In the second command, we are telling Octave to find a value for $f(t)$ at every point in time that we specified in the first command. The first argument is a handle for the function that computes g. The second argument is the initial population, $f(0) = 2$. The third argument is the vector containing the time values specified in the first command.

You now know the rat population at every point during the year! To see what this function looks like, plot the results.

```
octave:5> plot(T, Y, 'o-')
```

Your plot should look something like this:



The x-axis shows time from 0 to 365 days; the y-axis shows the rat population, which starts at 2 and grows to almost 80. The rate of growth is slow in the winter and summer, and faster in the spring and fall, but it also accelerates as the population grows.

1.6 ode45

A limitation of fixed-step solvers is that the time step is constant from one iteration to the next. But some parts of the solution are harder to estimate than others; if the time step is small enough to get the hard parts right, it is doing more work than necessary on the easy parts. The ideal solution is to adjust the time step as you go along. Methods that do that are called **adaptive**, and one of the best adaptive methods is the Dormand-Prince pair of Runge-Kutta formulas. Fortunately, you don't have to know what that means, because the nice people at Mathworks have implemented it in a function called `ode45`. The `ode` stands for "ordinary differential equation [solver];" the 45 indicates that it uses a combination of 4th and 5th order formulas.

When you call `ode45` without assigning the result to a variable, Octave displays the result in a figure:

1.7 Multiple output variables

`ode45` is one of many Octave functions that return more than one output variable. The syntax for calling it and saving the results is

```
octave:1> [T, Y] = ode45(@rats, [0, 365], 2);
```

The first return value is assigned to `T`; the second is assigned to `Y`. Each element of `T` is a time, t, where `ode45` estimated the population; each element of `Y` is an estimate of $f(t)$.

If you assign the output values to variables, `ode45` doesn't draw the figure; you have to do it yourself:

```
octave:1> plot(T, Y, 'bo-')
```

If you plot the elements of `T`, you'll see that the space between the points is not quite even. They are closer together at the beginning of the interval and farther apart at the end.

To see the population at the end of the year, you can display the last element from each vector:

```
octave:1> [T(end), Y(end)]

ans = 365.0000  76.9530
```

`end` is a special word in Octave; when it appears as an index, it means "the index of the last element." You can use it in an expression, so `Y(end-1)` is the second-to-last element of `Y`.

How much does the final population change if you double the initial population? How much does it change if you double the interval to two years? How much does it change if you double the value of a?

1.8 Analytic or numerical?

When you solve an ODE analytically, the result is a function, f, that allows you to compute the population, $f(t)$, for any value of t. When you solve an ODE numerically, you get two vectors. You can think of these vectors as a discrete approximation of the continuous function f: "discrete" because it is only defined for certain values of t, and "approximate" because each value F_i is only an estimate of the true value $f(t)$.

So those are the limitations of numerical solutions. The primary advantage is that you can compute numerical solutions to ODEs that don't have analytic solutions, which is the vast majority of nonlinear ODEs.

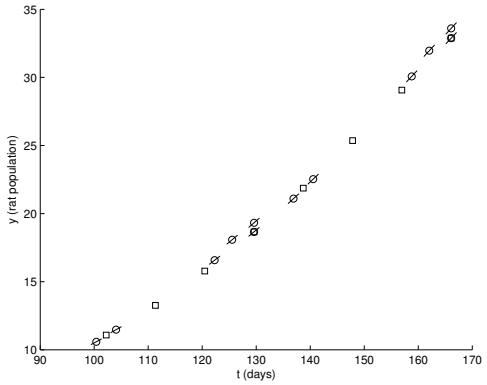
If you are curious to know more about how `ode45` works, you can modify `rats` to display the points, (t, y), where `ode45` evaluates g. Here is a simple version:

```
function res = rats(t, y)
  plot(t, y, 'bo')
  a = 0.01;
  omega = 2 * pi / 365;
  res = a * y * (1 + sin(omega * t));
end
```

Each time `rats` is called, it plots one data point; in order to see all of the data points, you have to use `hold on`.

```
octave:1> clf; hold on
octave:1> [T, Y] = ode45(@rats, [0, 10], 2);
```

This figure shows part of the output, zoomed in on the range from Day 100 to 170:



The circles show the points where `ode45` called `rats`. The lines through the circles show the slope (rate of change) calculated at each point. The rectangles show the locations of the estimates (T_i, F_i). Notice that `ode45` typically evaluates g several times for each estimate. This allows it to improve the estimates, for one thing, but also to detect places where the errors are increasing so it can decrease the time step (or the other way around).

1.9 What can go wrong?

Don't forget the `@` on the function handle. If you leave it out, Octave treats the first argument as a function call, and calls `rats` without providing arguments.

```
octave:1> ode45(rats, [0,365], 2)
??? Input argument "y" is undefined.

Error in ==> rats at 4
  res = a * y * (1 + sin(omega * t));
```

Again, the error message is confusing, because it looks like the problem is in `rats`. You've been warned!

Also, remember that the function you write will be called by `ode45`, which means it has to have the signature `ode45` expects: it should take two input variables, `t` and `y`, in that order, and return one output variable, `r`.

If you are working with a rate function like this:

$$g : t, y \to ay$$

You might be tempted to write this:

```
function res = rate_func(y)    % WRONG
  a = 0.1
  res = a * y
end
```

But that would be wrong. So very wrong. Why? Because when `ode45` calls `rate_func`, it provides two arguments. If you only take one input variable, you'll get an error. So you have to write a function that takes `t` as an input variable, even if you don't use it.

```
function res = rate_func(t, y)   % RIGHT
  a = 0.1
  res = a * y
end
```

Another common error is to write a function that doesn't make an assignment to the output variable. If you write something like this:

```
function res = rats(t, y)
  a = 0.01;
  omega = 2 * pi / 365;
  r = a * y * (1 + sin(omega * t))  % WRONG
end
```

And then call it from `ode45`, you get

```
octave:1> ode45(@rats, [0,365], 2)
??? Output argument "res" (and maybe others) not assigned during
call to "/home/downey/rats.m (rats)".

Error in ==> rats at 2
  a = 0.01;

Error in ==> funfun/private/odearguments at 110
f0 = feval(ode,t0,y0,args{:});  % ODE15I sets args{1} to yp0.

Error in ==> ode45 at 173
[neq, tspan, ntspan, next, t0, tfinal, tdir, y0, f0, odeArgs,
odeFcn, ...
```

This might be a scary message, but if you read the first line and ignore the rest, you'll get the idea.

Yet another mistake that people make with `ode45` is leaving out the brackets on the second argument. In that case, Octave thinks there are four arguments, and you get

```
octave:1> ode45(@rats, 0, 365, 2)
??? Error using ==> funfun/private/odearguments
When the first argument to ode45 is a function handle, the
tspan argument must have at least two elements.

Error in ==> ode45 at 173
[neq, tspan, ntspan, next, t0, tfinal, tdir, y0, f0, odeArgs,
odeFcn, ...
```

Again, if you read the first line, you should be able to figure out the problem (`tspan` stands for "time span", which we have been calling the interval).

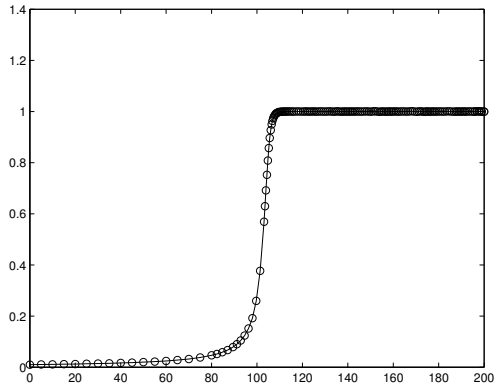
1.10 Stiffness

There is yet another problem you might encounter, but if it makes you feel better, it might not be your fault: the problem you are trying to solve might be **stiff**[†].

I won't give a technical explanation of stiffness here, except to say that for some problems (over some intervals with some initial conditions) the time step needed to control the error is very small, which means that the computation takes a long time. Here's one example:

$$f_t = f^2 - f^3$$

If you solve this ODE with the initial condition $f(0) = \delta$ over the interval from 0 to $2/\delta$, with $\delta = 0.01$, you should see something like this:



After the transition from 0 to 1, the time step is very small and the computation goes slowly. For smaller values of δ, the situation is even worse.

In this case, the problem is easy to fix: instead of `ode45` you can use `ode23s`, an ODE solver that tends to perform well on stiff problems (that's what the "s" stands for).

In general, if you find that `ode45` is taking a long time, you might want to try one of the stiff solvers. It won't always solve the problem, but if the problem is stiffness, the improvement can be striking.

Exercise 1.1 *Write a rate function for this ODE and use* `ode45` *to solve it with the given initial condition and interval. Start with* $\delta = 0.1$ *and decrease it by multiples of 10. If you get tired of waiting for a computation to complete, you can press the Stop button in the Figure window or press Control-C in the Command Window.*

Now replace `ode45` *with* `ode23s` *and try again!*

[†]The following discussion is based partly on an article from Mathworks available at `http://www.mathworks.com/company/newsletters/news_notes/clevescorner/may03_cleve.html`

1.11 Glossary

differential equation (DE): An equation that relates the derivatives of an unknown function.

ordinary DE: A DE in which all derivatives are taken with respect to the same variable.

partial DE: A DE that includes derivatives with respect to more than one variable

first order (ODE): A DE that includes only first derivatives.

linear: A DE that includes no products or powers of the function and its derivatives.

time step: The interval in time between successive estimates in the numerical solution of a DE.

first order (numerical method): A method whose error is expected to halve when the time step is halved.

fixed-step (solver): An ODE solver that uses a constant time step.

variable-step (solver): An ODE solver that has a time-step that changes as the function value changes.

adaptive: A method that adjusts the time step to control error.

stiffness: A characteristic of some ODEs that makes some ODE solvers run slowly (or generate bad estimates). Some ODE solvers, like `ode23s`, are designed to work on stiff problems.

parameter: A value that appears in a model to quantify some physical aspect of the scenario being modeled.

1.12 Exercises

Exercise 1.2 *Suppose that you are given an 8 ounce cup of coffee at 90 °C and a 1 ounce container of cream at room temperature, which is 20 °C. You have learned from bitter experience that the hottest coffee you can drink comfortably is 60 °C.*

Assuming that you take cream in your coffee, and that you would like to start drinking as soon as possible, are you better off adding the cream immediately or waiting? And if you should wait, then how long?

To answer this question, you will have to model the cooling process of a hot liquid in air. Hot coffee transfers heat to the environment by conduction, radiation, and evaporative cooling. Quantifying these effects individually would be challenging and unnecessary to answer the question as posed.

As a simplification, we can use Newton's Law of Cooling[‡]*:*

$$f_t = -r(f - e)$$

where f is the temperature of the coffee as a function of time and f_t is its time derivative; e is the temperature of the environment, which is a constant in this case, and r is a parameter (also constant) that characterizes the rate of heat transfer.

It would be easy to estimate r for a given coffee cup by making a few measurements over time. Let's assume that that has been done and r has been found to be 0.001 in units of inverse seconds, $1/s$.

- *Using mathematical notation, write the rate function, g, as a function of y, where y is the temperature of the coffee at a particular point in time.*
- *Create an M-file named* `coffee` *and write a function called* `coffee` *that takes no input variables and returns no output value. Put a simple statement like* `x=5` *in the body of the function and invoke* `coffee()` *from the Command Window.*
- *Add a function called* `rate_func` *that takes* `t` *and* `y` *and computes $g(t, y)$. Notice that in this case g does not actually depend on t; nevertheless, your function has to take t as the first input argument in order to work with* `ode45`*.*

  Test your function by adding a line like `rate_func(0,90)` *to* `coffee`*, the call* `coffee` *from the Command Window.*
- *Once you get* `rate_func(0,90)` *working, modify* `coffee` *to use* `ode45` *to compute the temperature of the coffee (ignoring the cream) for 60 minutes. Confirm that the coffee cools quickly at first, then more slowly, and reaches room temperature (approximately) after about an hour.*
- *Write a function called* `mix_func` *that computes the final temperature of a mixture of two liquids. It should take the volumes and temperatures of the liquids as parameters.*

  In general, the final temperature of a mixture depends on the specific heat of the two substances[§]*. But if we make the simplifying assumption that coffee and cream have the same density and specific heat, then the final temperature is $(v_1 y_1 + v_2 y_2)/(v_1 + v_2)$, where v_1 and v_2 are the volumes of the liquids, and y_1 and y_2 are their temperatures.*

  Add code to `coffee` *to test* `mix_func`*.*
- *Use* `mix_func` *and* `ode45` *to compute the time until the coffee is drinkable if you add the cream immediately.*

[‡] `http://en.wikipedia.org/wiki/Heat_conduction`
[§] `http://en.wikipedia.org/wiki/Heat_capacity`

- *Modify* `coffee` *so it takes an input variable* t *that determines how many seconds the coffee is allowed to cool before adding the cream, and returns the temperature of the coffee after mixing.*
- *Use* `fzero` *to find the time* t *that causes the temperature of the coffee after mixing to be* $60\,^\circ C$.
- *What do these results tell you about the answer to the original question? Is the answer what you expected? What simplifying assumptions does this answer depend on? Which of them do you think has the biggest effect? Do you think it is big enough to affect the outcome? Overall, how confident are you that this model can give a definitive answer to this question? What might you do to improve it?*