Chapter 12

Optimization and Interpolation

12.1 ODE Events

Normally when you call `ode45` you have to specify a start time and an end time. But in many cases, you don't know ahead of time when the simulation should end. Fortunately MATLAB provides a mechanism for dealing with this problem. The bad news is that it is a little awkward. Here's how it works:

1. Before calling `ode45` you use `odeset` to create an object called `options` that contains values that control how `ode45` works:

   ```
   options = odeset('Events', @events);
   ```

   In this case, the name of the option is `Events` and the value is a function handle. When `ode45` runs, it will invoke `events` after each timestep. You can call this function anything you want, but the name `events` is conventional.

2. The function you provide has to take the same input variables as your rate function. For example, here is an event function that would work with `projectile` from Section 11.6

   ```
   function [value,isterminal,direction] = events(t,X)
       value = X(2);        % Extract the current height.
       isterminal = 1;      % Stop the integration if height crosses zero.
       direction = -1;      % But only if the height is decreasing.
   end
   ```

`events` returns three output variables:

`value` determines when an event occurs. In this case `value` gets the second element of `X`, which is understood to be the height of the projectile. An "event" is a point in time when this value passes through 0.

`direction` determines whether an event occurs when `value` is increasing (`direction=1`), decreasing (`direction=-1`, or both `direction=0`.

`isterminal` determines what happens when an event occurs. If `isterminal=1`, the event is "terminal" and the simulation stops. If `isterminal=0`, the simulation continues, but `ode45` does some additional work to make sure that the solution in the vicinity of the event is accurate, and that one of the estimated values in the result is at the time of the event.

3. When you call `ode45`, you pass `options` as a fourth argument:

```
ode45(@projectile, [0,10], [0, 3, 40, 30], options);
```

Exercise 12.1 *How would you modify* `events` *to stop when the height of the projectile falls through 3m?*

12.2 Optimization

In Exercise 11.5, you were asked to find the optimal launch angle for a batted ball. "Optimal" is a fancy way of saying "best;" what that means depends on the problem. For the Green Monster Problem—finding the optimal angle for hitting a home run in Fenway Park, the meaning of "optimal" is not obvious.

It is tempting to choose the angle that yields the longest range (distance from home plate when it lands). But in this case we are trying to clear a 12m wall, so maybe we want the angle that yields the longest range when the ball falls through 12m.

Although either definition would be good enough for most purposes, neither is quite right. In this case the "optimal" angle is the one that yields the greatest height at the point where the ball reaches the wall, which is 97m from home plate.

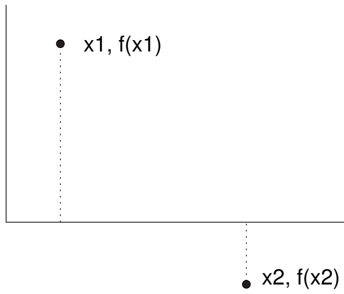
So the first step in any optimization problem is to define what "optimal" means. The second step is to define a range of values where you want to search. In this case the range of feasible values is between 0 degrees (parallel to the ground) and 90 degrees (straight up). We expect the optimal angle to be near 45 degrees, but we might not be sure how far from 45 degrees to look. To play it safe, we could start with the widest feasible range.

The simplest way to search for an optimal value is to run the simulation with a wide range of values and choose the one that yields the best result. This method is not very efficient, especially in a case like this where computing the distance in flight is expensive.

A better algorithm is a Golden Section Search.

12.3 Golden section search

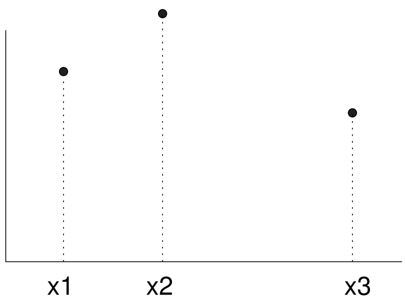
To present the Golden Section Search, I will start with a simplified version I'll call a Silver Section Search. The basic idea is similar to the methods for zero-finding we saw in Section 7.5. In the case of zero-finding, we had a picture like this:



We are given a function, f, that we can evaluate, and we want to find a root of f; that is, a value of x that makes $f(x) = 0$. If we can find a value, x_1, that makes $f(x_1)$ positive and another value, x_2, that makes $f(x_2)$ negative, then there has to be a root in between (as long as f is continuous). In this case we say that x_1 and x_2 "bracket" the root.

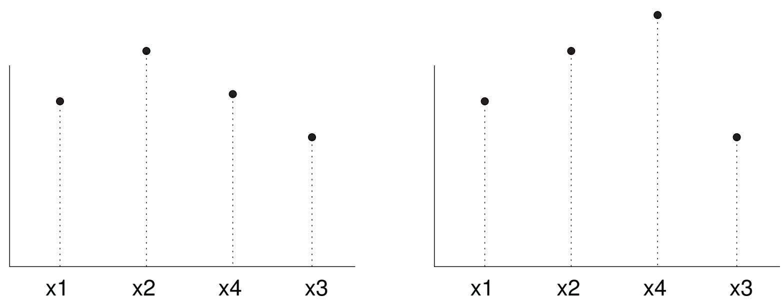
The algorithm proceeds by choosing a third value, x_3, between x_1 and x_2 and then evaluating $y = f(x_3)$. If y is positive, we can form a new pair, (x_3, x_2), that brackets the root. If y is negative then the pair (x_1, x_3) brackets the root. Either way the size of the bracket gets smaller, so our estimate of the location of the root gets better.

So that was root-finding. The Golden Section Search is similar, but we have to start with three values, and the picture looks like this:



This diagram shows that we have evaluated f in three places, x_1, x_2 and x_3, and found that x_2 yields the highest value. If f is continuous, then there has to be at least one local maximum between x_1 and x_3, so we would say that the triple (x_1, x_2, x_3) brackets a maximum.

The next step is to choose a fourth point, x_4, and evaluate $f(x_4)$. There are two possible outcomes, depending on whether $f(x_4)$ is greater than $f(x_2)$:



If $f(x_4)$ is less than than $f(x_2)$ (shown on the left), then the new triple (x_1, x_2, x_4) brackets the maximum. If $f(x_4)$ is greater than $f(x_2)$ (shown on the right), then (x_2, x_4, x_3) brackets the maximum. Either way the range gets smaller and our estimate of the optimal value of x gets better.

This method works for almost any value of x_4, but some choices are better than others. In the example, I chose to bisect the bigger of the ranges (x_1, x_2) and (x_2, x_3).

Here's what that looks like in MATLAB:

```
function res = optimize(V)
    x1 = V(1);
    x2 = V(2);
    x3 = V(3);

    fx1 = height_func(x1);
    fx2 = height_func(x2);
    fx3 = height_func(x3);

    for i=1:50
        if x3-x2 > x2-x1
            x4 = (x2+x3) / 2;
            fx4 = height_func(x4);
            if fx4 > fx2
                x1 = x2;  fx1 = fx2;
                x2 = x4;  fx2 = fx4;
            else
                x3 = x4;  fx3 = fx4;
            end
```

```
        else
            x4 = (x1+x2) / 2;
            fx4 = height_func(x4);
            if fx4 > fx2
                x3 = x2;  fx3 = fx2;
                x2 = x4;  fx2 = fx4;
            else
                x1 = x4;  fx1 = fx4;
            end
        end

        if abs(x3-x1) < 1e-2
            break
        end
    end
    res = [x1 x2 x3];
end
```

The input variable is a vector that contains three values that bracket a maximum; in this case they are angles in degrees. `optimize` starts by evaluating `height_func` for each of the three values. We assume that `height_func` returns the quantity we want to optimize; for the Green Monster Problem it is the height of the ball when it reaches the wall.

Each time through the `for` loop the function chooses a value of `x4`, evaluates `height_func`, and then updates the triplet `x1`, `x2` and `x3` according to the results.

After the update, it computes the range of the bracket, `x3-x1`, and checks whether it is small enough. If so, it breaks out of the loop and returns the current triplet as a result. In the worst case the loop executes 50 times.

Exercise 12.2 *I call this algorithm a Silver Section Search because it is almost as good as a Golden Section Search. Read the Wikipedia page about the Golden Section Search (`http://en.wikipedia.org/wiki/Golden_section_search`) and then modify this code to implement it.*

Exercise 12.3 *You can write functions that take function handles as input variables, just as* `fzero` *and* `ode45` *do. For example,* `handle_func` *takes a function handle called* `func` *and calls it, passing* `pi` *as an argument.*

```
function res = handle_func(func)
    func(pi)
end
```

You can call `handle_func` *from the Command Window and pass different function handles as arguments:*

```
>> handle_func(@sin)
```

```
ans = 0

>> handle_func(@cos)

ans = -1
```

Modify `optimize` *so that it takes a function handle as an input variable and uses it as the function to be optimized.*

Exercise 12.4 *The MATLAB function* `fminsearch` *takes a function handle and searches for a local minimum. Read the documentation for* `fminsearch` *and use it to find the optimal launch angle of a baseball with a given velocity.*

12.4 Discrete and continuous maps

When you solve an ODE analytically, the result is a function, which you can think of as a continuous map. When you use an ODE solver, you get two vectors (or a vector and a matrix), which you can think of as a discrete map.

For example, in Section 9.4, we used the following rate function to estimate the population of rats as a function of time:

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

The result from `ode45` is two vectors:

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

`T` contains the time values where `ode45` estimated the population; `Y` contains the population estimates.

Now suppose we would like to know the population on the 180th day of the year. We could search `T` for the value 180:

```
>> find(T==180)

ans = Empty matrix: 0-by-1
```

But there is no guarantee that any particular value appears in `T`. We can find the index where `T` crosses 180:

```
>> I = find(T>180); I(1)

ans = 23
```

`I` gets the indices of all elements of `T` greater than 180, so `I(1)` is the index of the *first* one.

Then we find the corresponding value from `Y`:

```
>> [T(23), Y(23)]

ans = 184.3451   40.3742
```

That gives us a coarse estimate of the population on Day 180. If we wanted to do a little better, we could also find the last value before Day 180:

```
>> [T(22), Y(22)]

ans = 175.2201   36.6973
```

So the population on Day 180 was between 36.6973 and 40.3742.

But where in this range is the best estimate? A simple option is to choose whichever time value is closer to 180 and use the corresponding population estimate. In the example, that's not a great choice because the time value we want is right in the middle.

12.5 Interpolation

A better option is to draw a straight line between the two points that bracket Day 180 and use the line to estimate the value in between. This process is called **linear interpolation**, and MATLAB provides a function named `interp1` that does it:

```
>> pop = interp1(T, Y, 180)

pop = 38.6233
```

The first two arguments specify a discrete map from the values in `T` to the values in `Y`. The third argument is the time value where we want to interpolate. The result is what we expected, about halfway between the values that bracket it.

`interp1` can also take a fourth argument that specifies what kind of interpolation you want. The default is `'linear'`, which does linear interpolation. Other choices include `'spline'` which uses a spline curve to fit two points on either side, and `'cubic'`, which uses piecewise cubic Hermite interpolation.

```
>> pop = interp1(T, Y, 180, 'spline')

pop = 38.6486

>> pop = interp1(T, Y, 180, 'cubic')

pop = 38.6491
```

In this case we expect the spline and cubic interpolations to be better than linear, because they use more of the data, and we know the function isn't linear. But we have no reason to expect the spline to be more accurate than the cubic, or the other way around. Fortunately, they are not very different.

We can also use `interp1` to project the rat population out beyond the values in `T`:

```
>> [T(end), Y(end)]

ans = 365.0000   76.9530

>> pop = interp1(T, Y, 370, 'cubic')

pop = 80.9971
```

This process is called **extrapolation**. For time values near 365, extrapolation may be reasonable, but as we go farther into the "future," we expect them to be less accurate. For example, here is the estimate we get by extrapolating for a whole year:

```
>> pop = interp1(T, Y, 365*2, 'cubic')

pop = -4.8879e+03
```

And that's wrong. So very wrong.

12.6 Interpolating the inverse function

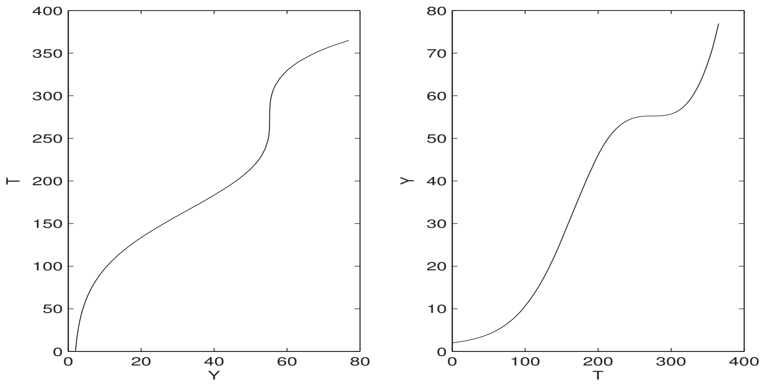
We have used `interp1` to find population as a function of time; by reversing the roles of `T` and `Y`, we can also interpolate time as a function of population. For example, we might want to know how long it takes the population to reach 20.

```
>> interp1(Y, T, 20)

ans = 133.4128
```

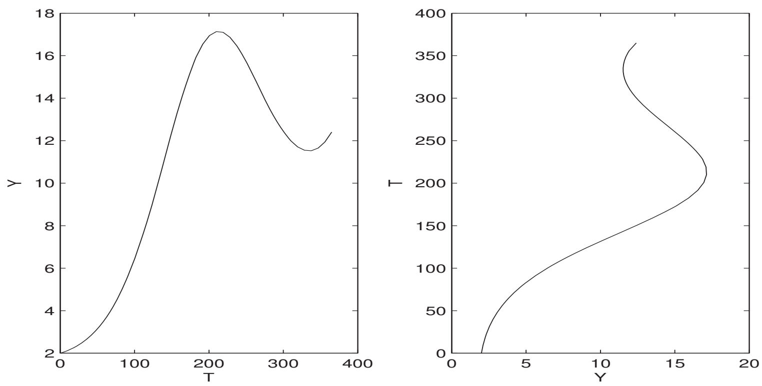
This use of `interp1` might be confusing if you think of the arguments as x and y. You might find it helpful to think of them as the range and domain of a map (where the third argument is an element of the range).

The following plot shows f (`Y` plotted as a function of `T`) and the inverse of f (`T` plotted as a function of `Y`).



In this case we can use `interp1` either way because f is a **single-valued mapping**, which means that for each value in the domain, there is only one value in the range that maps to it.

If we reduce the food supply so that the rat population decreases during the winter, we might see something like this:



We can still use `interp1` to map from `T` to `Y`:

```
>> interp1(T, Y, 260)

ans = 15.0309
```

So on Day 260, the population is about 15, but if we ask on what day the population was 15, there are two possible answers, 172.44 and 260.44. If we try to use `interp1`, we get the wrong answer:

```
>> interp1(Y, T, 15)

ans = 196.3833                    % WRONG
```

On Day 196, the population is actually 16.8, so `interp1` isn't even close! The problem is that `T` as a function of `Y` is a **multivalued mapping**; for some values in the range there are more than one values in the domain. This causes `interp1` to fail. I can't find any documentation for this limitation, so that's pretty bad.

12.7 Field mice

As we've seen, one use of interpolation is to interpret the results of a numerical computation; another is to fill in the gaps between discrete measurements.

For example*, suppose that the population of field mice is governed by this rate equation:

$$g : t, y \to ay - b(t)y^{1.7}$$

where t is time in months, y is population, a is a parameter that characterizes population growth in the absence of limitations, and b is a function of time that characterizes the effect of the food supply on the death rate.

Although b appears in the equation as a continuous function, we might not know $b(t)$ for all t. Instead, we might only have discrete measurements:

```
t          b(t)
-          ----
0          0.0070
1          0.0036
2          0.0011
3          0.0001
4          0.0004
5          0.0013
6          0.0028
7          0.0043
8          0.0056
```

If we use `ode45` to solve the differential equation, then we don't get to choose the values of t where the rate function (and therefore b) gets evaluated. We need to provide a function that can evaluate b everywhere:

```
function res = interpolate_b(t)
    T = 0:8;
    B = [70 36 11 1 4 13 28 43 56] * 1e-4;
    res = interp1(T, B, t);
end
```

Abstractly, this function uses a discrete map to implement a continuous map.

*This example is adapted from Gerald and Wheatley, *Applied Numerical Analysis*, Fourth Edition, Addison-Wesley, 1989.

Exercise 12.5 *Write a rate function that uses* `interpolate_b` *to evaluate g and then use* `ode45` *to compute the population of field mice from $t = 0$ to $t = 8$ with an initial population of 100 and $a = 0.9$.*

Then modify `interpolate_b` *to use spline interpolation and run* `ode45` *again to see how much effect the interpolation has on the results.*

12.8 Glossary

interpolation: Estimating the value of a function using known values on either side.

extrapolation: Estimating the value of a function using known values that don't bracket the desired value.

single-valued mapping: A mapping where each value in the range maps to a single value in the domain.

multivalued mapping: A mapping where at least one value in the range maps to more than one value in the domain.

12.9 Exercises

Exercise 12.6 *A golf ball*[†] *hit with backspin generates lift, which might increase the range, but the energy that goes into generating spin probably comes at the cost of lower initial velocity. Write a simulation of the flight of a golf ball and use it to find the launch angle and allocation of spin and initial velocity (for a fixed energy budget) that maximizes the horizontal range of the ball in the air.*

The lift of a spinning ball is due to the Magnus force[‡]*, which is perpendicular to the axis of spin and the path of flight. The coefficient of lift is proportional to the spin rate; for a ball spinning at 3000 rpm it is about 0.1. The coefficient of drag of a golf ball is about 0.2 as long as the ball is moving faster than 20 m/s.*

[†] See `http://en.wikipedia.org/wiki/Golf_ball`.
[‡] See `http://en.wikipedia.org/wiki/Magnus_effect`.