

# First examples of unconstrained optimization problems

Mark S. Gockenbach

## 1 An example in one variable

Here is an example of a common problem that one encounters in science. The mass of a radioactive material is known to obey the law

$$m = m_0 e^{-rt},$$

where  $m$  is the mass at time  $t$ ,  $t$  is the time in seconds, and  $r$  is the decay constant. If the decay constant  $r$  for a certain material is unknown, it can be determined by measuring the mass of a sample at various times. Assuming for simplicity that the initial mass (that is, the mass at  $t = 0$ ) is  $m_0 = 1$  gram, it suffices in principle to measure the mass at a single time  $t > 0$ . However, because of inevitable errors in measuring both  $m$  and  $t$ , it would be more usual to collect a number of data points  $(t_1, m_1), (t_2, m_2), \dots, (t_N, m_N)$ .

Since the data points are corrupted by data error, it is quite unlikely that any  $r$  would satisfy

$$e^{-rt_i} = m_i$$

exactly for all  $i = 1, 2, \dots, N$ . Instead, it makes sense to find the “best” value of  $r$ , best in the sense that the errors  $e^{-rt_i} - m_i$  are as small as possible. To define precisely what is meant by the optimal value of  $r$ , the total error must be defined, and it is common to use the *mean-square error*

$$E(r) = \frac{1}{2} \sum_{i=1}^N (e^{-rt_i} - m_i)^2. \quad (1)$$

It might seem more natural to use the following measure of error:

$$\sum_{i=1}^N |e^{-rt_i} - m_i|. \quad (2)$$

However, (1) is preferred over (2) for at least two reasons. First of all, the function  $E(r)$  defined by (1) is a smooth function of  $r$ , while the analogous function defined by (2) is not. Algorithms for optimizing smooth functions are much more effective (efficient and robust) than algorithms for optimizing nonsmooth functions. Second, there is a statistical justification for preferring (1), which, however, I will not describe here.

I can now define the desired optimization problem: Given the data  $(t_1, m_1), (t_2, m_2), \dots, (t_N, m_N)$ , find  $r$  to minimize the function  $E$  defined by (1). This problem can be abbreviated as

$$\min_{r \in \mathbb{R}} E(r),$$

and it is referred to as an *unconstrained minimization problem*. (The problem is called unconstrained because there are no constraints on  $r$ —any value of  $r$  is a potential solution.) The function  $E$  is referred to as the *objective function* since optimizing  $E$  is the objective or goal of the problem.

To give a specific example, I use the 10 data points in Table 1 to define  $E$ . Of course, evaluating  $E$  is simple, and in these days of computers and computer graphics, an obvious strategy for minimizing  $E$  is simple to evaluate  $E(r)$  for a large number of values of  $r$  and plot the results. The graph will then show (approximately) the optimal value of  $r$ . Following this approach, I graphed  $E$  using 20 values of  $r$ . The result is shown in Figure 1.

$t_i$	1	2	3	4	5	6	7	8	9	10
$m_i$	0.7927	0.6420	0.4995	0.4139	0.3046	0.2651	0.2192	0.1904	0.1463	0.1190

Table 1: The data for the first example.

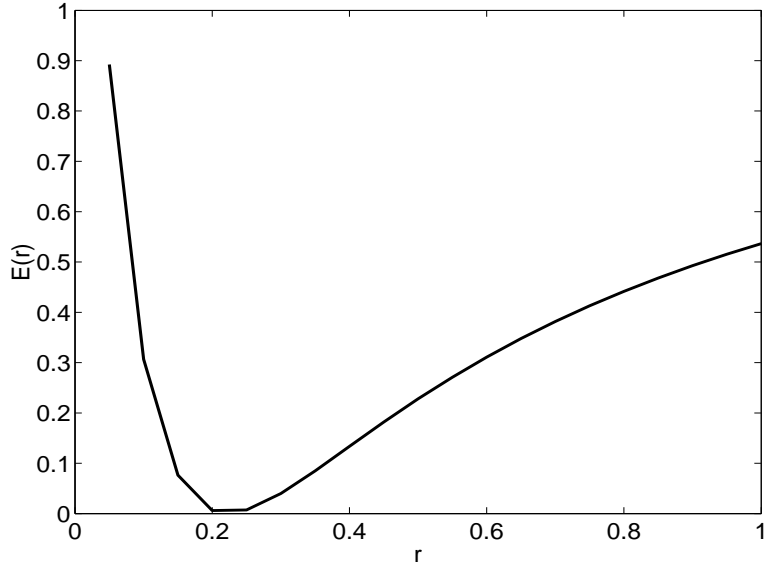


Figure 1: A graph of the function  $E$ .

Figure 1 shows that the optimal value of  $r$  is between 0.2 and 0.25. To get a more accurate value of  $r$ , I could sample  $E(r)$  for more values of  $r$  in the interval  $[0.2, 0.25]$  and eventually arrive at an accurate estimate of the minimizer, which is  $r \doteq 0.22194$ . The resulting exponential curve is plotted together with the data in Figure 2.

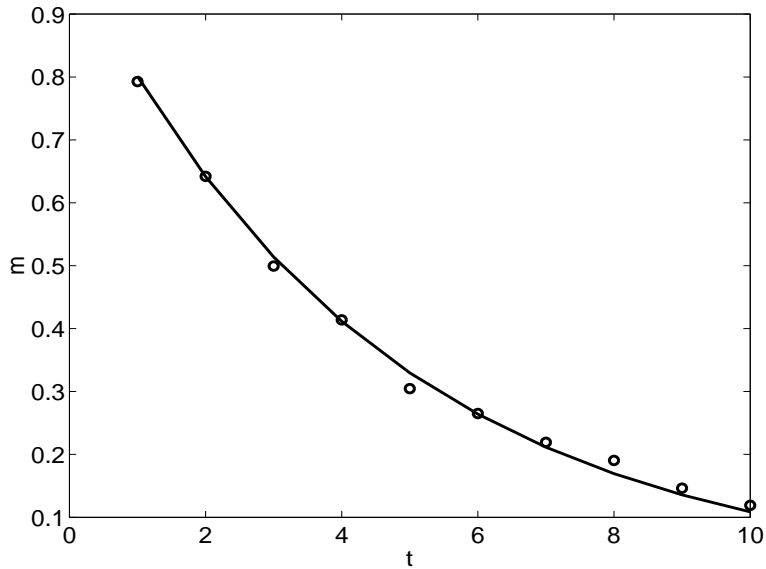


Figure 2: A graph of the function  $E$ .

## 2 An example with more variables

In the previous example, I found a crude estimate of the minimizer by sampling the objective function at 20 points. The graph of  $E$  was not really necessary; I could have just looked at the 20 values of  $E(r)$  and chosen the smallest to get an estimate of the minimum. The purpose of this next example is to show that the above method is impractical even for problems with just a few independent variables.

This example is similar to the last; I consider an experiment involving two variables  $t$  and  $m$  that are known (for theoretical reasons) to be related by

$$m = c_1 e^{-(t-c_2)^2/c_3^2} + c_4 e^{-(t-c_5)^2/c_6^2}.$$

If the parameters  $c_1, c_2, \dots, c_6$  are unknown, then it would be reasonable to collect data points  $(t_1, m_1), (t_2, m_2), \dots, (t_N, m_N)$ , as before (see Figure 3), and find the optimal values of  $c_1, c_2, \dots, c_6$  by minimizing

$$E(c_1, c_2, \dots, c_6) = \frac{1}{2} \sum_{i=1}^N \left( c_1 e^{-(t_i - c_2)^2/c_3^2} + c_4 e^{-(t_i - c_5)^2/c_6^2} - m_i \right)^2.$$

However, there are now six unknown variables. To determine an estimate of the optimal value as I did before, I should consider (say) 20 values of each independent variable. But then I would have to evaluate  $E(c_1, c_2, \dots, c_6)$   $20^6$ , or 64 million, times! Even this would give only a crude estimate of the best values of the parameters.

Of course, if the reader is not impressed by the number  $20^6$ , he or she need only imagine that the functional relationship between  $t$  and  $m$  depends on 10 or 20 or 50 parameters instead, in which case it might be necessary to evaluate  $E$   $20^{10}$  or  $20^{20}$  or  $20^{50}$  times!

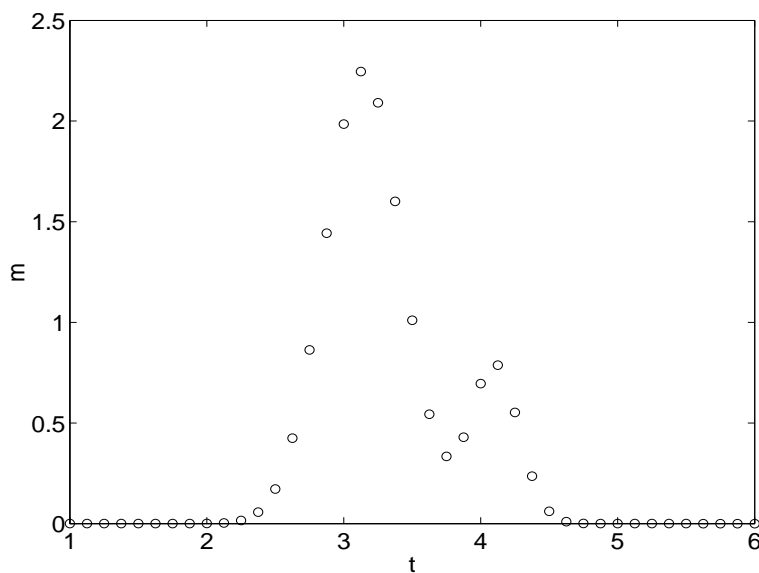


Figure 3: Possible data points for the second example.

The difficulty illustrated by this example is sometimes referred to as the *curse of dimensionality*. Any method for optimization that is based on sampling the objective function on a grid will quickly become impractical as the number of independent variables increases. It is necessary to look for more sophisticated techniques, which form the subject of numerical optimization.