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Optimization of function of two variables, a numerical approach

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Abstract: Teaching development in maximum value of a function of two variables is reported in this paper. Based on an experience in teaching numerical method, difficulty in determining step size of steepest ascent gives an idea to convert the function into one variable, so that we can solve numerically by standard method for that function, such as Newton method. Here, we present some examples to support that development.

Keywords: maximum value, function of two variables, steepest ascent, Newton's method

Introduction

Many problems in the technical and also social fields are solved qualitatively using mathematics as a tool. The problem formulation often comes to complicated equations or functions. Numerical approach is as the alternative in solving the problem. Wiryanto gave an example how to calculate the length of roll of rope by a line integral [1]. A simple model that can be introduced to students. Optimization is another problem that is often seen, such as to determine the extreme value of a function. For a simple function, analytical work can be done by theory of function derivative. A teaching development is presented in this paper especially for an un-simple function. Numerical approach is the alternative, but sometime the procedure is also un-simple.

Based on our teaching experiences, determining the extreme value of function is commonly introduced in first year university students. This topic is taught analytically, as application of derivative, see for example Varberg, et. al. [2]. For function of one variable, first or second derivative test is used to obtain the extreme value, depending on the type of the critical values of the function, which test is appropriate. In numerical approach, we know some methods such as golden section search, quadratic interpolation and Newton's methods, see Mathews [3], also [4, 5]. Each method has different formulation. We will review later in the next

section for Newton method, as it will be involved in our subject development.

On the other hand, for function of two variables, the critical values are determined by gradient, and then they should be checked by second partial derivative test, whether the critical value gives maximum, minimum or as saddle point of the function. For numerical approach, steepest ascent method is used to determine the maximum value of the function. This method is widely used in optimization. Denel, et. al reported the application in linear programming [6]. Meanwhile, Bazarraa, et. al. [7] worked on that method numerically for concave functions. In its formulation, we need to determine the direction and step size where each point would go, starting from the given initial value. Our observation indicates that for quadratic function, the step size can be formulated into an explicit form of step size, so that for the next iteration, we can use the same form. Meanwhile, for more complicated function, for example

$$f(x, y) = xe^{-(x^2 - xy + y^2)}$$

The step size for each iteration should be reformulated, this is not simple numerically.

Instead of the steepest ascent method, we propose to solve the problem by numerical method used in function of one variable. Modification is needed to the function before applying the numerical procedure. This is presented in this paper. We found that it is much help students in solving the problem and in understanding the numerical process.



Numerical Method

In this section we give a review of a numerical method in determining the extreme value of a function. Newton's method is a popular and widely used one for a function of one variable. We start by a function

$$y = f(x)$$

that is differentiable in an open interval, namely $x \in D$, and has a critical value x_0 giving maximum or minimum value of the function. This situation is mathematically presented by determining x_0 so that it satisfies $f'(x_0) = 0$.

Meanwhile, Newton method in solving an equation $g(x) = 0$ is expressed by iteration procedure in form

$$x^{(k+1)} = x^{(k)} - \frac{g(x^{(k)})}{g'(x^{(k)})} \quad (1)$$

where $x(k)$ is the iteration value at level k . Note that Newton's method requires initial value $x^{(0)}$ to get the next iteration calculation. A certain condition should be satisfied so that the iteration is convergent $x(k) \rightarrow x_0$, where x_0 is the root of the equation, satisfying $g(x_0) = 0$, see some references [8, 9].

Now, in determining the extreme value of $y = f(x)$ we can apply Newton's method (1) by formulating the iteration

$$x^{(k+1)} = x^{(k)} - \frac{f'(x^{(k)})}{f''(x^{(k)})} \quad (2)$$

Here we need second derivative of f instead of function g in (1).

As an example, we apply Newton's method above to get the maximum value of function

$$f(x) = x^2 - 81x^4 \quad (3)$$

using initial value $x^{(0)} = 0.1$. This is chosen as the plot of the function indicates that the function has maximum value in $x \in (0.05, 0.1)$. The iteration following (2) is given in Table 1. We found that the iteration reaches the convergence at $k = 4$, with $|x^{(4)} - x^{(3)}| < 10^{-5}$. $x^{(4)} = 0.07856742$ is the value giving maximum for $f(x)$.

Analytically, the result above is correct. There are three critical values $x = -\frac{1}{18}\sqrt{2}, 0, \frac{1}{18}\sqrt{2}$ from $f'(x) = 0$.

The third value $x = \frac{1}{18}\sqrt{2} \approx 0.07856742$ gives $f''(x) < 0$. It means $f(\frac{1}{18}\sqrt{2})$ is the maximum (second derivative test).

Table 1. Iteration of Newton's method for $f(x) = x^2 - 81x^4$

k	$x^{(k)}$	$f'(x^{(k)})$	$f''(x^{(k)})$
1	0.083937824	-0.023734333	-4.848282638
2	0.079042414	-0.001917238	-4.072767446
3	0.078571668	-1.69917E-05	-4.000648771
4	0.07856742	-1.37764E-09	-4.000000053

Now, we move to a function of two variables. Suppose we intend to determine the maximum value of

$$z = f(x, y).$$

A numerical method that can be used is steepest ascent. The method is iterative, constructed by determining the step size and direction from the previous position so that the next point tends to the maximum one. From the point $(x^{(k)}, y^{(k)})$ the direction is θ obtained from the gradient at that point, i.e.

$$\tan \theta = \frac{\frac{\partial f}{\partial y}(x^{(k)}, y^{(k)})}{\frac{\partial f}{\partial x}(x^{(k)}, y^{(k)})}$$

and the step size is namely h satisfying $g'(h) = 0$, where

$$g(h) = f\left(x^{(k)} + h \frac{\partial f}{\partial x}(x^{(k)}, y^{(k)}), y^{(k)} + h \frac{\partial f}{\partial y}(x^{(k)}, y^{(k)})\right)$$

Therefore, the position of the next point is

$$x^{(k+1)} = x^{(k)} + h \frac{\partial f}{\partial x}(x^{(k)}, y^{(k)}),$$

$$y^{(k+1)} = y^{(k)} + h \frac{\partial f}{\partial y}(x^{(k)}, y^{(k)})$$

This iteration is repeated until

$$|(x^{(k)}, y^{(k)}) - (x^{(k+1)}, y^{(k+1)})| < \epsilon,$$

where ϵ is a small number as the numerical tolerance.

The difficulty of the steepest ascent method is in determining step size h . For a simple function f , it would give a fix formula so that the numerical procedure can be written easily. However, each iteration in general should be derived the formula for h . This can be seen in the example as follows.

We work for

$$f(x, y) = xy - 2x^2 - y^4 \quad (4)$$

Steepest ascent method would be applied to that function using initial condition $(x^{(0)}, y^{(0)}) = (0.1, 0.5)$. The gradient of the function is

$$\nabla f = (y - 4x, x - 4y^3).$$

By substituting $x^{(0)}$ and $y^{(0)}$, we construct g as

$$g(h) = f(0.1 + 0.1h, 0.5 - 0.4h)$$

Giving

$$g(h) = -0.0325 + 0.17h - 0.3h^2 + 0.128h^3 - 0.0256h^4$$

and $g'(h) = 0$ for $h = 0.35722$, so that we obtain

$$x^{(1)} = 0.135722, y^{(1)} = 0.357112$$

That procedure is then repeated, obtain a different polynomial $g(h)$ and the next step size is $h = 0.18133$. We can continue the iteration, but it is not simple to write the numerical procedure as the function g changes every time iteration, and there are three roots of $g'(h) = 0$, luckily two are complex.

Based on that example for steepest ascent, we then develop the numerical method for function of two variables by converting into function of one variable and solve by Newton's method. We describe the procedure in the next section.

Optimization of Function of Two Variables

In this section, we determine the maximum value of a function of two variables through one variable. It is solved numerically by Newton's method. To do so, we consider the previous function (3) in the small domain $(x, y) \in (0.01, 0.07) \times (0.1, 0.3)$.

Geometrically, (4) is a surface. It is then cut with a plane $y = 3x$ so that we obtain a curve satisfying (3)

$$f(x, y = 3x) = x^2 - 81x^4$$

We have solved it by Newton's method to obtain the maximum value at $x = 0.07857$ which corresponds to $y = 0.23570$ and giving the maximum value $f(0.07857,$

$0.23570) = 0.00309$. This process is then generalized, the surface is cut by general plane $y = ax$ for various values of a . Newton's method is then used to determine x that correspond to the maximum value of f for each a . We then collect them for determining the extreme of the function of two variables.

Table 2. Result of Newton's method in determining the maximum of $g(x) = (a - 2)x^2 - a^4x^4$ for various parameter a

a	x	y	$g(x)$
2.5	0.08	0.2	0.0016
3	0.078567	0.235701	0.00308642
3.5	0.070696	0.247436	0.003748438
3.6	0.069014	0.24845	0.003810395
3.7	0.067345	0.249177	0.003855058
3.8	0.065698	0.249652	0.003884639
3.9	0.064081	0.249916	0.003901115
3.95	0.063286	0.24998	0.003904998
3.97	0.06297	0.249991	0.003905804
3.98	0.062813	0.249996	0.003906053
3.99	0.062656	0.249997	0.003906201
4	0.0625	0.25	0.00390625
4.01	0.062344	0.249999	0.003906201
4.02	0.062188	0.249996	0.003906057
4.03	0.062033	0.249993	0.003905817
4.04	0.061878	0.249987	0.003905484
4.05	0.061724	0.249982	0.003905059
4.1	0.060957	0.249924	0.003901604
4.2	0.059456	0.249715	0.003888555

Now, our problem is to determine the position x that gives maximum of $f(x, y = ax)$ for various values a . This can be solved by Newton's method. To simplify we denote the function of one variable

$$g(x) := f(x, y = ax) = (a - 2)x^2 - a^4x^4$$

The maximum of g can be obtained for $a > 2$.

As the result, our numerical calculation is presented in **Table 2**. Newton's method is applied by using initial value $x^{(0)} = 0.07$, and it gives the convergence value at 5th iteration using tolerance error less than 10^{-7} . We found that the maximum value for (4) at $a = 4.0$. This gives $x = 0.0625$, so that we can calculate $y = 0.25$, those correspond to $f = 0.00390625$ as the maximum value. Near $a = 4.0$ the calculation requires extra decimal for a to get accurate result, as shown in **Table 2**.

The optimization of function (4) was chosen as it can be compared the result analytically using Hessian determinant. Both results confirm. For another example, the numerical approach as presented above can be applied, for a function such as written in Introduction,

$$f(x, y) = xe^{-(x^2 - xy + y^2)}. \quad (5)$$

Steepest ascent method for that function needs more effort in design numerical procedure, but converting into one variable and using Newton's method can help in solving it. Otherwise, the above approach can be used as alternative in solving optimization in function of two variables.

Plot of (5) is shown in Figure 1a, given in $(x, y) \in (0, 2) \times (-1, 2)$ containing maximum of f . We can determine the position of the maximum value by converting (5) into function of one variable.

$$g(x) := f(x, y = ax)$$

instead of applying steepest ascent method. For some values of a we plot the curve as the intersection between the surface (5) and the plane $y = ax$. We present in Figure 1b the curve plotted using $a = 6, 2, 1$ and 0.5 from small to large curve, as indicated. In converting the function, we can also use other planes, such as $y = ax + 2$. But, it produces more difficult one-variable function.

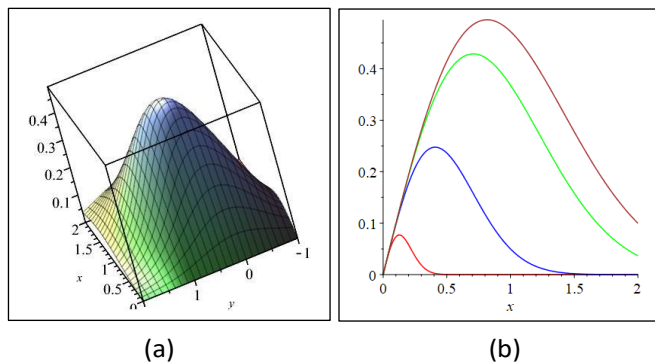


Figure 1. (a) 3D-plot of (5), (b) Curves of $g(x) = f(x, y = ax)$ for some different values of a as indicated

Now, our task is to determine the position x that gives maximum value of the curve for various a . Newton's method is used, and then we collect some calculation results similar to Table 2 to decide the maximum of f . Most of our calculations use initial value $x = 0.5$, and the method converges upto 7 decimal accuracy no more than 5 iterations. The result is shown in Table 3. We found that the maximum of f is achieved at $x = 0.81649658$ along the curve related to $a = 0.5$, accurate upto 2 decimal, and give the maximum value of f accurate upto 4 decimal. This can be increased the accuracy of f by increasing the decimal of a in the calculation.

Table 3. Result of Newton's method in determining the maximum of $g(x) = xe^{-(1-a+a^2)x^2}$ for various parameter a

a	x	$y = ax$	$f(x, y)$
2	0.40824829	0.81649658	0.247615105
1	0.70710678	0.70710678	0.428881942
0.7	0.79555728	0.556890096	0.482529884
0.6	0.81110711	0.486664266	0.491961328
0.55	0.81513915	0.448326533	0.494406884
0.54	0.81562704	0.440438602	0.494702808
0.53	0.81600712	0.432483774	0.494933339
0.52	0.81627894	0.424465049	0.495098201
0.51	0.81644215	0.416385497	0.495197198
0.5	0.81649658	0.40824829	0.49523021
0.49	0.81644215	0.400056654	0.495197198
0.48	0.81627894	0.391813891	0.495098201
0.45	0.81513915	0.366812618	0.494406884
0.4	0.81110711	0.324442844	0.491961328
0.3	0.79555728	0.238667184	0.482529884

Conclusions

We have presented a numerical approach in optimization of function of two variables. Instead of using steepest ascent, converting the function into one variable and using Newton's method can be used as an alternative solution. An example has been demonstrated and agreed with analytical work

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