THE GRADIENT AND EXTREME VALUES

DAVID BEN MCREYNOLDS

1. In One Variable

Let f be a function of one variable x with continuous first and second derivative. The following question motivates these notes.

Question 1. For what points does f have an extreme value?

A fundamental result of classical mathematics is the following.

Theorem 1.1. *If $f(x_0)$ is an extreme value, then*

$$f'(x_0) = 0.$$

Remark. In these notes, we do not concern ourselves with the scenario of f having a discontinuous derivative. In this case, an extreme value might occur at a discontinuity of the derivative.

This leads us to the following definition, where, again, we omit the case when the derivative could have a discontinuity.

Definition 1 (Critical Point)**.** We say that x_0 is a **critical point** if $f'(x_0) = 0$.

From Theorem 1.1, we see that the set of critical points contains the set of points whose image is an extreme value. This leads us to further analyze the critical points of a function. The result of such analysis is the following, which is called often called the **Second Derivative Test**.

Theorem 1.2 (Second Derivative Test)**.** *Let f be as above, and x_0 a critical point. Then*

(a) *If $f''(x_0) < 0$, then $f(x_0)$ is a local maximum.*
(b) *If $f''(x_0) > 0$, then $f(x_0)$ is a local minimum.*
(c) *If $f''(x_0) = 0$, then the test fails.*

We come back to Theorem 1.2 later to compare this with the higher dimensional case.

We give three examples to show that anything can happen in the case of (c).

Date: April 23, 2002.

Example 1.1.

Let $f(x) = x^3$. Then we see that

$$f'(0) = 0$$
$$f''(0) = 0.$$

By analyzing the graph of $f(x)$, we see that at $x = 0$, $f(0)$ is neither a local maximum or minimum.

Example 1.2.

Let $f(x) = x^4$. Then we see that

$$f'(0) = 0$$
$$f''(0) = 0.$$

Again, by analyzing the graph of $f(x)$, we see that at $x = 0$, $f(0)$ is a local minimum (in fact, it is a global minimum).

Example 1.3.

Let $f(x) = -x^4$. Then we see that

$$f'(0) = 0$$
$$f''(0) = 0.$$

Again, by analyzing the graph of $f(x)$, we see that at $x = 0$, $f(0)$ is a local maximum (in fact, it is a global maximum).

Since we are familiar with Taylor series, let us consider the following. We know that

$$P_1(x) = f(x_0) + f'(x_0)(x - x_0)$$

is the best first order or linear approximation of f at the point x_0. If $f'(x_0) = 0$, then this says that

$$P_1(x) = f(x_0).$$

Now, consider the best second order or quadratic approximation of f near x_0 given by (remember $f'(x_0) = 0$),

$$P_2(x) = f(x_0) + \frac{f''(x_0)}{2}(x - x_0)^2.$$

If $f''(x_0) \neq 0$, then we see that if $f''(x_0) < 0$, then $P_2(x)$ is a parabola pointing down. In this case, we see that $P_2(x)$ has a local maximum at x_0. If $f''(x_0) > 0$, then we see that $P_2(x)$ is a parabola pointing up. In this case, we see that $P_2(x)$ has a local minimum at x_0. From this, we see that Theorem 1.2 says that to decide whether or not f has a local maximum or local minimum at the point x_0, we only have to study the best second order approximation. Observe that when $f''(x_0) = 0$, the best second order approximation is

$$P_2(x) = f(x_0).$$

This has both a local minimum and local maximum at x_0. So we can see why the test fails in this case.

2. In Two Variables

As we have seen, the scene changes dramatically when we have two variables (or so it seems). First, the true analog of the derivative, the gradient, is now vector valued. Before we begin to ponder the extreme value question in this setting, we discuss the gradient.

Let $f(x, y)$ be a continuous function in two variables x and y, and taking values in the real numbers. Further, assume that $f(x, y)$ has continuous first and second order partial derivatives.

Definition 2 (Gradient)**.** We define the **gradient** of f to be the function

$$\nabla f(x, y) = (f_x, f_y).$$

That is,

$$\nabla f(x, y) = \frac{\partial f}{\partial x}\mathbf{i} + \frac{\partial f}{\partial y}\mathbf{j}.$$

Now, we would like to relate the gradient to the idea of the derivative in the case of just one dimension. To do this, observe that the equation

$$f(x) = y$$

is identical to

$$f(x) - y = 0.$$

This is a trivial observation granted, but we make the following use of it.

Let

$$F(x, y) = f(x) - y.$$

Now, the gradient of F is given by

$$\nabla F(x, y) = (f'(x), -1).$$

Next, recall that $f'(x)$, geometrically, gives the slope of the tangent line at $(x, f(x))$. Now, we know that lines are defined by a vector and a direction. So how do we turn the slope into a vector? Well, we know that the point $(x, f(x))$ in on the tangent line. From elementary algebra, we then know that $(x + 1, f(x) + f'(x))$ is also on the tangent line. Now that we have two points on the line, we can form the vector which starts at $(x, f(x))$ and ends at $(x + 1, f(x) + f'(x))$. This vector is given by

$$\begin{aligned}\mathbf{d} &= (x + 1, f(x) + f'(x)) - (x, f(x)) \\ &= (1, f'(x)).\end{aligned}$$

Lastly, observe that

$$\begin{aligned}\mathbf{d} \cdot \nabla F(x,y) &= (1, f'(x)) \cdot (f'(x), -1) \\ &= f'(x) - f'(x) \\ &= 0.\end{aligned}$$

Going back to our example, we see that gradient direction is orthogonal or normal to the tangent direction.

Lastly, recall that in 3 dimensions, we can describe a plane by the direction that is normal to the plane. We can do the same for a line in 2 dimensions.

If (x_0, y_0) is a fixed point on a line in $\mathbb{R}^2$, and $\mathbf{n} = (a,b)$, is the normal direction to the line, then we know that if (x,y) is a point on the line, then

$$\mathbf{n} \cdot (x - x,y - y_0) = 0. \tag{1}$$

That is, the vector that starts at (x_0, y_0) and ends at (x,y), which sits inside the line, must be normal to the vector $\mathbf{n}$. This is because $\mathbf{n}$ is the normal direction of the line. Expanding Equation (1) out, we get (if we assume that $b \neq 0$,

$$\begin{aligned}\mathbf{n} \cdot (x - x_0, y - y_0) &= 0 \\ (a,b) \cdot (x - x_0, y - y_0) &= 0 \\ a(x - x_0) + b(y - y_0) &= 0 \\ ax - ax_0 - by_0 + by &= 0 \\ ax - (ax_0 - by_0) &= -by \\ -\frac{a}{b}x + c &= y.\end{aligned}$$

Therefore, the slope of the line is given by

$$m = -\frac{a}{b}.$$

If we start at the origin, then the slope can be viewed as the vector

$$(b, -a).$$

Then, we see that

$$(b, -a) = \det \begin{pmatrix} \mathbf{i} & \mathbf{j} \\ a & b \end{pmatrix}.$$

From this, we see how the gradient generalizes the idea of a derivative.

3. The Gradient Revealed

If you have not had or are not currently taking Linear Algebra, then you might want to skip to the next section and read this later.

Now, working with the gradient of a function $f(x, y)$, we see that given a vector $\mathbf{v} \in \mathbb{R}^2$, we have

$$\nabla f(x_0, y_0) \cdot \mathbf{v} \in \mathbb{R}.$$

Let us denote this by

$$\nabla f_{(x_0,y_0)}(\mathbf{v}) = \nabla f(x_0, y_0) \cdot \mathbf{v}.$$

Observe that if we have two vectors $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^2$, and a and b be real numbers, then we have

$$\begin{aligned}\nabla f_{(x_0,y_0)}(a\mathbf{v}_1 + b\mathbf{v}_2) &= \nabla f(x_0, y_0) \cdot (a\mathbf{v}_1 + b\mathbf{v}_2)\\ &= a\nabla f(x_0, y_0) \cdot \mathbf{v}_1 + b\nabla f(x_0, y_0)\mathbf{v}_2\\ &= a\nabla f_{(x_0,y_0)}(\mathbf{v_1}) + b\nabla f_{(x_0,y_0)}(\mathbf{v}_2).\end{aligned}$$

So that $\nabla f_{(x_0,y_0)}$ is a linear map from $\mathbb{R}^2$ into $\mathbb{R}$. With not too much work, we can actually show that $\nabla f_{(x_0,y_0)}$ is the best linear approximation of $f(x, y)$ near the point (x_0, y_0). Compare this with the case of just one variable.

4. Approximating $f(x, y)$

The best linear approximation of $f(x)$ near x_0 was given by

$$P_1(x) = f(x_0) + f'(x_0)(x - x_0).$$

In the case of two variables, we might guess that the best linear approximation of $f(x, y)$ near (x_0, y_0) would be given by

$$P_1(x, y) = f(x_0, y_0) + f_x(x_0, y_0)(x - x_0) + f_y(x_0, y_0)(y - y_0). \tag{2}$$

Expanding this out, we see that

$$\begin{aligned}P_1(x, y) &= f(x_0, y_0) + f_x(x_0, y_0)(x - x_0) + f_y(x_0, y_0)(y - y_0)\\ &= f(x_0, y_0) + \nabla f(x_0, y_0) \cdot (x - x_0, y - y_0).\end{aligned}$$

Now, since we will make use of this later, what would the best quadratic or second order approximation look like? Well, we would want it to agree with $f(x, y)$ at the point (x_0, y_0), and agree on all the first and second partial derivatives. So that we would guess

$$\begin{aligned}P_2(x) = f(x_0, y_0) + \nabla f(x_0, y_0) \cdot (x - x_0, y - y_0) + \frac{f_{xx}(x_0, y_0)}{2}(x - x_0)^2\\ + \frac{f_{yy}(x_0, y_0)}{2}(y - y_0)^2 + f_{xy}(x_0, y_0)(x - x_0)(y - y_0).\end{aligned}$$

Let us write the second order piece, with

$$\frac{f_{xx}(x_0,y_0)}{2}(x-x_0)^2 = A(x-x_0)^2$$
$$\frac{f_{yy}(x_0,y_0)}{2}(y-y_0)^2 = C(y-y_0)^2$$
$$f_{xy}(x_0,y_0)(x-x_0)(y-y_0) = B(x-x_0)(y-y_0).$$

If we let $s = x - x_0$ and $t = y - y_0$, then we have for the second order terms,

$$As^2 + Ct^2 + Bst.$$

Recall from analytic geometry that we have the following cases: If $B^2 - 4AC > 0$, then

$$As^2 + Ct^2 + Bst = 0$$

is a hyperbola. If $B^2 - 4AC < 0$, then

$$As^2 + Ct^2 + Bst = 0$$

is an ellipse. If $B^2 - 4AC = 0$, then

$$As^2 + Ct^2 + Bst = 0$$

is a parabola. We will use this to analyze the critical points of a function in two variables.

5. Extreme Values in Two Dimensions

We are now ready to discuss extreme values in two dimensions. Again, let $f(x,y)$ have continuous first and second order partial derivatives. A classical result is the following, which we saw in the case of one variable.

Theorem 5.1. *Let $f(x,y)$ be as above. If $f(x_0,y_0)$ is an extreme value, then*

$$\nabla f(x_0,y_0) = (0,0).$$

That is

$$f_x(x_0,y_0) = 0$$
$$f_y(x_0,y_0) = 0.$$

So again, if we want to find the extreme values of a function $f(x,y)$, it suffices to consider only points where the gradient vanishes. This leads us the the following definition.

Definition 3 (Critical point)**.** We say that (x_0,y_0) is a **critical point** of $f(x,y)$ if

$$\nabla f(x_0,y_0) = 0.$$

Now, we again have the following result, which generalizes the Second Derivative test.

Theorem 5.2. *Let $f(x, y)$ be as above, and assume that (x_0, y_0) is a critical point. Then*

(a) *If*
$$(f_{xy}(x_0, y_0))^2 - f_{xx}(x_0, y_0)f_{yy}(x_0, y_0) < 0,$$
then $f(x_0, y_0)$ is an extreme value.

(b) *If*
$$(f_{xy}(x_0, y_0))^2 - f_{xx}(x_0, y_0)f_{yy}(x_0, y_0) > 0,$$
then $f(x_0, y_0)$ is a saddle point.

(c) *If*
$$(f_{xy}(x_0, y_0))^2 - f_{xx}(x_0, y_0)f_{yy}(x_0, y_0) = 0,$$
then the test fails

Furthermore, if (a) occurs, then we can decide whether or not $f(x_0, y_0)$ is a local maximum or local minimum depending on:

(i) *If $f_{xx} > 0$, then $f(x_0, y_0)$ is a local minimum.*
(ii) *If $f_{xx} < 0$, then $f(x_0, y_0)$ is a local maximum.*

Let us return to the best second order approximation. This was given by

$$P_2(x) = f(x_0, y_0) + \nabla f(x_0, y_0) \cdot (x - x_0, y - y_0) + \frac{f_{xx}(x_0, y_0)}{2}(x - x_0)^2 + \frac{f_{yy}(x_0, y_0)}{2}(y - y_0)^2 + f_{xy}(x_0, y_0)(x - x_0)(y - y_0).$$

Now, recall that if

$$(f_{xy}(x_0, y_0))^2 - 4\frac{f_{xx}(x_0, y_0)f_{yy}(x_0, y_0)}{4} > 0,$$

then

$$\frac{f_{xx}(x_0, y_0)}{2}(x-x_0)^2+\frac{f_{yy}(x_0, y_0)}{2}(y-y_0)^2+f_{xy}(x_0, y_0)(x-x_0)(y-y_0) = 0$$

is a hyperbola. If we graph

$$f(x_0, y_0)+\frac{f_{xx}(x_0, y_0)}{2}(x-x_0)^2+\frac{f_{yy}(x_0, y_0)}{2}(y-y_0)^2+f_{xy}(x_0, y_0)(x-x_0)(y-y_0) = z,$$

we will see that this is a saddle shaped surface. Further, the point (x_0, y_0) on the graph is located at the saddle point. So that $P_2(x_0, y_0)$ has (x_0, y_0) as a saddle point.

If

$$(f_{xy}(x_0, y_0))^2 - 4\frac{f_{xx}(x_0, y_0)f_{yy}(x_0, y_0)}{4} < 0,$$

then
$$\frac{f_{xx}(x_0,y_0)}{2}(x-x_0)^2+\frac{f_{yy}(x_0,y_0)}{2}(y-y_0)^2+f_{xy}(x_0,y_0)(x-x_0)(y-y_0)=0$$
is an ellipse. In this case,
$$\frac{f_{xx}(x_0,y_0)}{2}(x-x_0)^2+\frac{f_{yy}(x_0,y_0)}{2}(y-y_0)^2+f_{xy}(x_0,y_0)(x-x_0)(y-y_0)+f(x_0,y_0)=z$$
is an elliptic paraboloid. Recall, this surface looks like a bowl, and depending on whether it is facing up or down, (x_0, y_0) on the surface is a local minimum or maximum. Whether it faces up or down is completely determined by the sign of $f_{xx}(x_0, y_0)$.

Lastly, if
$$(f_{xy}(x_0,y_0))^2-4\frac{f_{xx}(x_0,y_0)f_{yy}(x_0,y_0)}{4}=0,$$
then
$$\frac{f_{xx}(x_0,y_0)}{2}(x-x_0)^2+\frac{f_{yy}(x_0,y_0)}{2}(y-y_0)^2+f_{xy}(x_0,y_0)(x-x_0)(y-y_0)=0$$
is a parabola. In this case, we see that we do not have enough information to decide whether or not $f(x_0, y_0)$ is a maximum or minimum.

We see that Theorem 5.2 says that to decide whether or not a critical point yields an extreme value, it suffices to studying the best second order approximation or quadratic surface.

6. A Different Spin on Extreme Values

Again, this section requires knowledge of linear algebra. So skip it if you want.

Consider the matrix
$$H_f(x_0,y_0)=\begin{pmatrix} f_{xx}(x_0,y_0) & f_{xy}(x_0,y_0) \\ f_{yx}(x_0,y_0) & f_{yy}(x_0,y_0)\end{pmatrix}.$$
This matrix is called the **Hessian** of f at the point (x_0, y_0). Observe that
$$-\det H_f(x_0,y_0)=(f_{xy}(x_0,y_0))^2-f_{xx}(x_0,y_0)f_{yy}(x_0,y_0),$$
if $f_{xy}(x_0, y_0) = f_{yx}(x_0, y_0)$. We will assume throughout that this is the case. This leads us to ask how $H_f(x_0, y_0)$ is related to deciding the nature of the critical point (x_0, y_0)? Then answer is the following:

Proposition 6.1. *Assume that* $\det H_f(x_0, y_0) \neq 0$. *Let* λ_1, λ_2 *be the eigenvalues of* $H_f(x_0, y_0)$. *Then we have the following*

(a) *If* $\lambda_1, \lambda_2 > 0$, *then* $f(x_0, y_0)$ *is a local minimum.*
(b) *If one of* λ_1 *and* λ_2 *is negative, then* (x_0, y_0) *is a saddle point.*

(c) *If* $\lambda_1, \lambda_2 < 0$*, then* $f(x_0, y_0)$ *is a local maximum.*

Anyone who has solved eigenvalue problems would agree that this does not make the problem better, since eigenvalue problems are generally quite difficult. On the other hand, this idea generalizes to higher dimensions, when the determinant alone is not sufficient in determining the nature of a critical point. Recall that the determinant is the product of the eigenvalues, using this, compare Proposition 6.1 with Theorem 5.2. Also, and you should ask this question, why are the eigenvalues of $H_f(x_0, y_0)$ real?

We close this section with some intuition on the above. The idea of how the eigenvalues of the Hessian determine the local geometry near a critical point is the following. If you have an eigenvalue λ of the Hessian, then if $\lambda < 0$, there is a direction in the xy-plane, where if we take a vertical slice of the surface through this direction, we would get, near the critical point, a parabola pointing down. Geometrically, this says that if you are at the point $(x_0, y_0, f(x_0, y_0))$, you can walk down in some direction. If $\lambda > 0$, then this says that you can walk up in some direction. Clearly, if you can walk up and down on the surface near the point $(x_0, y_0, f(x_0, y_0))$, then this point cannot be an extreme value. On the other hand, if you can only walk up, i.e., all the eigenvalues are positive, then the point is a local minimum. If you can only walk down, i.e. all the eigenvalues are negative, then the point is a local maximum.

University of Texas at Austin, Department of Mathematics
E-mail address: `dmcreyn@math.utexas.edu`