Hessians and Definiteness

Corrections to Dr Ian Rudy (http://people.ds.cam.ac.uk/iar1/contact.html) please.

This document describes how to use the Hessian matrix to discover the nature of a stationary point for a function of several variables. This issue involves deciding whether the Hessian is positive definite, negative definite or indefinite. We will take the case of a function of two variables, but the analysis extends to functions of more than two variables.

One way to study the stationary points of a function of several variables is to look at a Taylor Series for the function around a stationary point. Let's say we are studying a function f(x,y) at a specific point (a,b), which we know to be a stationary point. Then the Taylor Series of f(x,y) around (a,b) is:

$$f\big|_{(a+x,b+y)} \;=\; f\big|_{(a,b)} \;+\; xf_x\big|_{(a,b)} \;+\; yf_y\big|_{(a,b)} \;+\; \tfrac{1}{2}\left(x^2 f_{xx} + 2xyf_{xy} + y^2 f_{yy}\right)\Big|_{(a,b)} + \dots$$

which, slightly rearranged, gives:

$$f\big|_{(a+x,b+y)} \;-\; f\big|_{(a,b)} \;=\; xf_x\big|_{(a,b)} \;+\; yf_y\big|_{(a,b)} \;+\; \tfrac{1}{2}\left(x^2 f_{xx} + 2xyf_{xy} + y^2 f_{yy}\right)\Big|_{(a,b)} + \dots \qquad [1]$$

where the vertical bar just means "evaluated at" and the *x* and *y* suffices in f_x and f_y etc denote the partial derivatives of *f*. The other *x* and *y* quantities in the expression are small movements away from the stationary point.

We can work out the nature of the stationary point by looking at how $f\big|_{(a+x,b+y)} - f\big|_{(a,b)}$ behaves for various values of *x* and *y*. At a minimum, we would expect it to be *positive* for all *x* and *y*, because moving away from the minimum in any direction causes the function *f* to increase. At a maximum, we would expect it to be *negative* for all *x* and *y*. Because at a stationary point, f_x and f_y are both zero, everything depends on the term:

$$\tfrac{1}{2}\left(x^2 f_{xx} + 2xyf_{xy} + y^2 f_{yy}\right)\Big|_{(a,b)}. \qquad [2]$$

or, equivalently:

$$\tfrac{1}{2}\begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} f_{xx} & f_{xy} \\ f_{xy} & f_{yy} \end{pmatrix}\Bigg|_{(a,b)} \begin{pmatrix} x \\ y \end{pmatrix} \qquad [3]$$

This quantity is an example of what is known as a *quadratic form* (in that the highest power of x or y present is two). The matrix in the middle of expression [3] is known as the Hessian. If the quadratic form is positive for *all* values of *x* and *y*, then our stationary point must be a minimum, and we say that the (Hessian) matrix is *positive definite*. If the quadratic form is negative for *all* values of *x* and *y*, then our stationary point must be a maximum, and we say that the matrix is *negative definite*. If the quadratic form is positive for some values of x and y, but negative for others then we have a saddle point[1], and we say that the matrix is *indefinite*.

Our task is equivalent to working out whether the Hessian matrix is positive definite, negative definite, or indefinite. There are two main ways of doing this. One involves eigenvalues, which you will cover in the later Linear Algebra lectures. The other involves principal minors, and we will cover this method here.

For an n x n symmetric matrix, a k^{th} order leading principal minor is the determinant of the matrix obtained by deleting the last (n-k) rows and columns. Hence the 3rd order leading principal minor of:

$$\begin{pmatrix} z_{11} & z_{12} & z_{13} & z_{14} \\ z_{21} & z_{22} & z_{23} & z_{24} \\ z_{31} & z_{32} & z_{33} & z_{34} \\ z_{41} & z_{42} & z_{43} & z_{44} \end{pmatrix}$$

is:

$$\mathrm{D}_3 = \begin{vmatrix} z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \\ z_{31} & z_{32} & z_{33} \end{vmatrix}.$$

And the 2nd order leading principal minor is:

$$\mathrm{D}_2 = \begin{vmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{vmatrix}.$$

And the 1st order leading principal minor is:

$$\mathrm{D}_1 = |z_{11}| \text{ ie } z_{11}.$$

Gong back to the other extreme, the 4th order principal minor is just the determinant of the whole matrix:

$$\mathrm{D}_4 = \begin{vmatrix} z_{11} & z_{12} & z_{13} & z_{14} \\ z_{21} & z_{22} & z_{23} & z_{24} \\ z_{31} & z_{32} & z_{33} & z_{34} \\ z_{41} & z_{42} & z_{43} & z_{44} \end{vmatrix}.$$

[1] In this document, the phrase *saddle point* is used to mean a stationary point that is not a simple maximum or minimum; in some books, it is (entirely reasonably) used to mean one particular type of such stationary points, namely those that look like a horse saddle. We can discuss this further in supervisions.

There are a set of rules for working out whether a *symmetric* matrix is positive definite or negative definite (note the emphasis on the matrix being symmetric - the method will not work in quite this form if it is not symmetric). The rules are:

(a) If and only if all leading principal minors of the matrix are positive, then the matrix is positive definite. For the Hessian, this implies the stationary point is a minimum.
(b) If and only if the k^{th} order leading principal minor of the matrix has sign $(-1)^k$, then the matrix is negative definite. For the Hessian, this implies the stationary point is a maximum.
(c) If none of the leading principal minors is zero, and neither (a) nor (b) holds, then the matrix is indefinite. For the Hessian, this implies the stationary point is a saddle point.

If any of the leading principal minors is zero, then a separate analysis (to investigate whether the matrix could be positive semi-definite or negative semi-definite) is needed. In essence, one has to test all the principal minors, not just the leading principal minors, looking to see if they fit the rules (a)-(c) above, but with the requirement for the minors to be strictly positive or negative replaced by a requirement for the minors to be weakly positive or negative. In other words, minors are allowed to be zero. The implications of the Hessian being semi definite for the nature of the stationary point are not covered here.

Let's take a 2-variable example: find the stationary points of:

$$f = x^3 - 3x^2 + y^3 - 3y^2$$

We find:

$$f_x = 3x^2 - 6x \qquad\qquad f_y = 3y^2 - 6y$$
$$f_{xx} = 6x - 6 \qquad f_{xy} = 0 \qquad f_{yy} = 6y - 6$$

Hence the stationary points are at: $f_x = 3x^2 - 6x = 0$ and $f_y = 3y^2 - 6y = 0$. This gives four stationary points: (0,0), (2,0), (0,2), (2,2). The Hessian is:

$\begin{pmatrix} 6x-6 & 0 \\ 0 & 6y-6 \end{pmatrix}$ and hence at the four points it has the following values:

at (0,0): $\begin{pmatrix} -6 & 0 \\ 0 & -6 \end{pmatrix}$, which is negative definite ($D_1 = -6$, $D_2 = 36$), so a maximum;
at (2,0): $\begin{pmatrix} 6 & 0 \\ 0 & -6 \end{pmatrix}$, which is indefinite ($D_1 = 6$, $D_2 = -36$), so a saddle point;
at (0,2): $\begin{pmatrix} -6 & 0 \\ 0 & 6 \end{pmatrix}$, which is indefinite ($D_1 = -6$, $D_2 = -36$), so a saddle point;

at (2,2): $\begin{pmatrix} 6 & 0 \\ 0 & 6 \end{pmatrix}$, which is positive definite ($D_1 = 6$, $D_2 = 36$), so a minimum.

The Hessian can also be used to test for concavity and convexity. When testing for concavity, the analysis we need is effectively identical to that above for testing for a maximum. The only difference is that f_x and f_y are now not necessarily zero. Hence if the Hessian is is negative definite (ie the quadratic form [3] is everywhere negative), we must have a strictly concave function. Similarly, if the Hessian is positive definite, we must have a strictly convex function.