Extrema

Just as in one dimension we define a critical point as $df/dx = 0$ and all extrema are critical points; in higher dimensions a critical point is one where all the partial derivatives are zero. We saw that

$$\nabla_{\mathbf{w}} f = \mathbf{w} \cdot \nabla f \tag{1}$$

and so, given that the rate of change at an extremum must be zero in all directions, all extrema are critical points in higher dimensions too.

Distinguishing between maxima and minima is a small bit more complicated in higher dimesions; it relies on the *Hessian*, the matrix of second-order partial derivatives. Here we will look at two dimensions as an example, though the idea is similar for other numbers of dimensions. In two dimensions the Hessian is

$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix} \tag{2}$$

or, using the obvious notation

$$H = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix} \tag{3}$$

Also, note that for all but very weird functions $f_{xy} = f_{yx}$.

Now imagine the Hessian at a critical point looks like

$$H = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4}$$

then it would seem that we have a maximum since the x and y derivatives are falling at this point, just like the one-dimensional case. More generally though there are non-zero f_{xy} so what is important is not the diagonal elements but the eigenvalues. If both eigenvalues of the Hessian are negative at a critical point, then it's a maximum, if both are positive it is a minimum. There is another case, where one is positive and one is negative, that implies the critical point is a minumum in one direction and a maximum in another; that can happen in two dimensions and corresponds to a *saddlepoint*, like the point where two hills join and so the land goes up in one set of directions but down in another. Of course, there is always the possibility of a zero eigenvalue, this is like the one-dimensional case where the second derivative is zero, we could still have an extremum, but a very flat one, or it might not be an extremum at all.

This all seems to imply you need the eigenvalues of the Hessian to classify two-dimensional critical points and certainly if you have the eigenvalues and you can do the classification, however, you actually only need the signs of the two eigenvalues and you can usually work that out without actually knowing the eigenvalues. If λ_1 and λ_2 are the eigenvalues of a matrix H then

$$\det H = \lambda_1\lambda_2 \tag{5}$$

and

$$\mathrm{trH} = \lambda_1 + \lambda_2 \tag{6}$$

There are known as matrix invariants. It means that if the determinant is negative you have a saddlepoint, if it is positive then the two eigenvalues have the same sign, so if the trace is negative you have a maximum, if it is negative, a minimum. If the determinant is zero then there is a zero eigenvalue and the Hessian alone isn't enough to tell you what is happening.

Lets do an example:

$$f(x, y) = x^3 + x^2y - y^2 - 4y \tag{7}$$

Now $f_x = 3x^2 + 2xy$ and $f_y = x^2 - 2y - 4$. These equations are often a pain, it is hard to come up with good examples were the equations for the critical points are easy to solve. In this example, the first equation looks promising:

$$3x^2 + 2xy = 0 \implies x(3x + 2y) = 0 \tag{8}$$

so the solutions are $x = 0$ or $x = -2y/3$. If $x = 0$ then the second equation gives $y = -2$; if $x = -2y/3$ the second equation is

$$4y^2/9 - 2y - 4 = 0 \implies 2y^2 - 9y - 18 = 0 \tag{9}$$

and this factorizes into $(2y + 3)(y - 6) = 0$ so the solutions are $y = -3/2$ and $y = 6$. Hence the three critical points are $(0, -2)$, $(-4, 6)$ and $(1, -3/2)$. Now lets work out the Hessian:

$$H = \begin{pmatrix} 6x + 2y & 2x \\ 2x & -2 \end{pmatrix} \tag{10}$$

so for the point $(0, -2)$

$$H = \begin{pmatrix} -4 & 0 \\ 0 & -2 \end{pmatrix} \tag{11}$$

and since this is diagonal matrix we can read off the eigenvalues, they are -4 and -2 and so this is a maximum. For $(-4, 6)$ the Hessian is

$$H = \begin{pmatrix} -12 & -8 \\ -8 & -2 \end{pmatrix} \tag{12}$$

and hence the determinant of the Hessian is -40 which is negative and there is a saddle point. For $(1, -3/2)$ the Hessian is

$$H = \begin{pmatrix} 3 & 2 \\ 2 & -2 \end{pmatrix} \tag{13}$$

so the determinant is -10 and this is another saddle point.

For higher dimensions the story is much the same, but now there are more types of saddle point, for example in three dimensions there are saddle points with two up directions and one down and saddle points with one up direction and two down. These will correspond to two negative and one positive eigenvalues, or one negative and two positive eigenvalues for the Hessian.

Summary

In higher dimensions there is a critical point when the gradient is zero. To classify the critical point the Hessian is calculated, in two-dimension this is

$$H = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix} \tag{14}$$

If this has two positive eigenvalues at a critical point then it is a minimum, two negative, a maximum, one of each, a saddle point. If one, or both, of the eigenvalues is zero then it could be any of the three, or it might not be an extremum at all. The sign of the eigenvalues can be figured out from the determinant and trace since the determinant is the product of the eigenvalues and the trace is the sum.