Calculus and Optimization III

We now have a procedure for finding the stationary points of a known function $f(x)$ of one variable! Given an initial guess x_0, we find a sequence of approximations

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}, \quad k = 0, 1, 2, \ldots$$

which hopefully converge to a stationary point of f.

Now let's see if we can extend these ideas to find the stationary points of a function of two variables $f(x, y)$.

1. Create a local approximation of f at given point (x, y):

$$f(x + a_x, y + a_y) \approx f(x, y) + ??$$

2. Could we use this approximation to find the roots of the function $f(x, y)$?
3. Modify your result and develop a procedure for finding a stationary point of $f(x, y)$.
4. Use your iterative procedure to find a stationary point of the function

$$f(x, y) = (e^x - x)(e^y - 2y)$$

with initial guess $(x, y)_0 = (1, 1)$.

(1) $f(x+a_x, y+a_y) \approx f(x,y) + a_x \frac{\partial f}{\partial x}(x,y) + a_y \frac{\partial f}{\partial y}(x,y)$

$= f(x,y) + a^T \nabla f(x,y)$

local linear approximation in 2-variables.

$a = \begin{bmatrix} a_x \\ a_y \end{bmatrix}$ is a direction or step vector.

$\nabla f(x) = \begin{bmatrix} \partial f/\partial x \\ \partial f/\partial y \end{bmatrix}$ is the gradient vector.

(2) Suppose we wish to find locations where $f=0$ starting from point (x,y). We would need to find a step vector a such that

$$0 = f(x+a_x, y+a_y) \approx f(x,y) + a^T \nabla f(x,y).$$

This is one equation in 2 unknowns (a_x and a_y). The solution set is the level line of $f=0$ in the linear approximation.

(3) Take the gradient of the approximation in (1):

$$\nabla f(x+a_x, y+a_y) \approx \nabla f(x,y) + \nabla\left(a^T \nabla f(x,y)\right)$$

$$\cancel{\neq \nabla f(x,y) + \begin{bmatrix} \frac{\partial}{\partial x} a^T \nabla f(x,y) \\ \frac{\partial}{\partial y} a^T \nabla f(x,y) \end{bmatrix}}$$

$$= \nabla f(x,y) + \nabla\left[a_x \frac{\partial f}{\partial x}(x,y) + a_y \frac{\partial f}{\partial y}(x,y)\right]$$

$$= \nabla f(x,y) + \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} \begin{bmatrix} a_x \\ a_y \end{bmatrix}$$

$$= \nabla f(x,y) + \nabla^2 f(x,y)\, a$$

So, to move a step a so that $\nabla f(x+a_x, y+a_y) = 0$:

$$a = -(\nabla^2 f)^{-1} \nabla f$$

And let $a = x_{k+1} - x_k \Rightarrow \boxed{x_{k+1} = x_k - (\nabla^2 f)^{-1} \nabla f}$

(4) Suppose $f(x,y) = (e^x - x)(e^y - 2y)$.

$$\nabla f = \begin{bmatrix} (e^x-1)(e^y-2y) \\ (e^x-x)(e^y-2) \end{bmatrix}$$

$$\nabla^2 f = \begin{bmatrix} e^x(e^y-2y) & (e^x-1)(e^y-2) \\ (e^x-1)(e^y-2) & (e^x-x)e^y \end{bmatrix}$$

(a) start with $(x_0, y_0) = (1,1)$.

$$\nabla f \approx \begin{bmatrix} 1.2342 \\ 1.2342 \end{bmatrix} \qquad \nabla^2 f \approx \begin{bmatrix} 1.9525 & 1.2342 \\ 1.2342 & 4.6708 \end{bmatrix}$$

$$(x_1, y_1) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 1.9525 & 1.2342 \\ 1.2342 & 4.6708 \end{bmatrix}^{-1} \begin{bmatrix} 1.2342 \\ 1.2342 \end{bmatrix}$$

$$(x_1, y_1) = \begin{bmatrix} 0.44165 \\ 0.88330 \end{bmatrix}$$

(b) continuing ...

$$(x_2, y_2) = \begin{bmatrix} 0.11792 \\ 0.73808 \end{bmatrix} \qquad \nabla f(x_2, y_2) = \begin{bmatrix} 0.36218 \\ 0.46644 \end{bmatrix}$$

$$(x_3, y_3) = \begin{bmatrix} 0.00741 \\ 0.69475 \end{bmatrix} \qquad \nabla f(x_3, y_3) = \begin{bmatrix} 0.07706 \\ 0.09259 \end{bmatrix}$$

$$(x_4, y_4) = \begin{bmatrix} 0.00003 \\ 0.69315 \end{bmatrix} \qquad \nabla f(x_4, y_4) = \begin{bmatrix} 0.00456 \\ 0.00320 \end{bmatrix}$$

Notice that ∇f appears to be converging to $\nabla f = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

We can solve directly for the location of any stationary points. It is reasonably straightforward to show that the only stationary point is at $(x,y) = (0, \ln 2)$ which is very close to our 4^{th} approximation. Evaluation of the Hessian matrix will show that this point is a local minimizer of $f(x,y)$.

How would we terminate our iterative procedure in part (3)?

Two typical tests are to stop if either of the following occur:

(a) $\| x_{k+1} - x_k \| < \varepsilon$

(b) $\| \nabla f(x_k) \| < \delta$

where ε and δ are user-defined values.

The iterative procedure can fail to reach a stationary point.

(i) No stationary point may exist

(ii) sequence of $\{x_k\}$ may not converge

(iii) $\nabla^2 f$ may not be invertible, or nearly so.