COMS10013 - Analysis - WS4

Solutions

1. **Gradient descent:** In this question we're going to study the function

$$E(x, y) = x^2 + y^2$$

   (a) $\nabla E(x, y) = (2x, 2y)$

   (b) We have the initial value $(x, y) = (1, 2)$ and step $\eta = 0.1$.

   - $\mathbf{x}_0 = (1, 2)$ (because it's just the initial value).
   - $\mathbf{x}_1 = (1, 2) = 0.1 \times (2, 4) = (0.8, 1.6)$
   - $\mathbf{x}_2 = (0.64, 1.28)$
   - $\mathbf{x}_3 = (0.512, 1.024$

   and $E(\mathbf{x}_3) = 1.3107...$ (to 4 decimal places). Observe the powers of two that arise!

   (c) Using the same initial value, calculate $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ taking

   (i) $\eta = 0.5$: we get $\mathbf{x}_0 = \mathbf{x}_1 = \mathbf{x}_2 = \mathbf{x}_3 = (0, 0)$. So following the pattern (which one can prove inductively) we get $\mathbf{x}_n = (0, 0)$.

   (ii) $\eta = 1$: we get $\mathbf{x}_0 = \mathbf{x}_2 = (1, 2)$ and $\mathbf{x}_1 = \mathbf{x}_3 = (-1, -2)$ So following the pattern (that again, we could prove inductively, we get $\mathbf{x}_n = (-1)^n(1, 2)$

   The first choice of η is actually (accidentally) a great choice, because (see the next part) it instantly minimises the function. However, it isn't obvious that this is what has happened; for example, we could have hit a local minimum.

   The second choice of η is definitely poor: we're flipping between two values, rather than 'honing in' on the minimal solution.

   (d) Find all minima of E using calculus: First of all, we'll find the critical points of E by looking at ∇E: if $\nabla E = (0, 0)$, then $x = y = 0$. This is the only critical point; now we can argue that $(0, 0)$ is a minimum by using the fact that $x^2 + y^2 \geq 0$, and $E(0, 0) = 0$.

   (e) Pick a new initial starting point (not a minimum value that you found in (d)!), and calculate $E(\mathbf{x}_3)$ using $\eta = 0.1$. Compare this to what you found in (b) – is it a better starting point? Is this what you'd expect given what you found in (d)?
   For example, let's pick the initial starting point $(5, 8)$. A couple of rounds of this gives $E(\mathbf{x}_3) \approx 23$, which is further from the minimum than the results from (c) – this makes it a worse initial starting point. This isn't hugely surprising because this point is further away from the actual minimum than $(1, 2)$, and we're using a very symmetric function with the same value of η. If our function of choice were less regular, then the distance from the actual minimum wouldn't necessarily matter so much.

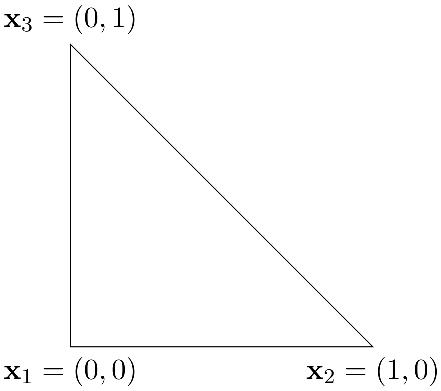
2. **Nelder-Mead Method:** In this question, we're going to study the function

$$E(x, y) = x^2 + y^2 \, .$$

The eagle-eyed amongst you will notice that this is the same function as in question 1. This means that we already know what the minimum should be; the purpose of this question is to use the downhill simplex method to find the minimum.

We'll start with the initial simplex points: $(0, 0), (1, 0), (0, 1)$.

(a) Draw the initial simplex and assign values $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ to the initial simplex points so that $E(\mathbf{x}_1) \leq E(\mathbf{x}_2) \leq E(\mathbf{x}_3)$.



Since $E(\mathbf{x}_2)+E(\mathbf{x}_3)$, it's equally correct to have swapped the assignment of these two values.

(b) The centroid is given by

$$\mathbf{x}_0 = \frac{1}{2}\left(\begin{pmatrix}0\\0\end{pmatrix} + \begin{pmatrix}1\\0\end{pmatrix}\right) = \begin{pmatrix}\frac{1}{2}\\0\end{pmatrix}$$

If you had the other assignment of the $\mathbf{x}_2$ and $\mathbf{x}_3$ variables, then the centroid is instead given by $\begin{pmatrix}0\\\frac{1}{2}\end{pmatrix}$.

The reflection point $\mathbf{x}_r$ is

$$\mathbf{x}_r = \mathbf{x}_0 + (\mathbf{x}_0 - \mathbf{x}_3) = \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\\-1\end{pmatrix}$$

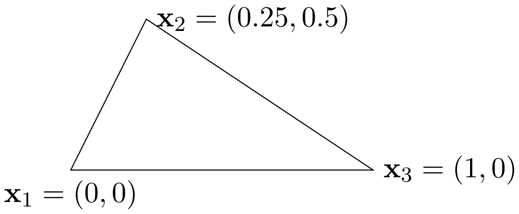
Hence $E(\mathbf{x}_r) = 2$.

(c) Notice that $E(\mathbf{x}_r)$ is a worse outcome in terms of this minimisation outcome (i.e. it gives a bigger output). This is bad! We won't proceed using this new point – instead the algorithm tells us to find a contraction point:

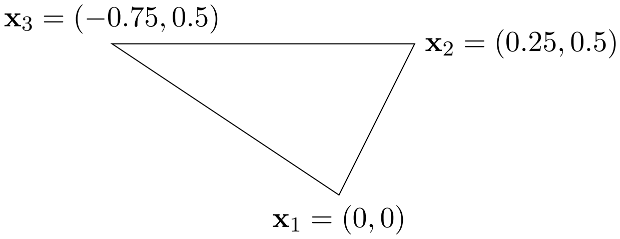
$$\begin{aligned}\mathbf{x}_c &= \mathbf{x}_0 - \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_3) \\ &= \begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} - \frac{1}{2}\left[\begin{pmatrix}\frac{1}{2}\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\right] \\ &= \begin{pmatrix}\frac{1}{4}\\\frac{1}{2}\end{pmatrix} \, .\end{aligned}$$

Now $E(\mathbf{x}_c) = \frac{1}{16} + \frac{1}{4} = \frac{5}{16}$, so our output has (as desired) decreased. This means our new point is $\begin{pmatrix} \frac{1}{4} \\ \frac{1}{2} \end{pmatrix}$.

Let's have a look at our new simplex:



(d) The subsequent centroid is $\begin{pmatrix} 0.125 \\ 0.25 \end{pmatrix}$ and the next $\mathbf{x}_r$ value is $\begin{pmatrix} -0.75 \\ 0.5 \end{pmatrix}$. Thus $E(\mathbf{x}_r) - 0.8125$, which is less than $E(\mathbf{x}_3)$, so we'll swap in $\mathbf{x}_r$:



Let us continue:
the next centroid is still $(0.125, 0.25)$. The next reflection point is

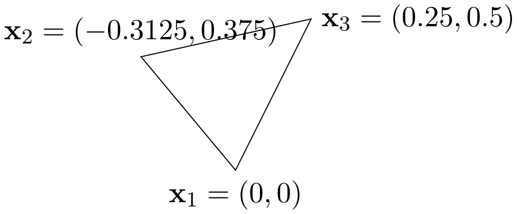
$$(0.25, 0.5) - (-0.75, 0.5) = (1, 0);$$

this is a familiar point and would result in us going in a circle. The algorithm tells us to turn to a contraction point again:

$$\mathbf{x}_c = \begin{pmatrix} 0.125 \\ 0.25 \end{pmatrix} - \frac{1}{2}\left(\begin{pmatrix} 0.125 \\ 0.25 \end{pmatrix} - \begin{pmatrix} -0.75 \\ 0.5 \end{pmatrix}\right) = \begin{pmatrix} -0.3125 \\ 0.375 \end{pmatrix}$$

and $E(\mathbf{x}_c) = 0.223828125$.

So our contraction point becomes a new point in our simplex:



(e) In this picture, we're iteratively swapping out either $\mathbf{x}_2$ or $\mathbf{x}_3$ until the simplex (i.e. the triangle) gets closer to the point $(0, 0)$. Because $\mathbf{x}_1$ is the actual minimum, we won't touch it when creating new points.

A sensible stopping condition might be after a certain number of steps, or when then rate of change of the $E(\mathbf{x}_0)$ (the centroid at a given iteration) begins to slow.

These suggestions are by no means exclusive.

Extra questions

These are extra questions you might attempt in the workshop or at a later time. Some parts of these questions require a computer (e.g. using Python).

1. **Gradient descent:** In this question we're going to aim to minimise the function

$$f(x, y) = e^{-x} \cos(x) y^2$$

using Gradient descent.

(a) $\nabla f(x, y) = (-e^{-x} \cos(x) y^2 - e^{-x} \sin(x) y^2, 2e^{-x} \cos(x) y)$

(b-d) 'Solutions' on this depend very much on what you've picked. Here's some code that I used in Python:

```
import math

def grad(x,y):
    return [-math.exp(-x)*math.cos(x)*pow(y,2)-math.sin(x)*math.exp(-x)*pow(y,2),
           2*math.exp(-x)*math.cos(x)*y]

vec = [1,2] # your random vector here

eta = 0.01
#eta = 0.1
#eta = 0.5

iters = 0
limit = 100

while iters < limit:
    [x,y] = [vec[0],vec[1]]
    newgrad = grad(x,y)
    vec = [x - eta*newgrad[0], y - eta*newgrad[1]]
    iters += 1
    print(iters, vec, math.exp(-x)*math.cos(x)*y**2) # prints i, x_i, , f(x_i)
```

(e) Look again at f; what do you expect the minimum value to be?
To minimise f, we want to take x and y to make it as negative as possible; e^{-x} and y^2 are always positive, so we're going to have to take x so that $\cos(x)$ is as negative as possible - this means that $\cos x = -1$. Now we can take $y \to \infty$, so we get $f(x, y) = -\infty$. Outputs from (c) and (d) should aim to therefore be as small and as negative as possible; a good performance would be going quickly towards this minimum value.

2. **Nelder-Mead:** There are no 'sample' solutions here because there's a myriad of ways that you could implement this and seeing a method that isn't yours isn't hugely helpful. Feel free to discuss your solution in person.