Operations Research Techniques and Algorithms (620-361)

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Today's Lecture

Introduction

Unimodal 1-D unconstrained optimisation

- Fibonacci search
- Golden section, false position and Newton's method

Today's Lecture

In step 1 of this algorithm, we need to find the smallest value of n such that $(b-a)/F_n < 2\epsilon$. We could do this by generating numbers F_n using the recursive formula, until $F_n > (b-a)/2\epsilon$.

An alternative to generating the numbers F_n using the recursive formula, is to use the explicit formula for F_n.

This is derived as follows.

Note that

$$F_n = F_{n-1} + F_{n-2}. \tag{1}$$

is a difference equation with constant coefficients. We solve these by trying a solution of the form $F_n = \lambda^n$. This leads to the *characteristic equation*

$$\lambda^2 = \lambda + 1 \tag{2}$$

and so

$$\lambda = \frac{1 \pm \sqrt{5}}{2}. \tag{3}$$

Thus

$$F_n = A\left(\frac{1+\sqrt{5}}{2}\right)^n + B\left(\frac{1-\sqrt{5}}{2}\right)^n$$

The initial conditions give us

$$A = \frac{\sqrt{5}+1}{2\sqrt{5}}$$

and

$$B = \frac{\sqrt{5}-1}{2\sqrt{5}},$$

so that

$$F_n = \frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1}\right]. \tag{4}$$

The Golden Section Search

The Fibonacci Search reduces the size of an interval in which the minimum occurs in the most efficient way possible. However, at iteration k, we have to choose the points q and p so that the ratios

$$(q-a)/(b-a) = (b-p)/(b-a) = F_{k-1}/F_k$$

depend on k, and the entire search therefore depends on n. Also, we have to pre-compute the values of the Fibonacci numbers in some way.

To remove these dependencies, we can approximate the Fibonacci Search as follows: choose the position of q and p so that the above ratio is equal to

$$\gamma = \lim_{k \to \infty} F_{k-1}/F_k.$$

This is called the Golden Section search.

The Golden Section Search Let $\gamma_k = F_{k-1}/F_k$. Then, from (4),

$$\begin{aligned}\gamma_k &= \frac{\left(\frac{1+\sqrt{5}}{2}\right)^k - \left(\frac{1-\sqrt{5}}{2}\right)^k}{\left(\frac{1+\sqrt{5}}{2}\right)^{k+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{k+1}} \\ &= \frac{1 - \left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^k}{\frac{1+\sqrt{5}}{2} - \frac{1-\sqrt{5}}{2}\left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^k}.\end{aligned} \tag{5}$$

Since $|1-\sqrt{5}| < |1+\sqrt{5}|$, the second terms in both the denominator and numerator decay as $k \to \infty$. Thus

$$\begin{aligned} \gamma &\equiv \lim_{k\to\infty} \gamma_k && (6)\\ &= \frac{1}{\frac{1+\sqrt{5}}{2}} \\ &= \frac{\sqrt{5}-1}{2} \\ &\approx 0.618 && (7) \end{aligned}$$

We could also note that, by equation (1),

$$\gamma_k + \gamma_k \gamma_{k-1} = 1.$$

Letting $k \to \infty$, we see that

$$\gamma + \gamma^2 = 1. \tag{8}$$

The only point in the interval $[0, 1]$ that satisfies this equation is $(\sqrt{5} - 1)/2$, which agrees with our calculation above. The interesting thing about equation (8) is that it shows us that the ratio of γ to 1 is the same as the ratio of $1 - \gamma$ to γ. The number γ is known as the *golden ratio*, a ratio that is supposed to possess many aethestic properties.

Golden Section Search Algorithm

To minimise a unimodal function f over $[a, b]$ to within tolerance ϵ.

1. Set

$$
\begin{aligned}
k &= 1 \\
p &= b - \gamma(b - a) \\
q &= a + \gamma(b - a)
\end{aligned}
$$

   Calculate $f(p)$ and $f(q)$.

2. Set $k = k + 1$. If $f(p) \le f(q)$, then set

$$\begin{aligned} b &= q \\ q &= p \\ p &= b - \gamma(b - a) \end{aligned}$$

Calculate $f(p)$. If $f(p) > f(q)$, then set

$$\begin{aligned} a &= p \\ p &= q \\ q &= a + \gamma(b - a) \end{aligned}$$

Calculate $f(q)$. Repeat until $(b - a) < 2\epsilon$.

Methods Using the Derivative

Now let us assume not only that f is continuous, but that it is also differentiable and that we have a "black box" for f' as well as one for f. We still assume that f is unimodal on $[a, b]$.

The problem of minimising f now reduces to the problem of finding the point x^*, where $f'(x^*) = 0$.

The Method of False Position

Let g be a continuous and increasing function on $\mathbb{R}$. The method of false position is a recursive method for finding the point x^* where $g(x^*) = 0$.

Assume that we can find two points a and b such that $g(a) < 0$ and $g(b) > 0$. The line through the points $(a, g(a))$ and $(b, g(b))$ has equation

$$y = \frac{g(b) - g(a)}{b - a}(x - a) + g(a). \tag{9}$$

The value of the right hand side of (9) is equal to zero at the point

$$x^*_{estimate} = a + \frac{(b - a)g(a)}{g(a) - g(b)}. \tag{10}$$

$x^*_{estimate}$ is a linear estimate for the point x^* at which $g(x^*) = 0$.

- If $g(x^*_{estimate}) = 0$ (to within some tolerance), then we have found a "near enough" approximation to the point x^*.
- If $g(x^*_{estimate}) < 0$, then we use $x^*_{estimate}$ as the lower bound for a new interval.
- If $g(x^*_{estimate}) > 0$, then we use $x^*_{estimate}$ as the upper bound for a new interval.

We can extend this to develop a recursive algorithm as follows.

Algorithm for the Method of False Position

For an increasing, continuous function g on $[a, b]$, to find a point x^* where $|g(x^*)| < \epsilon$.

1. Set

$$\begin{aligned} k &= 1 \\ p &= a + \frac{(b-a)g(a)}{g(a)-g(b)} \end{aligned}$$

   Calculate $g(p)$.

2. Set $k = k + 1$.
If $g(p) < 0$, then set

$$\begin{aligned} a &= p \\ p &= a + \frac{(b-a)g(a)}{g(a)-g(b)} \end{aligned}$$

Calculate $g(p)$.

2. If $g(p) > 0$, then set

$$\begin{aligned} b &= p \\ p &= a + \frac{(b-a)g(a)}{g(a)-g(b)} \end{aligned}$$

Calculate $g(p)$.

Repeat until $|g(p)| < \epsilon$.

If f is convex, then f' is increasing and so we can use the algorithm for the method of false position with $g = f'$ to find the minimum of f.

Newton's Method (Single Variable case)

Another method that we can use to find the point at which an increasing function g is equal to zero is Newton's Method.

The method is both simple to implement and typically converges very quickly. For this method, we need black boxes for both the function g and its derivative g'.

The underlying idea of Newton's Method is that we calculate an estimate of the point x^* at which $g(x^*) = 0$ by calculating the point at which the tangent to g at some point a would cross the x-axis.

The tangent to g at the point $(a, g(a))$ has slope $g'(a)$, and so its equation is

$$y = g'(a)(x - a) + g(a). \tag{11}$$

Thus $y = 0$ when $x = a - g(a)/g'(a)$.

We incorporate this into a recursive algorithm by calculating the value of $g(x)$ and $g'(x)$ at then a subsequent new estimate for the point at which $g = 0$.

One thing we need to beware of is that we do not "divide by zero". Thus we need to test whether $g'(a)$ is very small. In fact if there is a zero of g' close to the zero of g, then Newton's Method doesn't work. Can you explain this physically?

Algorithm for Newton's Method

For an increasing, continuous function g on $\mathbb{R}$ and an initial starting point a, to find a point x^* where $|g(x^*)| < \epsilon$.

1. Set

$$\begin{aligned} k &= 1 \\ \text{if} \quad g'(a) &< \epsilon \quad \text{then} \quad \text{signal} \quad \text{and} \quad \text{stop.} \\ \text{else} \quad p &= a - \frac{g(a)}{g'(a)} \end{aligned}$$

2. Set $k = k + 1$.

$$\begin{array}{rrcl} & a & = & p \\ \text{if} & g'(a) & < & \epsilon \quad \text{then} \quad \text{signal} \quad \text{and} \quad \text{stop.} \\ \text{else} & p & = & a - \dfrac{g(a)}{g'(a)} \end{array}$$

Repeat until $|g(p)| < \epsilon$.

As with the method of false position, we can find the minimum of a convex and twice differentiable function f by using Newton's Method with $g = f'$ and $g' = f''$.