One-Dimensional Search Methods

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In addition to solving nonlinear optimization problems with a single variable, we require an algorithm to do "line searches" as part of a multi-dimensional nonlinear optimization problem:

$$\underset{t}{\text{Minimize}}\ f\left(x^k + t\ d^k\right)$$

where x^k = the k^{th} iterate, $x^k \in R^n$
d^k = (feasible) direction of descent
t = step size
$x^{k+1} = x^k + t^*\ d^k$ for optimal stepsize t^*

- an analytic expression for $f(x)$ might be unknown... $f(x)$ might be "evaluated" by performing a laboratory or simulation experiment, for example
- it is assumed that the function f is *unimodal*, i.e., a local optimum will be globally optimal.
- the result of minimization will be a "sufficiently small" *interval of uncertainty* containing the optimum.
- the derivative of f need not be computed in many of these methods.

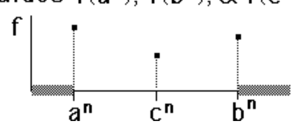
Three-Point Equi-Interval Search

Simple, but inefficient.... not recommended!

Assume that at the n^{th} iteration we have the interval of uncertainty $[a^n,b^n]$ and its midpoint

$$c^n = \frac{a^n + b^n}{2},$$

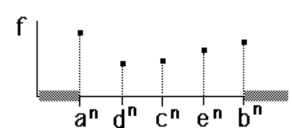
along with the function values $f(a^n)$, $f(b^n)$, & $f(c^n)$



Find the midpoints of the two subintervals $[a^n,c^n]$ and $[c^n,b^n]$:

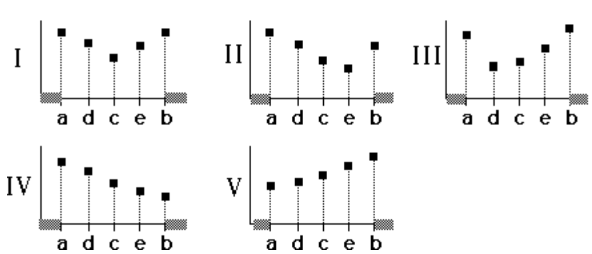
$$d^n = \frac{3a^n + b^n}{4},\quad e^n = \frac{a^n + 3b^n}{4}$$

and evaluate $f(d^n)$ and $f(e^n)$:

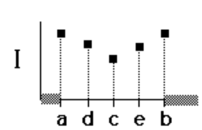


Consider the relative magnitudes of the function at these five points:

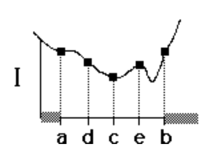
There are several cases to consider:



For example, suppose that f(c) is lower than f(d) and f(e).



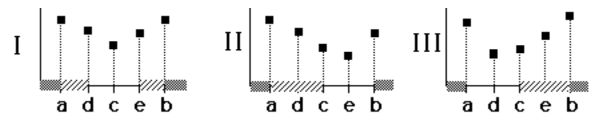
Assuming that the function is unimodal, the minimum cannot be in the interval [e,b]!



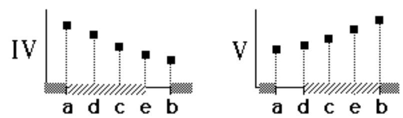
And so, using our assumption of unimodality, this allows us to eliminate portions of the interval [a,b] as possible locations for the optimum.

x cannot be in [a,d) or (e,b]:*

We therefore choose
$a^{n+1} = d^n$, $c^{n+1} = c^n$, $b^{n+1} = e^n$
to begin iteration n+1.



In cases I, II, and III, 50% of the interval is eliminated.

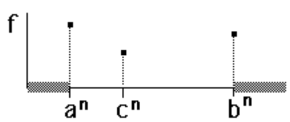


In cases IV and V, 75% of the interval is eliminated!

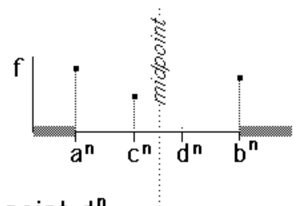
In the event that the smallest of f(a), f(b), f(c), f(d), & f(e) is not unique, less than 25% of the interval can be eliminated.

This event will generally be very rare, especially given round-off errors, etc.

Golden-Section Search



As in 3-point equi-interval search, at the n iteration we have an interval of uncertainty $[a^n,b^n]$ and an interior point $c^n \in (a^n,b^n)$, but c^n is *not the midpoint*!
We insert a *single* additional point d^n so that c^n and d^n are *symmetric* about the midpoint of the interval $[a^n,b^n]$ and compare the values of $f(a^n)$, $f(b^n)$, $f(c^n)$, & $f(d^n)$.

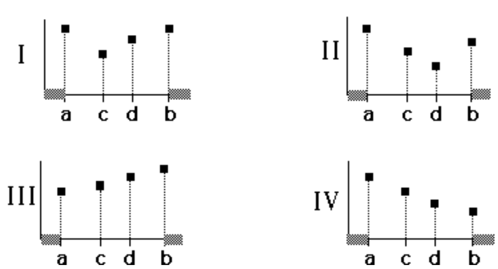


The new point d^n is selected so as to be symmetric to c^n in the interval.

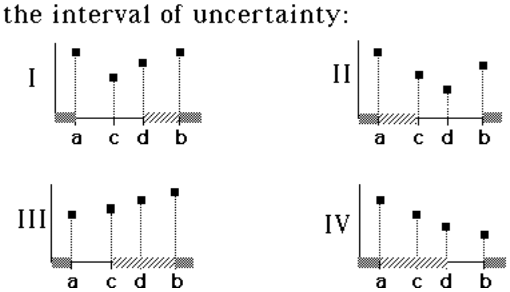
$$b^n - d^n = c^n - a^n$$

$$\Rightarrow \boxed{d^n = a^n + b^n - c^n}$$

Assuming unimodality, we can eliminate a segment from the interval of uncertainty



The shaded segments (▨) can be eliminated from the interval of uncertainty:



Once the location of c^o has been determined within the original interval of uncertainty $[a^o,b^o]$, the location of subsequent points is determined (by symmetry).

?☞ How should c^o be located within $[a^o,b^o]$? ☜?

In "Golden Section" search, this is done so that the ratio $\frac{c^n - a^n}{b^n - a^n}$ is constant (α) $\forall$ n (assuming points are labeled so that $c^n < d^n$)

This requirement uniquely determines

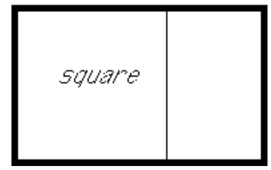
$$\alpha = \frac{c^n - a^n}{b^n - a^n} = \frac{3-\sqrt{5}}{2} \quad \forall\ n$$

$$= 0.381966$$

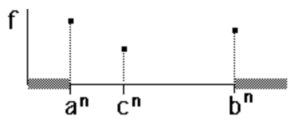
$$\beta = 1 - \alpha = 0.618034$$

known to early Greek mathematicians as the "Golden Section"

If a rectangle with ratio width:length = β is cut to yield a square, the other rectangle also has width:length = β ☚



Fibonacci Search



As is the case with Golden Section Search, this method begins each iteration with an interval of uncertainty [a ,b] and one interior point c , and then inserts another interior point d which is symmetric to c .

In Fibonacci search, however, the ratio $\frac{c^n - a^n}{b^n - a^n}$ is not constant, but converges to $\frac{1}{2}$!

Given: $[a^1,b^1]$ = initial interval of uncertainty

$I_k = b^k - a^k$

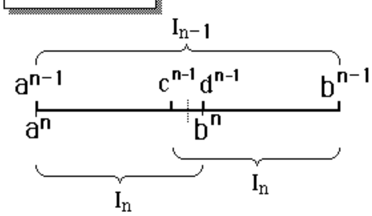
$I_n = b^n - a^n$ = desired length of interval of uncertainty

ε = "distinguishability constant" >0

(i.e., x & y are indistinguishable if $|x-y| < \varepsilon$)

For ease of discussion, assume $I_1 = b^1 - a^1 = 1$

At the last iteration



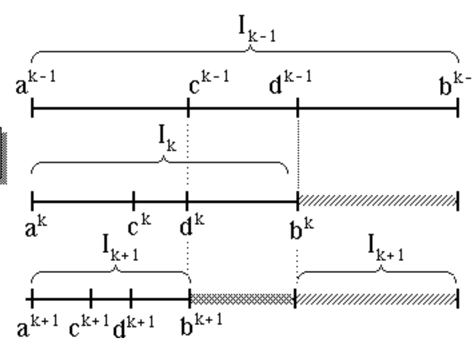
The distance between c^n and d^n will be ε

$$I_{n-1} = 2\ I_n - \varepsilon$$

The final interval of uncertainty will be one of these two intervals

In general, we have

$$I_{k-1} = I_k + I_{k+1}$$



$$I_{k-1} = I_k + I_{k+1}$$

"Fibonacci Numbers"

$$\Longrightarrow \begin{aligned} I_{n-1} &= 2\ I_n - \varepsilon &&= F_2\, I_n - F_0\ \varepsilon \\ I_{n-2} &= 3\ I_n - \varepsilon &&= F_3\, I_n - F_0\ \varepsilon \\ I_{n-3} &= 5\ I_n - 2\ \varepsilon &&= F_4\, I_n - F_1\ \varepsilon \\ I_{n-4} &= 8\ I_n - 3\ \varepsilon &&= F_5\, I_n - F_2\ \varepsilon \\ I_{n-5} &= 13\ I_n - 5\ \varepsilon &&= F_6\, I_n - F_3\ \varepsilon \\ &\vdots \\ I_{n-k} &= F_{k+1}\, I_n - F_{k-1}\ \varepsilon \\ &\vdots \\ 1 = I_1 &= F_n\, I_n - F_{n-2}\ \varepsilon \end{aligned}$$

Fibonacci Numbers

Leonardo of Pisa, son of Bonacci ("Fibonacci") 1202 AD.

Rule for Generating the Sequence:

$$F_0 = F_1 \equiv 1$$

$$F_n = F_{n-1} + F_{n-2}\ ,\ n \geq 2$$

$$\Longrightarrow \begin{aligned} F_2 &= F_1 + F_0 = 1+1 = 2 \\ F_3 &= F_2 + F_1 = 2+1 = 3 \\ F_4 &= F_3 + F_2 = 3+2 = 5 \\ F_5 &= F_4 + F_3 = 5+3 = 8 \\ &\vdots \end{aligned}$$

n	F_n
0	1
1	1
2	2
3	3
4	5
5	8
6	13
7	21
8	34
9	55
10	89

$$I_1 = F_n I_n - F_{n-2}\,\varepsilon$$

Solving for the "reduction ratio" $\frac{I_1}{I_n}$

$$\frac{I_1}{I_n} = \frac{F_n}{1 + F_{n-2}\,\varepsilon}$$

Given a desired reduction ratio, we can find **n**, the required number of iterations.

Example

Suppose we desire $I_n \le 0.01\, I_1$

i.e., $\frac{I_1}{I_n} \ge 100$

and suppose $\varepsilon \approx 0$

Then $\frac{I_1}{I_n} = \frac{F_n}{1 + F_{n-2}\,\varepsilon} \approx F_n$

Choose n so that $F_n \ge 100$

$\Rightarrow n = 11$

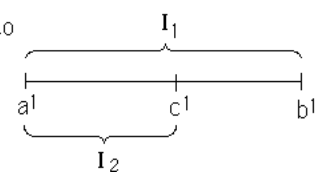
n	F_n
0	1
1	1
2	2
3	3
4	5
5	8
6	13
7	21
8	34
9	55
10	89
11	144
⋮	⋮

Once we have determined n (the # of iterations), we can compute

$$I_2 = F_{n-1}\left[\frac{1 + F_{n-2}\,\varepsilon}{F_n}\right] - F_{n-3}\,\varepsilon$$

$$= \frac{F_{n-1}}{F_n} + \left[\frac{F_{n-1}F_{n-2}}{F_n}\right]\varepsilon$$

This will tell us where to put our initial interior point c^1 within $[a^1, b^1]$.



Example

For example, suppose $n = 11$ and $\varepsilon \approx 0$

$$I_2 \approx \frac{F_{10}}{F_{11}} \approx 0.6180555$$

Throughout the remainder of the iterations, the other interior points are located to retain the symmetry of c^k and d^k.

Polynomial Interpolation

In quadratic & cubic interpolation methods, we use information about the function at two or more points to determine a polynomial in agreement with the known information about the function f.

A minimum point is then computed for the interpolating polynomial to obtain a new point interior to the interval of uncertainty [a,b].

Polynomial	Given information
Quadratic	a, f(a), b, f(b), c (a,b), f(c)
Cubic	a, f(a), f'(a), b, f(b), f'(b)

Polynomial Interpolation

- ☞ Lagrange's Interpolating Polynomials
  polynomials p(x) with p(a)=f(a), etc.
- ☞ Quadratic Interpolation
- ☞ Hermite Interpolating Polynomials
  polynomials p(x) with p(a)=f(a), p'(a)=f'(a)
- ☞ Cubic Interpolation

Lagrange's Interpolating Polynomials

Assume that we are given the n+1 values

$$\{x_0, x_1, x_2, \cdots x_n\}$$

and function values $f(x_i)$,

What is the polynomial p(x) of degree n which agrees exactly with f(x) at the values x_i, i=0,1,2,...n ?

Define

$$\mathcal{L}_j(x) = \prod_{k \neq j} \frac{x - x_k}{x_j - x_k} = \frac{x - x_0}{x_j - x_0} \times \frac{x - x_1}{x_j - x_1} \times \cdots \times \frac{x - x_n}{x_j - x_n}$$

Properties:

$\mathcal{L}_j(x)$ is a polynomial of degree n
$\mathcal{L}_j(x_j) = 1$
$\mathcal{L}_j(x_k) = 0$ for $k \neq j$

That is, for each x_j we define a polynomial of degree n which is 1 at x_j but zero for $x_k, k \neq j$.

Lagrange's interpolating polynomial is

$$p(x) = \sum_{j=0}^{n} f(x_j)\, \mathcal{L}_j(x)$$

This polynomial agrees exactly with the function f at $x_0, x_1, x_2, \cdots x_n$

i.e., $p(x_k) = \sum_{j=0}^{n} f(x_j)\, \mathcal{L}_j(x_k) = f(x_k)\ \forall k=0,1,2,\ldots n$

Hermite Interpolating Polynomials

Assume that we are given the n+1 triplets of values

$x_0, f(x_0), f'(x_0)$
$x_1, f(x_1), f'(x_1)$
$\vdots$
$x_n, f(x_n), f'(x_n)$

We want to find a polynomial p(x) such that

$$p(x_i) = f(x_i), \quad p'(x_i) = f'(x_i) \quad \forall\ i=0,1,\ldots n$$

Notation

$f_i \equiv f(x_i)$

$f'_i \equiv f'(x_i) = \frac{df}{dx}(x_i)$

The polynomial p(x) will be of the form

$$p(x) = \sum_{j=0}^{n} f_j\, h_j(x) + \sum_{j=0}^{n} f'_j\, \bar{h}_j(x)$$

In order that $p(x_i) = f(x_i)$, h_j and $\bar{h}_j$ will satisfy

$h_j(x_j) = 1$
$h_j(x_k) = 1\ \forall\ k \neq j$
$\bar{h}_j(x_k) = 0\ \forall\ k\&j$

Differentiating $p(x) = \sum_{j=0}^{n} f_j\, h_j(x) + \sum_{j=0}^{n} f'_j\, \bar{h}_j(x)$

yields $p'(x) = \sum_{j=0}^{n} f_j\, h'_j(x) + \sum_{j=0}^{n} f'_j\, \bar{h}'_j(x)$

We would therefore like h_j and $\bar{h}_j$ to satisfy

$$h'_j(x_k) = 0\ \forall\ k\&j$$

$$\bar{h}'_j(x_k) = \begin{cases} 1 & \text{if } k = j \\ 0 & \text{if } k \neq j \end{cases}$$

The following functions have the desired properties:

$$h_j(x) = \left[1 - 2(x - x_j)\, \mathcal{L}'_j(x_j)\right] \mathcal{L}_j^2(x)$$

$$\bar{h}_j(x) = (x - x_j)\, \mathcal{L}_j^2(x)$$

Quadratic Interpolation

Given: a, b, c
and f(a), f(b), f(c)

The interpolating quadratic polynomial is

$$p(x) = f(a)\frac{x-b}{a-b}\times\frac{x-c}{a-c} + f(b)\frac{x-a}{b-a}\times\frac{x-c}{b-c} + f(c)\frac{x-a}{c-a}\times\frac{x-b}{c-b}$$

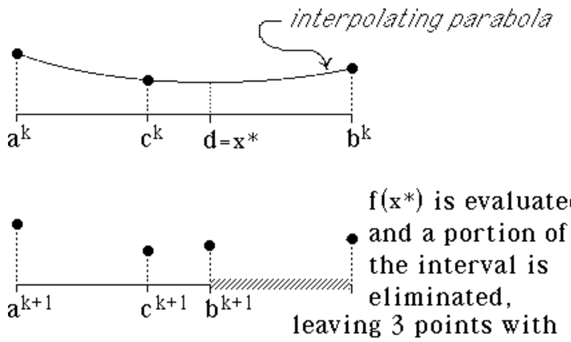
We want to find the minimum of this polynomial,

and so we will find x such that $\frac{dp(x)}{dx} = 0$

$$\frac{dp(x)}{dx} = \frac{f(a)}{(a-b)(a-c)}(2x-b-c) + \frac{f(b)}{(b-a)(b-c)}(2x-a-c) + \frac{f(c)}{(c-a)(c-b)}(2x-a-b) = 0$$

$$\Rightarrow \quad x^* = \frac{1}{2}\, \frac{f(a)\,(b^2 - c^2) + f(b)\,(c^2 - a^2) + f(c)\,(a^2 - b^2)}{f(a)\,(b - c) + f(b)\,(c - a) + f(c)\,(a - b)}$$

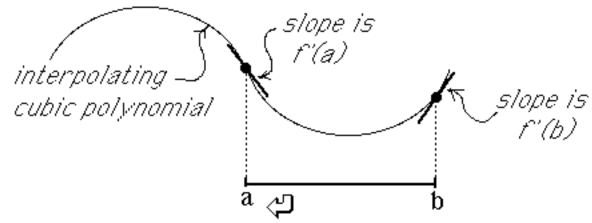
Having located this 4th point (call it d), evaluate f(d) and proceed as in Golden Section or Fibonacci search, eliminating a portion of the interval [a,b]



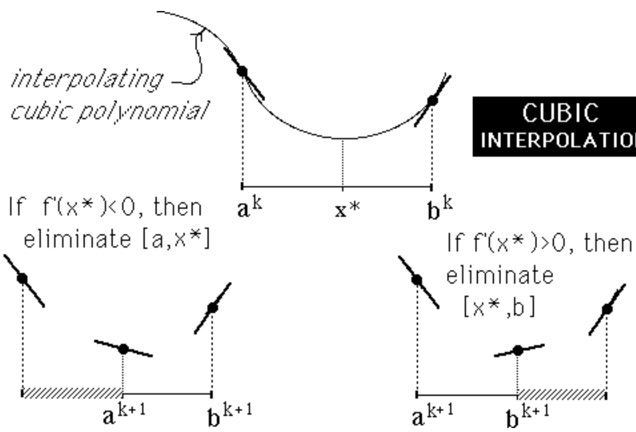
$f(x^*)$ is evaluated and a portion of the interval is eliminated, leaving 3 points with which to begin the next iteration

Cubic Interpolation

Given a, $f(a)$, $f'(a)$, and b, $f(b)$, $f'(b)$, there is a unique cubic polynomial which passes through the points $(a, f(a))$, $(b,f(b))$ and is tangent to the graph at these points.



CUBIC INTERPOLATION



Cubic Interpolation, Using Hermite Polynomials

Given a, $f(a)$, $f'(a)$, and b, $f(b)$, $f'(b)$

The interpolating CUBIC polynomial is

$$p(x) = f(a)h_0(x) + f(b)\,h_1(x) + f'(a)\bar{h}_0(x) + f'(b)\bar{h}_1(x)$$

where

$$h_0(x) = \left[1 - 2\,\frac{x-a}{a-b}\right]\left[\frac{x-b}{a-b}\right]^2 \qquad \bar{h}_0(x) = (x-a)\left[\frac{x-b}{a-b}\right]^2$$

$$h_1(x) = \left[1 - 2\,\frac{x-b}{b-a}\right]\left[\frac{x-a}{b-a}\right]^2 \qquad \bar{h}_1(x) = (x-b)\left[\frac{x-a}{b-a}\right]^2$$

Finding the stationary point of p(x) in [a,b]

Step 1: $z = f'(a) + f'(b) + 3\left[\frac{f(a) - f(b)}{b - a}\right]$

Step 2: $w = \sqrt{\max\,\{0,\ z^2 - f'(a)\times f'(b)\ \}}$

Step 3: $x^* = b - \dfrac{(b-a)(f'(b) + w - z)}{f'(b) + 2w - f'(a)}$