One-Dimensional Minimization

Lectures for PHD course on Non-linear equations and numerical optimization

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March 2005



Outline

- Golden Section minimization
 - Convergence Rate
- Pibonacci Search Method
 - Convergence Rate
- 3 Polynomial Interpolation



The problem

Definition (Global minimum)

Given a function $\phi:[a,b]\mapsto\mathbb{R}$, a point $x^\star\in[a,b]$ is a global minimum if

$$\phi(x^*) \le \phi(x), \quad \forall x \in [a, b].$$

Definition (Local minimum)

Given a function $\phi: [a,b] \mapsto \mathbb{R}$, a point $x^* \in [a,b]$ is a local minimum if there exist a $\delta > 0$ such that

$$\phi(x^*) \le \phi(x), \quad \forall x \in [a, b] \cap (x^* - \delta, x^* + \delta).$$

Finding a global minimum is generally not an easy task even in the 1D case. The algorithms presented in the following approximate local minima.



Interval of Searching

- In many practical problem, $\phi(x)$ is defined in the interval $(-\infty,\infty)$; if $\phi(x)$ is continuous and coercive (i.e. $\lim_{x\mapsto\pm\infty}f(x)=+\infty$), then there exists a global minimum.
- A simple algorithm can determine an interval [a,b] which contains a local minimum. The method searches 3 consecutive points $a, \, \eta, \, b$ such that $\phi(a) > \phi(\eta)$ and $\phi(b) > \phi(\eta)$ in this way the interval [a,b] certainly contains a local minima.
- In practice the method start from a point a and a step-length h>0; if $\phi(a)>\phi(a+h)$ then the step-length k>h is increased until we have $\phi(a+k)>\phi(a+h)$.
- if $\phi(a) < \phi(a+h)$, then the step-length k > h is increased until we have $\phi(a+h-k) > \phi(a)$.
- This method is called forward-backward method.



Interval of Search

Algorithm (forward-backward method)

- Let us be given α and h > 0 and a multiplicative factor t > 1 (usually 2).
- ② If $\phi(\alpha) > \phi(\alpha + h)$ goto forward step otherwise goto backward step
- **3** *forward step*: $a \leftarrow \alpha$; $\eta \leftarrow \alpha + h$;

 - 2 if $\phi(b) \ge \phi(\eta)$ then return [a, b];

 - goto step 1;
- **1 backward step**: $\eta \leftarrow \alpha$; $b \leftarrow \alpha + h$;
 - $\bullet \quad h \leftarrow h \, t \colon \quad a \leftarrow b h \colon$
 - **2** if $\phi(a) \geq \phi(\eta)$ then return [a,b];
 - $b \leftarrow \eta; \ \eta \leftarrow a;$
 - goto step 1;





Unimodal function

Definition (Unimodal function)

A function $\phi(x)$ is unimodal in [a,b] if there exists an $x^* \in (a,b)$ such that $\phi(x)$ is strictly decreasing on $[a,x^*)$ and strictly increasing on $(x^*,b]$.

Another equivalent definition is the following one

Definition (Unimodal function)

A function $\phi(x)$ is unimodal in [a,b] if there exists an $x^* \in (a,b)$ such that for all $a < \alpha < \beta < b$ we have:

- if $\beta < x^*$ then $\phi(\alpha) > \phi(\beta)$;
- if $\alpha > x^*$ then $\phi(\alpha) < \phi(\beta)$;



Unimodal function

Golden search and Fibonacci search are based on the following theorem

Theorem (Unimodal function)

Let $\phi(x)$ unimodal in [a,b] and let be $a < \alpha < \beta < b$. Then

- if $\phi(\alpha) \leq \phi(\beta)$ then $\phi(x)$ is unimodal in $[a, \beta]$
- ② if $\phi(\alpha) \ge \phi(\beta)$ then $\phi(x)$ is unimodal in $[\alpha, b]$

Proof.

- From definition $\phi(x)$ is strictly decreasing over $[a, x^*)$, since $\phi(\alpha) \leq \phi(\beta)$ then $x^* \in (a, \beta)$.
- ② From definition $\phi(x)$ is strictly increasing over $(x^*, b]$, since $\phi(\alpha) \ge \phi(\beta)$ then $x^* \in (\alpha, b)$.

In both cases the function is unimodal in the respective intervals.



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Let $\phi(x)$ an unimodal function on [a,b], the golden section scheme produce a series of intervals $[a_k,b_k]$ where

- $[a_0, b_0] = [a, b];$
- $[a_{k+1}, b_{k+1}] \subset [a_k, b_k];$
- $\lim_{k\to\infty} b_k = \lim_{k\to\infty} a_k = x^*$;

Algorithm (Generic Search Algorithm)

- **1** Let $a_0 = a$, $b_0 = b$
- $oldsymbol{0}$ for k = 0, 1, 2, ... $oldsymbol{choose} a_k < \lambda_k < \mu_k < b_k;$
 - \bullet if $\phi(\lambda_k) \leq \phi(\mu_k)$ then $a_{k+1} = a_k$ and $b_{k+1} = \mu_k$;
 - \bullet if $\phi(\lambda_k) > \phi(\mu_k)$ then $a_{k+1} = \lambda_k$ and $b_{k+1} = b_k$;





- When an algorithm for choosing the observations λ_k and μ_k is defined, the generic search algorithm is determined.
- Apparently the previous algorithm needs the evaluation of $\phi(\lambda_k)$ and $\phi(\mu_k)$ at each iteration.
- In the golden section algorithm, a fixed reduction of the interval τ is used, i.e:

$$b_{k+1} - a_{k+1} = \tau(b_k - a_k)$$

Due to symmetry the observations are determined as follows

$$\lambda_k = b_k - \tau(b_k - a_k)$$

$$\mu_k = a_k + \tau (b_k - a_k)$$

• By a carefully choice of τ , golden search algorithm permits to evaluate only one observation per step.



Consider case 1 in the generic search: then,

$$\lambda_k = b_k - \tau(b_k - a_k), \qquad \mu_k = a_k + \tau(b_k - a_k)$$

and

$$a_{k+1} = a_k, b_{k+1} = \mu_k = a_k + \tau(b_k - a_k)$$

Now, evaluate

$$\lambda_{k+1} = b_{k+1} - \tau(b_{k+1} - a_{k+1}) = a_k + (\tau - \tau^2)(b_k - a_k)$$

$$\mu_{k+1} = a_{k+1} + \tau(b_{k+1} - a_{k+1}) = a_k + \tau^2(b_k - a_k)$$

The only value that can be reused is λ_k so that we try $\lambda_{k+1}=\lambda_k$ and $\mu_{k+1}=\lambda_k$.





• If $\lambda_{k+1} = \lambda_k$, then

$$b_k - \tau(b_k - a_k) = a_k + (\tau - \tau^2)(b_k - a_k)$$

and $1-\tau=\tau-\tau^2$ \Rightarrow $\tau=1$. In this case there is no reduction so that λ_{k+1} must be computed.

• If $\mu_{k+1} = \lambda_k$, then

$$b_k - \tau(b_k - a_k) = a_k + \tau^2(b_k - a_k)$$

and

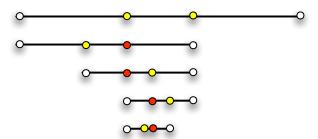
$$1 - \tau = \tau^2$$
 \Rightarrow $\tau^{\pm} = \frac{-1 \pm \sqrt{5}}{2}$

By choosing the positive root, we have $\tau=(\sqrt{5}-1)/2\approx 0.618.$ In this case, μ_{k+1} does not need to be computed.



Graphical structure of the Golden Section algorithm.

- White circles are the extrema of the successive
- Yellow circles are the newly evaluated values;
- Red circles are the already evaluated values;





Algorithm (Golden Section Algorithm)

Let $\phi(x)$ be an unimodal function in [a,b],

- Set k = 0, $\delta > 0$ and $\tau = (\sqrt{5} 1)/2$. Evaluate $\lambda = b \tau(b a)$, $\mu = a + \tau(b a)$, $\phi_a = \phi(a)$, $\phi_b = \phi(b)$, $\phi_{\lambda} = \phi(\lambda)$, $\phi_{\mu} = \phi(\mu)$.
- ② If $\phi_{\lambda} > \phi_{\mu}$ go to step 3; else go to step 4
- If $b-\lambda \leq \delta$ stop and output μ ; otherwise, set $a \leftarrow \lambda$, $\lambda \leftarrow \mu$, $\phi_{\lambda} \leftarrow \phi_{\mu}$ and evaluate $\mu = a + \tau(b-a)$ and $\phi_{\mu} = \phi(\mu)$. Go to step 5
- If $\mu a \leq \delta$ stop and output λ ; otherwise, set $b \leftarrow \mu$, $\mu \leftarrow \lambda$, $\phi_{\mu} \leftarrow \phi_{\lambda}$ and evaluate $\lambda = b \tau(b a)$ and $\phi_{\lambda} = \phi(\lambda)$.

 Go to step 5
- **5** $k \leftarrow k+1$ goto step 2.





Golden Section convergence rate

- At each iteration the interval length containing the minimum of $\phi(x)$ is reduced by τ so that $b_k a_k = \tau^k (b_0 a_0)$.
- Due to the fact that $x^* \in [a_k, b_k]$ for all k then we have:

$$(b_k - x^*) \le (b_k - a_k) \le \tau^k (b_0 - a_0)$$

 $(x^* - a_k) \le (b_k - a_k) \le \tau^k (b_0 - a_0)$

• This means that $\{a_k\}$ and $\{b_k\}$ are r-linearly convergent sequence with coefficient $\tau \approx 0.618$.



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- In the Golden Search Method, the reduction factor τ is unchanged during the search.
- If we allow to change the reduction factor at each step we have a chance to produce a faster minimization algorithm.
- In the next slides we see that there are only two possible choice of the reduction factor:
 - The first choice is $\tau_k = (\sqrt{5} 1)/2$ and gives the golden search method.
 - \bullet The second choice takes τ_k as the ratio of two consecutive Fibonacci numbers and gives the so-called Fibonacci search method.





Consider case 1 in the generic search: the reduction step au_k can vary with respect to the index k as

$$\lambda_k = b_k - \tau_k (b_k - a_k), \qquad \mu_k = a_k + \tau_k (b_k - a_k)$$

and

$$a_{k+1} = a_k, b_{k+1} = \mu_k = a_k + \tau_k (b_k - a_k)$$

Now, evaluate

$$\lambda_{k+1} = b_{k+1} - \tau_{k+1}(b_{k+1} - a_{k+1}) = a_k + (\tau_k - \tau_k \tau_{k+1})(b_k - a_k)$$

$$\mu_{k+1} = a_{k+1} + \tau_{k+1}(b_{k+1} - a_{k+1}) = a_k + \tau_k \tau_{k+1}(b_k - a_k)$$

The only value that can be reused is λ_k , so that we try $\lambda_{k+1} = \lambda_k$ and $\mu_{k+1} = \lambda_k$.





• If $\lambda_{k+1} = \lambda_k$, then

$$b_k - \tau_k (b_k - a_k) = a_k + (\tau_k - \tau_k \tau_{k+1})(b_k - a_k)$$

and $1 - \tau_k = \tau_k - \tau_k \tau_{k+1}$. By searching a solution of the form $\tau_k = z_{k+1}/z_k$, we have the recurrence relation:

$$z_k - 2z_{k+1} + z_{k+2} = 0$$

which has a generic solution of the form

$$z_k = c_1 + c_2(k+1)$$

In general, we have $\lim_{k\to\infty} \tau_k = 1$, so that reduction is asymptomatically worse than golden section.





• If $\mu_{k+1} = \lambda_k$, then

$$b_k - \tau_k(b_k - a_k) = a_k + \tau_k \tau_{k+1}(b_k - a_k)$$

and $1 - \tau_k = \tau_k \tau_{k+1}$. By searching a solution of the form $\tau_k = z_{k+1}/z_k$, we have the recurrence relation:

$$z_k = z_{k+1} + z_{k+2}$$

which is a reverse Fibonacci succession. The computation of z_k involves complex number.





• A simpler way to compute z_k is to take the length of the reduction step constant, say n and compute the Fibonacci sequence up to n as follows

$$F_0 = F_1 = 1,$$
 $F_{k+1} = F_k + F_{k-1}$

then, set $z_k = F_{n-k+1}$ so that $\tau_k = F_{n-k}/F_{n-k+1}$.

- In the Fibonacci search we evaluate reduction factor τ_k by choosing the number of reductions before starting the algorithm
- \bullet A way to evaluate this number is to choose a tolerance δ so that

$$b_n - a_n \le \delta$$





9 From the definition of the reduction factor τ_k , it is easy to evaluate $b_n - a_n$:

$$b_n - a_n = \frac{F_1}{F_2} (b_{n-1} - a_{n-1}) = \frac{F_1}{F_2} \frac{F_2}{F_3} (b_{n-2} - a_{n-2})$$
$$= \frac{F_1}{F_2} \frac{F_2}{F_3} \cdots \frac{F_n}{F_{n+1}} (b_0 - a_0) = \frac{b_0 - a_0}{F_{n+1}}$$

② In this way the number of reductions n is deduced from:

$$F_{n+1} \ge \frac{b_0 - a_0}{\delta}$$





Algorithm (Fibonacci Search Algorithm)

Let $\phi(x)$ be an unimodal function in [a,b]

- Set k=0, $\delta>0$ and n such that $F_{n+1}\geq (b_0-a_0)/\delta$. Evaluate $\tau=F_n/F_{n+1}$, $\lambda=b-\tau(b-a)$, $\mu=a+\tau(b-a)$, $\phi_a=\phi(a)$, $\phi_b=\phi(b)$, $\phi_\lambda=\phi(\lambda)$, $\phi_\mu=\phi(\mu)$.
- ② If $\phi_{\lambda} > \phi_{\mu}$ go to step 3; else go to step 4
- If $b-\lambda \leq \delta$ stop and output μ ; otherwise set $a \leftarrow \lambda$, $\lambda \leftarrow \mu$, $\phi_{\lambda} \leftarrow \phi_{\mu}$ evaluate $\mu = a + \tau(b-a)$ and $\phi_{\mu} = \phi(\mu)$. Go to step 5
- If $\mu-a \leq \delta$ stop and output λ ; otherwise set $b \leftarrow \mu$, $\mu \leftarrow \lambda$, $\phi_{\mu} \leftarrow \phi_{\lambda}$ evaluate $\lambda = b \tau(b-a)$ and $\phi_{\lambda} = \phi(\lambda)$.

 Go to step 5
- **5** set $k \leftarrow k+1$ and $\tau \leftarrow F_{n-k}/F_{n-k+1}$ goto step 2.





Fibonacci Search convergence rate

• At each iteration, the interval length containing the minimum of $\phi(x)$ is

$$b_k - a_k = (b_0 - a_0)(F_{n-k+1}/F_{n+1})$$

• Due to the fact that $x^* \in [a_k, b_k]$ for all k, we have:

$$(b_k - x^*) \le (b_k - a_k) \le (F_{n-k+1}/F_{n+1})(b_0 - a_0)$$

$$(x^* - a_k) \le (b_k - a_k) \le (F_{n-k+1}/F_{n+1})(b_0 - a_0)$$



Fibonacci Search convergence rate

ullet To estimate convergence rate we need the expression of F_k

$$F_k = rac{1}{\sqrt{5}} \left\{ \left(rac{1 + \sqrt{5}}{2}
ight)^{k+1} - \left(rac{1 - \sqrt{5}}{2}
ight)^{k+1}
ight\}$$

and for large k

$$F_k pprox rac{1}{\sqrt{5}} \left(rac{1+\sqrt{5}}{2}
ight)^{k+1}$$

• in this way we can approximate

$$\frac{F_{n-k+1}}{F_{n+1}} \approx \left(\frac{1+\sqrt{5}}{2}\right)^{-k} = \left(\frac{\sqrt{5}-1}{2}\right)^k$$





Fibonacci Search convergence rate

- This means that $\{a_k\}$ and $\{b_k\}$ are r-linearly convergent sequences with coefficient $\tau \approx 0.618$.
- So, golden search and Fibonacci search perform similarly for large n. Golden search is easier, for this reason, normally Golden search is preferre to Fibonacci search.





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- Fibonacci and golden search are r-linearly convergent methods.
- Approximating the function $\phi(x)$ with a polynomial model and minimizing the polynomial result in algorithms which are normally superior to Fibonacci and golden search.





- Suppose that an initial guess x_0 is known, and the interval $[0, x_0]$ contains a minimum.
- We can form the quadratic approximation p(x) to $\phi(x)$ by interpolating $\phi(0)$, $\phi(x_0)$ and $\phi'(0)$.

$$q(x) = \frac{\phi(x_0) - \phi(0) - x_0 \phi'(0)}{x_0^2} x^2 + \phi'(0)x + \phi(0).$$

The new trial minimum is defined as the minimum of the polynomial approximation q(x), an takes the value:

$$x_1 = -\frac{\phi'(0)x_0^2}{2[\phi(x_0) - \phi(0) - \phi'(0)x_0]}$$





• If $\phi'(x_1)$ is small enough (we are near a stationary point) we can stop the iteration, otherwise we can construct a cubic polynomial that interpolates $\phi(0)$, $\phi'(0)$, $\phi(x_0)$ and $\phi(x_1)$.

$$c(x) = A_1 x^3 + B_1 x^2 + \phi'(0)x + \phi(0).$$

where

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{x_0^2 x_1^2 (x_1 - x_0)} \begin{pmatrix} x_0^2 & -x_1^2 \\ -x_0^3 & x_1^3 \end{pmatrix} \begin{pmatrix} \phi(x_1) - \phi(0) - \phi'(0) x_1 \\ \phi(x_0) - \phi(0) - \phi'(0) x_0 \end{pmatrix}$$

The new trial minimum is defined as the minimum of the polynomial approximation c(x).





• By differentiating c(x) and taking the root nearest the 0 values we obtain:

$$x_2 = \frac{-B_1 + \sqrt{B_1^2 - 3A_1\phi'(0)}}{A_1}$$
$$= \frac{-\phi'(0)}{B_1 + \sqrt{B_1^2 - 3A_1\phi'(0)}}$$

where for stability reason we use the first expression when $B_1 < 0$, the second expression when $B_1 \ge 0$.

• If the new trial minimum is not accepted, we repeat the procedure with $\phi(0)$, $\phi'(0)$, $\phi(x_1)$ and $\phi(x_2)$.





• In general we can approximate the minimum by the procedure

$$x_{k+1} = \frac{-B_k + \sqrt{B_k^2 - 3A_k\phi'(0)}}{A_k}$$
$$= \frac{-\phi'(0)}{B_k + \sqrt{B_k^2 - 3A_k\phi'(0)}}$$

where

$$\begin{pmatrix} A_k \\ B_k \end{pmatrix} = \frac{1}{x_{k-1}^2 x_k^2 (x_k - x_{k-1})} \begin{pmatrix} x_{k-1}^2 & -x_k^2 \\ -x_{k-1}^3 & x_k^3 \end{pmatrix} \times \begin{pmatrix} \phi(x_k) - \phi(0) - \phi'(0) x_k \\ \phi(x_{k-1}) - \phi(0) - \phi'(0) x_{k-1} \end{pmatrix}$$





References



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