One-Dimensional Minimization

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

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Outline

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

$$\phi(x^\star) \leq \phi(x), \qquad \forall x \in [a, b].$$

Definition (Local minimum)

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

$$\phi(x^\star) \leq \phi(x), \qquad \forall x \in [a, b] \cap (x^\star - \delta, x^\star + \delta).$$

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, η, 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)

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

Unimodal function

Definition (Unimodal function)

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

Another equivalent definition is the following one

Definition (Unimodal function)

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

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

1. *if $\phi(\alpha) \leq \phi(\beta)$ then $\phi(x)$ is unimodal in $[a, \beta]$*
2. *if $\phi(\alpha) \geq \phi(\beta)$ then $\phi(x)$ is unimodal in $[\alpha, b]$*

Proof.

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

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

Outline

Golden Section minimization

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

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

Algorithm (Generic Search Algorithm)

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

Golden Section minimization

- 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.

Golden Section minimization

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

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

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 $\mu_{k+1} = \lambda_k$.

Golden Section minimization

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

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

  and $1 - \tau = \tau - \tau^2 \quad \Rightarrow \quad \tau = 1$. 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

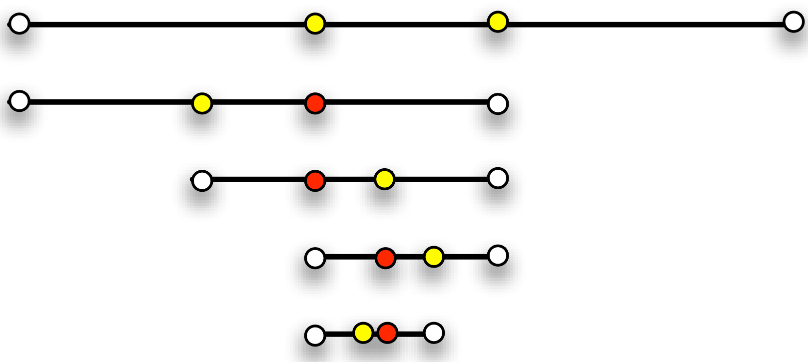
$$1 - \tau = \tau^2 \qquad \Rightarrow \qquad \tau^{\pm} = \frac{-1 \pm \sqrt{5}}{2}$$

  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.

Golden Section minimization

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* $[a, b]$*,*

1. *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
3. *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
4. *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 $x^\star \in [a_k, b_k]$ for all k then we have:

$$(b_k - x^\star) \leq (b_k - a_k) \leq \tau^k(b_0 - a_0)$$

$$(x^\star - a_k) \leq (b_k - a_k) \leq \tau^k(b_0 - a_0)$$

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

Outline

Fibonacci Search Method

- 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.
  - The second choice takes τ_k as the ratio of two consecutive Fibonacci numbers and gives the so-called Fibonacci search method.

Fibonacci Search Method

Consider case 1 in the generic search: the reduction step τ_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

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

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 $\mu_{k+1} = \lambda_k$.

Fibonacci Search Method

- 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 $\lim_{k\mapsto\infty} \tau_k = 1$, so that reduction is asymptomatically worse than golden section.

Fibonacci Search Method

- 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.

Fibonacci Search Method

- 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

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

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
- A way to evaluate this number is to choose a tolerance δ so that

$$b_n - a_n \leq \delta$$

Fibonacci Search Method

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

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

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

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

Algorithm (Fibonacci Search Algorithm)

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

1. *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*
3. *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*
4. *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 $x^\star \in [a_k, b_k]$ for all k, we have:

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

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

Fibonacci Search convergence rate

- To estimate convergence rate we need the expression of F_k

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

- and for large k

$$F_k \approx \frac{1}{\sqrt{5}} \left(\frac{1+\sqrt{5}}{2} \right)^{k+1}$$

- 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.

Outline

Polynomial Interpolation

- 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.

Polynomial Interpolation

- 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:

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

Polynomial Interpolation

Polynomial Interpolation

- 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 $\phi(x_1)$.

$$c(x) = A_1x^3 + B_1x^2 + \phi'(0)x + \phi(0).$$

where

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

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

Polynomial Interpolation

- 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 $B_1 \geq 0$.

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

Polynomial Interpolation

Polynomial Interpolation

- 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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