Computational Maths 2

Introduction to Numerical Optimization

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Optimization in dimension 1

- Methods of order zero (without derivatives)
- Methods of order one and above (with derivatives)

Some basic definitions

Let $f : K \to \mathbb{R}$ be a regular function and K be an interval.

1. x^* is a local minimum of f on K if there exists $\varepsilon > 0$ such that $f(x^*) \le f(x)$ for every $x \in (x^* - \varepsilon, x^* + \varepsilon)$
2. x^* is a local maximum of f on K if there exists $\varepsilon > 0$ such that $f(x^*) \ge f(x)$ for every $x \in (x^* - \varepsilon, x^* + \varepsilon)$
3. x^* is a global minimum of f on K if $f(x^*) \le f(x)$ for every $x \in K$
4. x^* is a global maximum of f on K if $f(x^*) \ge f(x)$ for every $x \in K$
5. x^* is an local/global extremum of f on K if it is a local/global minimum or maximum of f

Existence of a minimizer

Compact interval

Let $f : [a, b] \to \mathbb{R}$ be a continuous function. Then f is bounded and it attains its upper and lower bounds on $[a, b]$, i.e. f admits global minima and maxima.

$\star$ a classical condition to recover existence on the whole space is what we call "infinite at infinity"

Existence on $\mathbb{R}$

Let $f : \mathbb{R} \to \mathbb{R}$ be a continuous function such that $f(x) \to +\infty$ when $|x| \to +\infty$ then f admits global minimizers on $\mathbb{R}$.

$\star$ Uniqueness is not guaranteed, in general.

Classical method in the calculus of variations

- lower bound on f: existence of a minimizing sequence
- compactness: extract a converging subsequence
- continuity: conclude that a limit point of the minimizing sequence is a solution

Necessary conditions of optimality

Suppose that f is a C^1 function defined on an interval $K \subset \mathbb{R}$ and that f has a local extremum at x^* which is an interior point of K. Then $f'(x^*) = 0$.

Proof: Classical. Just write $f'(x^*) = \lim_{x \to x^*} \dfrac{f(x) - f(x^*)}{x - x^*}$.

$\star$ points x such that $f'(x) = 0$ are called critical points.

$\star$ what happens if the extremum is attained at the end of the interval?

Euler's inequality

Let $f : [a, b] \to \mathbb{R}$ be a C^1 function on an open set containing $[a, b]$. Then

- if a is a local minimum then $f'(a) \geq 0$
- if b is a local minimum then $f'(b) \leq 0$
- if a is a local maximum then $f'(a) \leq 0$
- if b is a local maximum then $f'(b) \geq 0$

Proof: the same idea.

Before going further...

$\star$ Recall the Taylor expansion formula around a: suppose that f is smooth and x is "close to a". Then

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \dots$$

Before going further...

Proposition 1 (Taylor theorem with remainder)

Suppose that $f : \mathbb{R} \to \mathbb{R}$ is of class C^k at a. Then

$$f(x) = \sum_{i=0}^{k} \frac{f^{(i)}(a)}{i!}(x-a)^i + R_k(x)$$

where the remainder $R_k(x)$ is equal to one of the following:

- $R_k(x) = h_k(x)(x-a)^k$ *with* $\lim_{x\to a} h_k(x) = 0$. *In other words* $R_k(x) = o(|x-a|^k)$ *as* $x \to a$.
- *if f is of class C^{k+1} then*
$$R_k(x) = \frac{f^{(k+1)}(\xi_L)}{(k+1)!}(x-a)^{k+1}$$
with ξ_L between a and x. This is the Lagrange form of the remainder.

$\star$ Recall the Little-o and Big-O notations:

$$|O(x)| \leq C|x| \text{ and } \frac{o(x)}{|x|} \to 0 \text{ as } |x| \to 0$$

What about sufficient conditions?

⋆ in general, we may have critical points which are not local extrema

Example: $f(x) = x^3$ has a unique critical point $x = 0$, but $x = 0$ is not a local minimizer.

⋆ the first option is to look at second order conditions

Second order necessary and sufficient conditions

1. Suppose $f : \mathbb{R} \to \mathbb{R}$ is of class C^2 and $x^* \in \mathbb{R}$. Then
$$x^* \text{ is a local minimum of } f \implies f'(x^*) = 0 \text{ and } f''(x^*) \geq 0$$
$$x^* \text{ is a local maximum of } f \implies f'(x^*) = 0 \text{ and } f''(x^*) \leq 0$$

2. Suppose $f : \mathbb{R} \to \mathbb{R}$ is of class C^2 and $x^* \in \mathbb{R}$. Then
$$f'(x^*) = 0 \text{ and } f'' \geq 0 \text{ on } (x^* - \varepsilon, x^* + \varepsilon) \implies x^* \text{ is a local minimum of } f.$$

This implies the following weaker sufficient condition:
$$f'(x^*) = 0 \text{ and } f''(x^*) > 0 \implies x^* \text{ is a local minimum of } f.$$

⋆ proof idea: $f(x)$ is above $f(x^*)$ plus a "positive parabola" centered at x^*.

Important particular case

⋆ the class of convex functions is important from the optimization point of view
⋆ we can have results of existence and uniqueness of minimizers
⋆ first order optimality conditions are necessary and sufficient

Definition 2 (Convex functions)

Let $f : \mathbb{R} \to \mathbb{R}$ be a function.
f is convex if $\forall t \in [0,1],\ \forall x, y \in \mathbb{R}$ we have

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y)$$

Equivalent definitions:
⋆ f is below its secants
⋆ f is above its tangents (where f is regular)

⋆ if we replace the inequality above with a strict one, we obtain the class of strictly convex functions

Existence and uniqueness: convex case

Proposition 3

Let $f : \mathbb{R} \to \mathbb{R}$ be a convex function. If f is convex then any local minimum of f is a global minimum.

Proposition 4 (Uniqueness)

Let $f : \mathbb{R} \to \mathbb{R}$ be a convex function. If f is strictly convex then there exists at most one minimum of f on $\mathbb{R}$.

$\star$ We cannot say more with strict convexity alone! In particular, strict convexity does not guarantee existence. Consider $f(x) = \exp(x)$.

Proposition 5 (Existence and Uniqueness)

Let $f : \mathbb{R} \to \mathbb{R}$ be a function. Then if

- $f(x) \to +\infty$ *when* $|x| \to \infty$
- f *is strictly convex*

then there exists a unique minimizer x^* of f on $\mathbb{R}$.

Exercise: Prove that a convex function $f : [a, b] \to \mathbb{R}$ is continuous on (a, b).

Optimality conditions: convex case

Proposition 6

Suppose that $f : \mathbb{R} \to \mathbb{R}$ is a convex function of class C^1 and $x^* \in \mathbb{R}$. Then the following statements are equivalent:

- x^* *is a global minimum of* f
- x^* *is a local minimum of* f
- $f'(x^*) = 0$

$\star$ convexity gives convenient tools for proving convergence results regarding numerical algorithms

$\star$ it is one of the rare hypotheses which can guarantee the convergence of an algorithm to the global minimum

$\star$ numerical algorithms will be applied to general functions, but in general we can only hope to converge to a local minimum

Importance of the 1D case

⋆ It gives an initial framework, to be extended to higher dimensions
⋆ most efficient optimization algorithms use a line-search routine

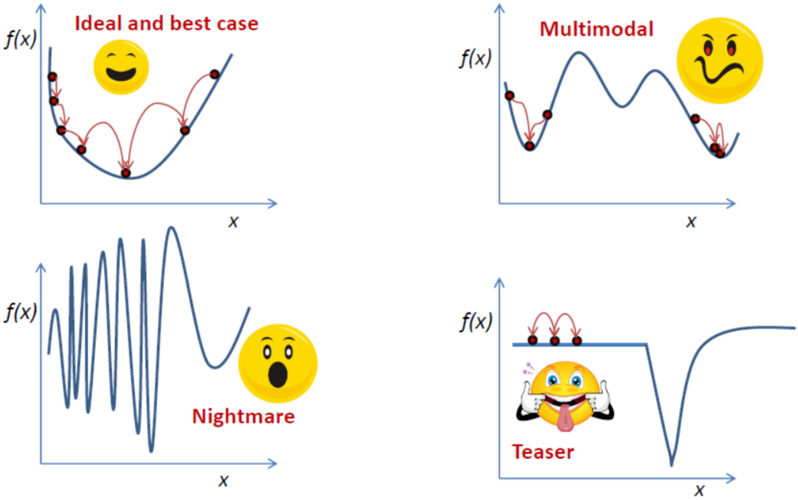
Example of optimization algorithm

Optimization of a function $f : \mathbb{R}^n \to \mathbb{R}$ starting from an initial point x_0
At iteration i

- Point x_n: find a descent direction d_n
- Find a reasonable step size such that $f(x_n + \gamma d_n)$ is significantly smaller than $f(x_n)$

⋆ The second step is essentially a one dimensional optimization routine
⋆ Often it is not reasonable to solve an optimization problem at every iteration

What to expect?



[photo from Ziv Bar-Joseph, used with permision]

Assumption: the function f is unimodal on the segment $[a, b]$, i.e. it possesses a unique local minimum on $[a, b]$

Optimization in dimension 1

- Methods of order zero (without derivatives)
- Methods of order one and above (with derivatives)

Motivation

⋆ some practical objective functions don't have derivatives available

Examples:

a) physical proprieties of a given material
b) trajectory of an object in a gravitational field
c) general "black box" functions

⋆ function evaluations can cost money in real life: achieve best results for a given number of function evaluations

Simplest idea: grid search

Given $f : [a, b] \to \mathbb{R}$:

- Discretize $[a, b]$ using N points $x_1, ..., x_N$
- Evaluate $f(x_i)$ and select the smallest value
- If N is large enough and f is not oscillating too much, this method will give a first indication concerning the global minimizer

$\star$ the precision depends on N
$\star$ lots of unnecessary evaluations of f away from the local minimizers
$\star$ **Advantage:** it gives indication on the position of global minimizers (under regularity assumptions...)
$\star$ a more localized approach should be used in order to achieve faster converging algorithms.

Bracketing algorithms: unimodal case

⋆ f is unimodal on $[a, b]$: it possesses a unique local minimum $x^* \in [a, b]$

Proposition 7

If f is unimodal on $[a, b]$ with minimum x^* then:
⋆ f is strictly decreasing on $[a, x^*]$ and strictly increasing on $[x^*, b]$.
⋆ f is unimodal on every sub-interval $[a', b'] \subset [a, b]$

⋆ We wish to reduce the size of the interval $[a, b]$ containing x^* by computing the value of f at some intermediary points
⋆ Without the use of derivatives, one intermediary point is not enough. Are two intermediary points enough?

Consider two points $x^+, x^- \in (a, b)$ such that $a < x^- < x^+ < b$.
Case 1: $f(x^-) \leq f(x^+) \Rightarrow$ ...
Case 2: $f(x^-) \geq f(x^+) \Rightarrow$ ...

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Case 1: $f(x^-) \leq f(x^+) \Rightarrow$ x^* is to the left of x^+
Case 2: $f(x^-) \geq f(x^+) \Rightarrow$ x^* is to the right of x^-

Bracketing algorithms: unimodal case

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Consider two points $x^+, x^- \in (a,b)$ such that $a < x^- < x^+ < b$.
Case 1: $f(x^-) \leq f(x^+) \Rightarrow$ x^* is to the left of x^+ $\Rightarrow$ replace $[a,b]$ with $[a,x^+]$
Case 2: $f(x^-) \geq f(x^+) \Rightarrow$ x^* is to the right of x^- $\Rightarrow$ replace $[a,b]$ with $[x^-,b]$

Generic Algorithm

Algorithm 1 (Zero-order minimization of a unimodal function)

Initialization: *Initial segment* $S_0 = [a, b]$*, iteration number* $i = 1$
Step i*: Given previous segment* $S_{i-1} = [a_{i-1}, b_{i-1}]$

- *choose points* x_i^-, x_i^+*:* $a_{i-1} < x_i^- < x_i^+ < b_{i-1}$
- *compute* $f(x_i^-)$ *and* $f(x_i^+)$
- *define the new segment as follows*
  - *if* $f(x_i^-) \leq f(x_i^+)$ *then* $S_i = [a_{i-1}, x_i^+]$
  - *if* $f(x_i^-) \geq f(x_i^+)$ *then* $S_i = [x_i^-, b_{i-1}]$
- *go to step* $i + 1$

⋆ Why does the algorithm work?

- at each step we guarantee that x^* belongs to S_i
- the length of S_i is diminished at each iteration

⋆ Stopping criterion: the length of the segment S_i is smaller than a tolerance $\varepsilon > 0$

Rate of convergence

⋆ measure the speed of convergence of the iterates to the optimum

⋆ define an error function $\text{err}(x_i)$: for example $\text{err}(x_i) = |x_i - x^*|$

⋆ in the following, denote $r_i = \text{err}(x_i)$

Standard classification

- linear convergence: there exists $q \in (0,1)$ such that $r_{i+1} \leq q r_i$
  - ⋆ the constant $q \in (0,1)$ is called the convergence ratio
  - ⋆ it is easy to show that $r_i \leq q^i r_0$, so in particular $r_i \to 0$.
- sublinear convergence: $r_i \to 0$ but is not linearly converging
- superlinear convergence: $r_i \to 0$ with any positive convergence ratio
  - ⋆ sufficient condition: $\lim\limits_{i \to \infty} (r_{i+1}/r_i) = 0$
- convergence of order $p > 1$: there exists $C > 0$ such that for i large enough

$$r_{i+1} \leq C r_i^p$$

  - ⋆ p is called the order of convergence
  - ⋆ the case $p = 2$ has a special name: quadratic convergence

Rates of convergence - Examples

Let $\gamma \in (0,1)$. Then:

- (γ^n) converges linearly to zero, but not superlinearly
- (γ^{n^2}) converges superlinearly to zero, but not quadratically
- (γ^{2^n}) converges to zero quadratically

Quadratic convergence is much faster than linear convergence

Plotting the order of convergence

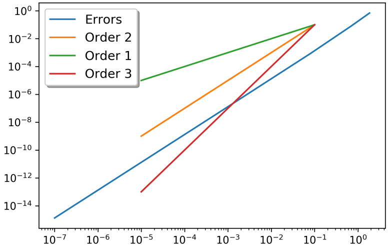
For the convergence of order p we have $r_{i+1} \approx C r_i^p$.

$\star$ representing this directly does not illustrate clearly the power p

$\star$ taking logarithms we get $\log \operatorname{err}(x_{i+1}) \approx \log C + p \log \operatorname{err}(x_i)$

$\star$ therefore, plotting the next error in terms of the previous error in a log-log scale gives the line $y = \log C + px$

$\star$ the slope of the line shows the order of the method!



Trisection algorithm

⋆ the interval S_i gives an approximation of x^* with error at most $|S_i|$

Trisection algorithm

Define intermediary points by

$$x_i^- = \frac{2}{3}a_{i-1} + \frac{1}{3}b_{i-1} \quad x_i^+ = \frac{1}{3}a_{i-1} + \frac{2}{3}b_{i-1}$$

Then $|S_i| = 2/3|S_{i-1}|$ and we achieve linear convergence rate.

⋆ if x_i is an arbitrary point in S_i then

$$|x^* - x_i| \leq \left(\frac{2}{3}\right)^i |b-a|.$$

⋆ if x_i is an approximation of x^* after k function evaluations then

$$|x^* - x_i| \leq \left(\frac{2}{3}\right)^{\lfloor k/2 \rfloor} |b-a|.$$

⋆ in terms of function evaluations the convergence ratio is $\sqrt{2/3} \approx 0.816$

⋆ it is possible to be more efficient by doing one function evaluation when changing from S_{i-1} to S_i

Fibonacci search

⋆ the Fibonacci sequence is defined by

$$F_0 = 1,\ F_1 = 1,\ F_{n+1} = F_n + F_{n-1}.$$

⋆ first few terms are: $1, 1, 2, 3, 5, 8, 13, 21, 34, 55...$

⋆ Fibonacci search: when you know from advance the number of function evaluations N you want to make

Algorithm 2 (Fibonacci search)

Initialization: *Start with $S_0 = [a_0, b_0]$ and perform N steps as follows:* **For** $i = 1, ..., N-1$

- *choose x_i^- and x_i^+ such that*

$$|a_{i-1} - x_i^+| = |b_{i-1} - x_i^-| = \frac{F_{N-i}}{F_{N-i+1}} |a_{i-1} - b_{i-1}|$$

- *compute $f(x_i^-)$ or $f(x_i^+)$ (which one was not computed before)*
- *define the new segment as follows*
  - *if $f(x_i^-) \leq f(x_i^+)$ then $S_i = [a_{i-1}, x_i^+]$*
  - *if $f(x_i^-) \geq f(x_i^+)$ then $S_i = [x_i^-, b_{i-1}]$*
- *go to step $i+1$*

Why is this choice ok?

Proposition 8

We need to do only one function evaluation per iteration.

⋆ $|b_i - a_i| = \frac{F_{N-i}}{F_{N-i+1}} \dots \frac{F_{N-1}}{F_N} |b_0 - a_0| = \frac{F_{N-i}}{F_N} |b_0 - a_0|$

⋆ in the end $|x^* - x_N| = |b_N - a_N| = \frac{|b_0 - a_0|}{F_N}$

⋆ Formula: $F_n = \frac{1}{\lambda+2} \left[(\lambda+1)\lambda^n + (-1)^n \lambda^{-n}\right],\ \lambda = \frac{1+\sqrt{5}}{2}$

⋆ In the end: $|x^* - x_N| \leq C\lambda^{-N} |b_0 - a_0|(1 + o(1))$ which gives a linear convergence rate with ratio $\lambda^{-1} = \frac{2}{1+\sqrt{5}} = 0.61803\dots$

⋆ the previous method gave a rate of convergence of $\sqrt{2/3} = 0.81649\dots$ in terms of the number of evaluations

⋆ this is the best we can do in a given number of iterations

[J. Kiefer, *Sequential minimax search for a maximum*]

Fun fact - computing Fibonacci numbers

Question

What algorithm do you use to compute F_n given n?

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What algorithm do you use to compute F_n given n?

Trivial algorithm

Initialize $F_0 = 1, F_1 = 1$, at each step compute $F_i = F_{i-1} + F_{i-2}$.
Complexity:

Don't store all values F_i if they are not needed: diminish memory consumption
Don't use recursive algorithms(!!!): exponential complexity

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Efficient algorithm

If $M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$ then $M^n = \begin{pmatrix} F_{n+1} & F_n \\ F_n & F_{n-1} \end{pmatrix}$.
Complexity:

Fun fact - computing Fibonacci numbers

Question

What algorithm do you use to compute F_n given n?

Trivial algorithm

Initialize $F_0 = 1, F_1 = 1$, at each step compute $F_i = F_{i-1} + F_{i-2}$.
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If $M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$ then $M^n = \begin{pmatrix} F_{n+1} & F_n \\ F_n & F_{n-1} \end{pmatrix}$.
Complexity: $O(\log n)$

$\star$ Exponentiation is very fast if done properly: search for "exponentiation by squaring" or "fast exponentiation" if you are interested
$\star$ If you want other tricky problems where maths can significantly reduce the complexity of the problem take a look at Project Euler

Other ways of computing Fibonacci numbers

Use the following recursion formulas:

$$F_{2n} = F_n(2F_{n+1} - F_n)$$
$$F_{2n+1} = F_{n+1}^2 + F_n^2$$

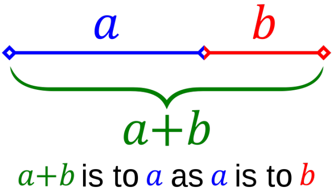
$\star$ This will again give you a $O(\log n)$ algorithm since you can always go from n to $2n$ or $2n+1$: the number of steps is the length of the binary expansion of n
$\star$ All this is nice, but be aware that Fibonacci numbers grow exponentially fast:

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

$\star$ Note that $F_n \approx \frac{1}{\sqrt{5}}\lambda^{n+1}$
$\star$ in NumPy you will quickly go beyond the 16 digit precision: there is no need to be extremely efficient...

Golden search

⋆ Fibonacci search: one needs to know in advance the number of function evaluations N
⋆ Golden ratio: $\lambda = \frac{1+\sqrt{5}}{2}$
⋆ Essential property:



Algorithm

Algorithm 3 (Golden search)

Initialization: *Start with* $S_0 = [a_0, b_0]$ *and define* $\lambda = \dfrac{\sqrt{5}+1}{2}$

Iterate

- *choose* x_i^- *and* x_i^+ *such that*

$$x_i^- = \frac{\lambda}{\lambda+1} a_{i-1} + \frac{1}{\lambda+1} b_{i-1} \qquad x_i^+ = \frac{1}{\lambda+1} a_{i-1} + \frac{\lambda}{\lambda+1} b_{i-1}$$

- *compute* $f(x_i^-)$ *or* $f(x_i^+)$ *(which one was not computed before)*
- *define the new segment as follows*
  - *if* $f(x_i^-) \leq f(x_i^+)$ *then* $S_i = [a_{i-1}, x_i^+]$
  - *if* $f(x_i^-) \geq f(x_i^+)$ *then* $S_i = [x_i^-, b_{i-1}]$
- *go to step* $i+1$

Until $|S_i|$ *is small enough*

⋆ Consequence: One of $f(x_i^-)$ and $f(x_i^+)$ was computed previously. Only one evaluation per iteration is needed

⋆ $|S_N| = \lambda^{-N}|b_0 - a_0|$: same ratio as Fibonacci search

Other methods...

Parabolic approximation knowing the values of f at points a, b, c approximate f by a parabola and choose the next point as

$$x = b - \frac{1}{2}\frac{(b-a)^2(f(b)-f(c))-(b-c)^2(f(b)-f(a))}{(b-a)(f(b)-f(c))-(b-c)(f(b)-f(a))}$$

$\star$ this method converges fast if f is close to being quadratic

$\star$ in general, faster methods are combined with robust methods: if the fast method gives an aberrant result at the current iterate, run the robust method instead

Important drawback

⋆ when using zero-order methods we compare values of the function for different arguments: up to which precision can we detect such differences?
⋆ if f is smooth near the optimum x^* we have

$$f(x) \approx f(x^*) + \frac{1}{2} f''(x^*)(x - x^*)^2$$

⋆ if $0.5 f''(x^*)(x - x^*)^2 < \varepsilon f(x^*)$ where ε is the machine epsilon (typically around 10^{-16} for double precision) then numerically we don't see any difference between $f(x)$ and $f(x^*)$
⋆ in conclusion, the algorithm will not be able to tell the difference between $f(x)$ and $f(x^*)$ if

$$|x - x^*| \leq \sqrt{\varepsilon} |x^*| \sqrt{\frac{2|f(x^*)|}{(x^*)^2 |f''(x^*)|}}$$

⋆ in these cases (in practice, most of the time!), zero-order methods will not be able to obtain precision higher than $\sqrt{\varepsilon}$!!!

Conclusion - zero-order methods

- we may achieve linear convergence rate even with the simple trisection method
- it is important to minimize the number of function evaluations in order to minimize the computational cost of the methods
- with Fibonacci or Golden search we arrive at the best possible convergence ratio of $\lambda^{-1} = 0.61803...$
- if the number of function evaluations is known: use Fibonacci search
- else use Golden search: **one function evaluation per iteration**!

All of this is to be used when you can't compute the derivatives of f.
!!! As soon as you have access to the derivative, even the most basic algorithm is better than Fibonacci and Golden search, as we will see in the next section !!!

Optimization in dimension 1

- Methods of order zero (without derivatives)
- Methods of order one and above (with derivatives)

Using derivatives...

Assumptions: f is unimodal on $[a, b]$ and is smooth (admits as many derivatives as we want)
Suppose that x^* is a local minimum of f on $[a, b]$

Proposition 9 (Classical result - optimality conditions)

- *If* $x^* \in (a, b)$ *then* $f'(x^*) = 0$ *(x^* is a critical point)*
- *If* $x^* = a$ *then* $f'(x^*) \geq 0$
- *If* $x^* = b$ *then* $f'(x^*) \leq 0$

$\star$ The second and third conditions are called Euler inequalities

Towards an algorithm...

$\star$ Direct consequence of unimodality: if $a < x^* < b$ is the minimizer of f on $[a, b]$ then

$$f'(x) < 0 \text{ for } x \in [a, x^*) \quad \text{and} \quad f'(x) > 0 \text{ for } x \in (x^*, b]$$

$\star$ Therefore, if we choose one intermediary point $a < x_n < b$ then we know the position of x^* w.r.t. x_n by looking at $f'(x_n)$

$\star$ Note that, compared to zero-order methods, one intermediary point is enough in order to reduce the size of the search interval

Simplest algorithm

Algorithm 4 (Bisection)

Initialization: $S_0 = [a_0, b_0]$, $i = 1$

Loop:

- *choose* $x_i = 0.5(a_{i-1} + b_{i-1})$
- *compute* $f'(x_i)$
  - **if** $f'(x_i) < 0$ *then* $S_i = [x_i, b]$
  - **if** $f'(x_i) > 0$ *then* $S_i = [a, x_i]$
  - **if** $f'(x_i) = 0$ *then* $x^* = x_i$ *and* **stop**
- *replace* i *with* $i + 1$ *and continue until the desired precision is reached*

$\star$ the third option ($f'(x_i) = 0$ can (almost) never be verified numerically) when working with fixed machine precision for general functions f

Simplest algorithm

Algorithm 4 (Bisection)

Initialization: $S_0 = [a_0, b_0]$, $i = 1$
Loop:

- *choose* $x_i = 0.5(a_{i-1} + b_{i-1})$
- *compute* $f'(x_i)$
  - **if** $f'(x_i) \leq 0$ *then* $S_i = [x_i, b]$
  - **if** $f'(x_i) > 0$ *then* $S_i = [a, x_i]$
  - ~~**if** $f'(x_i) = 0$ *then* $x^* = x_i$ *and* **stop**~~
- *replace* i *with* $i + 1$ *and continue until the desired precision is reached*

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Convergence rate

Proposition 10

The Bisection algorithm converges linearly with ratio 0.5.

Proof: $|S_i| = 0.5|S_{i-1}|$ therefore

$$|x^* - x_N| \leq 0.5^N(b-a).$$

$\star$ Already better than the Fibonacci/Golden search algorithms.

$\star$ Is there a contradiction between the optimality of their claimed optimal rate/ratio of convergence and the result stated above?

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$\star$ Bisection method can be seen as a search for a zero of f'. For a general function f such that $f'(a)f'(b) \leq 0$ it will converge to a critical point of f

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$\star$ Bisection method can be seen as a search for a zero of f'. For a general function f such that $f'(a)f'(b) \leq 0$ it will converge to a critical point of f
$\star$ Can we reach machine precision using the bisection method? The answer is yes: we compare the values of f' with 0!

Further improvements...

⋆ all methods presented so far possess global linear convergence assuming that f is unimodal.

⋆ Can we hope for something better?

Further improvements...

⋆ all methods presented so far possess global linear convergence assuming that f is unimodal.

⋆ Can we hope for something better?

Use curve fitting: approximate f locally by a simple function with analytically computable minimum.

Basic ideas:

- for each iteration: a set of working points for which we compute the values and (eventually) the derivatives
- construct an approximating polynomial p
- find analytically the minimum of p and update the family of working points

First example: Newton's method

$\star$ suppose that given x we can compute $f(x), f'(x), f''(x)$

Algorithm 5 (Newton's method in dimension one)

Initialization: *Choose the starting point* x_0

Step i**:**

- *Compute* $f(x_{i-1}), f'(x_{i-1}), f''(x_{i-1})$ *and approximate* f *around* x_{i-1} *by its second-order Taylor expansion*

$$p(x) = f(x_{i-1}) + f'(x_{i-1})(x - x_i) + \frac{1}{2} f''(x_{i-1})(x - x_{i-1})^2.$$

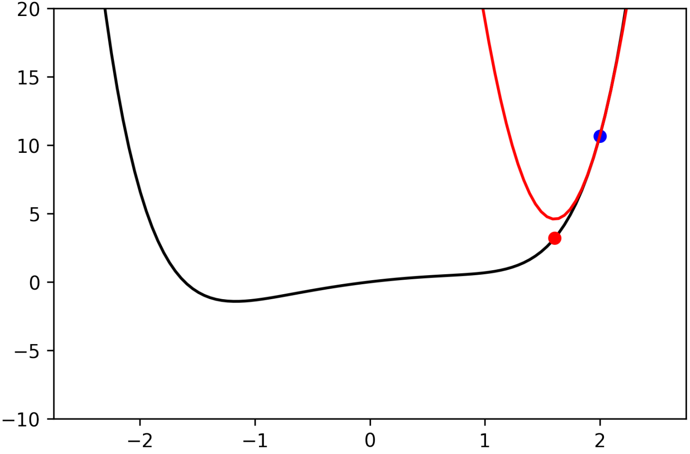
- *choose* x_i *as the critical point of the quadratic function* p*:*

$$x_i = x_{i-1} - \frac{f'(x_{i-1})}{f''(x_{i-1})}.$$

- *replace* i *with* $i+1$ *and loop*

Example

$f(x) = x^6/6 - x^2/2 + x$ on $[-2.5, 2.5]$, $x_0 = 2$.



Fast convergence...

Proposition 11

Let $x^* \in \mathbb{R}$ be a local minimizer of a smooth function f such that $f'(x^*) = 0$ and $f''(x^*) > 0$. Then the Newton method converges to x^* quadratically, provided that the starting point x_0 is close enough to x^*.

Fast convergence...

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Let $x^* \in \mathbb{R}$ be a local minimizer of a smooth function f such that $f'(x^*) = 0$ and $f''(x^*) > 0$. Then the Newton method converges to x^* quadratically, provided that the starting point x_0 is close enough to x^*.

All the hypotheses are essential!

- What happens for $f(x) = x^4$? Which hypothesis is not verified? Does the algorithm converge for every starting point x_0? What is the observed convergence rate of the algorithm?
- What happens for $f(x) = \sqrt{1+x^2}$? Does the algorithm converge for every starting point x_0?

Fast convergence...

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All the hypotheses are essential!

- What happens for $f(x) = x^4$? Which hypothesis is not verified? Does the algorithm converge for every starting point x_0? What is the observed convergence rate of the algorithm?
  Answer: $x^* = 0$, $f''(x^*) = 0$, $x_i = \frac{2}{3}x_{i-1}$. The convergence rate is linear.
- What happens for $f(x) = \sqrt{1+x^2}$? Does the algorithm converge for every starting point x_0?
  Answer: $x^* = 0$, $f''(x^*) > 0$, $x_i = -x_{i-1}^3$. The convergence rate is cubic when $|x_0| < 1$, but the algorithm does not converge at all for $|x_0| \geq 1$.

Proof ideas

- Denote $g = f'$ and observe that $g(x^*) = 0, g'(x^*) > 0$,
  $g(x^*) = g(x_i) + g'(x_i)(x^* - x_i) + \frac{1}{2}g''(\xi_i)(x^* - x_i)^2$
- Use $g(x^*) = 0$ and reformulate:
  $$\frac{g(x_i)}{g'(x_i)} + (x^* - x_i) = -\frac{g''(\xi_i)}{2g'(x_i)}(x^* - x_i)^2.$$
- Use the definition of the Newton iterations to see that
  $$x^* - x_{i+1} = \frac{-g''(\xi_i)}{2g'(x_i)}(x^* - x_i)^2.$$
- use the hypotheses to conclude!

Another point of view

⋆ Newton's method can be seen a linearization method for finding the zeros of $g = f'$.

⋆ Indeed, $g(x) = g(x_{i-1}) + g'(x_{i-1})(x - x_{i-1}) + o(|x - x_{i-1}|)$

⋆ Imposing that the linear part is zero amounts to

$$x = -\frac{g(x_{i-1})}{g'(x_{i-1})} + x_{i-1}$$

which is exactly the Newton method

Modified Newton: degenerate case

⋆ it is possible to show that when $f''(x^*) = 0$ then the rate of convergence is linear

⋆ if the multiplicity m of the root x^* of f' is known then the following modified Newton method converges quadratically (if it is well defined...)

$$x_{n+1} = x_n - m\frac{f'(x_n)}{f''(x_n)}.$$

⋆ in practice this does not really help: you don't know the multiplicity *a priori* for a general function f!

A second example: Regula Falsi

⋆ approximate f again by a quadratic polynomial
⋆ we consider two working points with first order information
⋆ given the two last iterates x_{i-1} and x_{i-2} we may approximate $f''(x_{i-1})$ using finite differences

$$f''(x_{i-1}) \approx \frac{f'(x_{i-1}) - f'(x_{i-2})}{x_{i-1} - x_{i-2}}$$

A second example: Regula Falsi

Algorithm 6 (False Position Method)

Initialization: *Choose the starting points* x_0, x_1.

Step $i \geq 2$**:**

- *Compute* $f(x_{i-1}), f'(x_{i-1}), f'(x_{i-2})$ *and approximate* f *around* x_{i-1} *with a second-order polynomial*

$$p(x) = f(x_{i-1}) + f'(x_{i-1})(x - x_i) + \frac{1}{2}\frac{f'(x_{i-1}) - f'(x_{i-2})}{x_{i-1} - x_{i-2}}(x - x_{i-1})^2.$$

- *choose* x_i *as the minimizer of the quadratic function* p*:*

$$x_i = x_{i-1} - f'(x_{i-1})\frac{x_{i-1} - x_{i-2}}{f'(x_{i-1}) - f'(x_{i-2})}.$$

- *replace* i *with* $i + 1$ *and loop*

Remarks

⋆ The method is symmetric with respect to x_{i-1} and x_{i-2}. It is equivalent to

$$x_i = x_{i-2} - f'(x_{i-2})\frac{x_{i-1} - x_{i-2}}{f'(x_{i-1}) - f'(x_{i-2})}$$

⋆ this can be viewed again as a search for a zero of $g = f'$: approximate f' by a straight line through points $(x_{i-1}, f'(x_{i-1}))$ and $(x_{i-2}, f'(x_{i-2}))$.

⋆ for a non degenerate minimizer x^* of a smooth function f $(f'(x^*) = 0,\ f''(x^*) > 0)$ and for x_0, x_1 close enough to x^* the method converges to x^* superlinearly with order of convergence

$$\lambda = (1 + \sqrt{5})/2.$$

⋆ the Regula Falsi method has a slower convergence rate than Newton's method, but it does not need the knowledge of the second derivative

Proof ideas

- **Lemma:** Let (r_n) be a sequence of positive reals verifying $r_{n+1} \leq r_n r_{n-1}$ for $n \geq 1$. If $r_0, r_1 \in (0,1)$ then
$$\text{there exists a constant } C > 0 \text{ such that } r_n \leq C r^{\lambda^n},$$
where $r \in (0,1)$ and $\lambda = \frac{\sqrt{5}+1}{2}$ is the golden ratio
- Show that the errors $e_n = |x^* - x_n|$ verify an inequality of the form
$$e_{n+1} \leq M e_n e_{n-1}.$$

Cubic fit

$\star$ consider two working points x_1 and x_2 with zero and first order information

$\star$ define the cubic polynomial such that

$$p(x_1) = f(x_1), p(x_2) = f(x_2), p'(x_1) = f'(x_1), p'(x_2) = f'(x_2)$$

$\star$ as the next iterate, choose the local minimizer of p.

$\star$ if x^* is non degenerate and the method starts sufficiently close to x^* then the method converges quadratically

$\star$ formulas: complicated, if you are interested, ask for references

$\star$ curve fitting is used with polynomials of small degree: we need to be able to compute analytically position of the minima: therefore, there is no point using approximating polynomials of degree higher than four!

Conclusion: curve fitting - towards descent methods

- when the algorithm works we achieve superlinear convergence
- the convergence results are local
- when applying these methods in the general case they might converge to a local maximum or a critical point
- What to do when these methods do not work?
  - alternate zero-order or bisection search methods with curve fitting (in cases where curve fitting gives iterates outside the desired search region)
  - at each iteration be sure to decrease the objective function using a line-search method

Descent direction in 1D

- if $f'(x) \neq 0$ there are only two options: go left or go right
- choose the direction $d \in \{-1, +1\}$ which decreases f.
- first order Taylor expansion:
$$f(x + \gamma d) = f(x) + \gamma d \cdot f'(x) + o(\gamma)$$
- if $d \cdot f'(x) < 0$ then if γ is small enough then
$$f(x + \gamma d) < f(x)$$

Examples when $f'(x) \neq 0$

1. $d = -f'(x)$
2. The Newton direction $d = -f'(x)/f''(x)$ is a descent direction if and only if $f''(x) > 0$.
3. The direction $d = -f'(x_{i-1})\frac{x_{i-1}-x_{i-2}}{f'(x_{i-1})-f'(x_{i-2})}$ from the Secant method is a descent direction if f is strictly convex.

Inexact line search

⋆ big question: how to choose a descent step?
⋆ the 1D reasoning will be useful in higher dimensions

Denote $q(t) = f(x + td)$ where d is a descent direction (with $d \in \{\pm 1\}$ in 1D or general in nD), sometimes called merit function.
⋆ Note that if d is a descent direction, then $q'(0) = d \cdot f'(x) < 0$

We perform a test for t, with three options

a) t is good
b) t is too big
c) t is too small

We should be able to answer these questions by looking at $q(t)$ and $q'(t)$.
⋆ perform an iterative process for constructing confidence interval $[t_l, t_r]$ for t
⋆ ideally the condition a) should be attained as quickly as possible!

Generic line-search algorithm

Algorithm 7 (Line-search)

Start with $t_l = 0, t_r = 0$ and pick an initial $t > 0$.

Iterate:

Step 1:

If *a) then exit: you found a good t*

If *b) then $t_r = t$: you found a new upper bound for t*

If *c) then $t_l = t$: you found a new lower bound for t*

Step 2:

If *no valid t_r exists we choose a new $t > t_l$, like $t = 2t_l$ (extrapolation step)*

Else *choose a new $t \in (t_l, t_r)$, like $t = 0.5(t_l + t_r)$ (interpolation step)*

- ⋆ a), b), c) should form a partition of $\mathbb{R}_+$
- ⋆ if t is big enough c) should be false
- ⋆ each interval $[t_l, t_r]$ should contain a non-trivial sub-interval verifying a)

Armijo's rule

- ⋆ $m_1 \in (0,1)$ and $\eta > 1$ are chosen constants.
- ⋆ we fix an initial choice of $t = t_0$ (for example $t = 1$)
- ⋆ recall that $q'(0) < 0$

a) $\dfrac{q(t)-q(0)}{t} \leq m_1 q'(0) \iff q(t) \leq q(0) + t(m_1 q'(0))$ (t is good)

b) $m_1 q'(0) < \dfrac{q(t)-q(0)}{t} \iff q(t) > q(0) + t(m_1 q'(0))$ (t is too big, $t_r = t$)

c) never

- ⋆ if t is too big, then the next t is chosen as t/η (a popular choice is $\eta = 2$).

Proposition 12

Suppose that q is of class C^1 and $q'(0) < 0$. Then the line-search with Armijo's rule finishes in a finite number of steps.

Armijo's rule may lead to slow convergence: we choose once and for all a **maximal step**.

Goldstein-Price rule

⋆ $m_1 < m_2 \in (0,1)$ are chosen constants

⋆ recall that $q'(0) < 0$

a) $m_2 q'(0) \leq \frac{q(t)-q(0)}{t} \leq m_1 q'(0)$
$\iff q(0) + t(m_2 q'(0)) \leq q(t) \leq q(0) + t(m_1 q'(0))$ (good t)

b) $m_1 q'(0) < \frac{q(t)-q(0)}{t} \iff q(t) > q(0) + t(m_1 q'(0))$ (t is too big)

c) $\frac{q(t)-q(0)}{t} < m_2 q'(0) \iff q(t) < q(0) + t(m_2 q'(0))$ (t is too small)

Proposition 13

Suppose that $q \in C^1$ is bounded from below and $q'(0) < 0$. Then the line-search with the Goldstein-Price rule finishes in a finite number of steps.

⋆ What about the choice of the constants m_1, m_2?

Wolfe rule

⋆ $m_1 < m_2 \in (0,1)$ are chosen constants
⋆ recall that $q'(0) < 0$

a) $\frac{q(t)-q(0)}{t} \leq m_1 q'(0)$ and $q'(t) \geq m_2 q'(0)$ (good t)

b) $\frac{q(t)-q(0)}{t} > m_1 q'(0)$ (t is too big)

c) $\frac{q(t)-q(0)}{t} \leq m_1 q'(0)$ and $q'(t) < m_2 q'(0)$ (t is too small)

Proposition 14

Suppose that $q \in C^1$ is bounded from below and $q'(0) < 0$. Then the line-search with the Wolfe rule finishes in a finite number of steps.

⋆ The condition on $q'(t)$ is called curvature condition. Wolfe's rule is widely used in line-search algorithms: it gives good convergence properties
⋆ the first condition in a) assures that the value of f decreases while the second assures that the slope reduces
⋆ What about the choice of the constants m_1, m_2?

The quadratic case

Proposition 15

Suppose that q is quadratic with minimum t^*: $q(t) = (x - t^*)^2 + a$. Then: $q'(t) = 2(x - t^*)$ and $q(t^*) = q(0) + \frac{1}{2}q'(0)t^*$.

⋆ we should not refuse the optimal step when q is quadratic!

$$\frac{q(t^*) - q(0)}{t^*} = \frac{1}{2}q'(0).$$

Armijo: $\frac{1}{2}q'(0) \leq m_1 q'(0)$
Goldstein-Price: $m_2 q'(0) \leq \frac{1}{2}q'(0) \leq m_1 q'(0)$
Wolfe: $\frac{1}{2}q'(0) \leq m_1 q'(0)$ and $q'(t^*) \geq m_2 q'(0)$

In conclusion it is recommended to:

⋆ choose $m_1 < 0.5$ (for Armijo, Goldstein-Price and Wolfe)
⋆ choose $0.5 < m_2 < 1$ (for Goldstein-Price)

Finally...

Algorithm 8 (Generic gradient descent algorithm)

Initialization: *Choose an initial point* x_0 *and the eventual parameters for the line-search algorithm*

Step i:

- *compute the function value* $f(x_{i-1})$ *and the derivative* $f'(x_{i-1})$
- *perform the line-search algorithm in order to find a descent step* t.
- *choose the next iterate*

$$x_i = x_{i-1} - tf'(x_{i-1}).$$

Stopping criterion: $|f'(x_i)|$ *is small,* $|f(x_{i-1}) - f(x_i)|$ *is small, the descent step* t *is too small, maximum number of iterations reached, etc.*

⋆ $f'(x_{i-1})$ can be replaced with any descent direction d.

⋆ various simplified variants exist: fixed descent step, variable descent step

⋆ the generalization to higher dimensions is straightforward

Convergence rate?

$\star$ it is a order 1 algorithm so *a priori* we cannot expect more than linear convergence
$\star$ if $f(x) = x^2$ and we use a fixed step algorithm then the update at each iteration is

$$x_i = x_{i-1} - tf'(x_{i-1}) = (1-2t)x_{i-1}.$$

therefore, for $t < 0.5$ we have linear convergence to the optimum.
$\star$ the function $f(x) = x^2$ is strictly convex and quadratic: the ideal case. Therefore we cannot expect something better.
$\star$ locally, around a minimizer x^* the function f is convex. Therefore, if convergence is proved for convex functions, it will follow, that locally, around the minimizer, the convergence of GD is linear

Example of global convergence result

Proposition 16 (Convergence rate for the gradient descent with fixed step)

Suppose that $f : \mathbb{R} \to \mathbb{R}$ is of class C^2 with f' Lipschitz continuous on $\mathbb{R}$: there exists $M > 0$ such that

$$|f'(x) - f'(y)| \leq M|x - y|, \ \forall x, y \in \mathbb{R}.$$

Moreover, suppose that f is α-strictly convex ($f''(x) \geq \alpha > 0$) and that f is ∞ at infinity (so that a minimizer exists).
Then the Gradient Descent algorithm with fixed step t converges to the minimum linearly when t is small enough.

Proof: Define the application $\mathcal{F} : \mathbb{R} \to \mathbb{R}$

$$\mathcal{F}(x) = x - tf'(x)$$

and prove that for t small enough $\mathcal{F}$ is a contraction:

$$|\mathcal{F}(x) - \mathcal{F}(y)| \leq k|x - y|, \quad k \in (0, 1).$$

$\star$ then we know that the fixed point iteration $x_{n+1} = \mathcal{F}(x_n)$ converges to the unique fixed point, which is exactly the optimum.

Example of local result

Proposition 17 (Local convergence rate)

Suppose that $f : [a, b] \to \mathbb{R}$ is unimodal and has a unique minimizer x^* in $[a, b]$. Then if f is of class C^2 and $f''(x^*) > 0$ the gradient descent algorithm with fixed step t converges linearly to x^* if t is chosen small enough and x_0 is close enough to x^*.

⋆ Taylor expansion for f' around x^* gives a recurrence relation for the error!

⋆ the condition $f''(x^*) > 0$ cannot be ommited: degenerate minimizers will lead to sublinear rate of convergence. Example $f(x) = x^4$.

⋆ using more involved techniques, it is possible to prove that the gradient descent always converges to a local minimizer, with an eventual sublinear rate of convergence

⋆ various convergence results can be formulated when using line-search procedures instead of a fixed step: guaranteeing descent is essential for convergence

⋆ Wolfe's rule gives good convergence results!

Improve the speed of convergence

$\star$ we saw that Newton's method or the Secant method give superlinear convergence under the right hypotheses, but they offer no guarantee of convergence

$\star$ modify the gradient descent algorithm by changing the descent direction:

$$x_{i+1} = x_i + \gamma d_i$$

where d_i is either

- $-f'(x_i)/f''(x_i)$ (if $f''(x_i) > 0$)
- $-f'(x_i)\frac{x_i - x_{i-1}}{f'(x_i) - f'(x_{i-1})}$ (if this is indeed a descent direction)

$\star$ combine this with a line-search procedure with initial step size $t = 1$.
$\star$ the new algorithm will eventually attain a superlinear rate of convergence provided we can choose the step $\gamma = 1$ for all iterations $i \geq n_0$

$\star$ this idea is useful in higher dimensions where the family of descent directions is richer

Conclusions - optimization in dimension one

- there are efficient zero-order algorithms (when derivatives are not available)
- as soon as derivatives can be computed, the convergence is accelerated
- curve-fitting methods give increased convergence rates, but they are sensitive to the initialization
- line-search procedures play an important role even in higher dimensions
- inexact line-search: sometimes searching for an optimum is not the main objective but attaining a significant decrease in the objective function is enough
- gradient descent algorithms (almost) always converge to a local minimzer, but the rate of convergence is linear at best