Computational Maths 2

Introduction to Numerical Optimization

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What this course is about?

- theoretical aspects in optimization
- algorithms for numerical optimization
- implementation of optimization algorithms

Objectives

After this course you should:

1. know the basic optimization algorithms: gradient descent, Newton, etc.
2. implement optimization algorithms for problems of reasonable size
3. translate the contents of a problem into an optimization algorithm
4. know how to use existing libraries in order to solve particular classes of optimization problems

Grading

- 50%: evaluation of your work during practical sessions
  - activity points: at the end of each session you should provide a working Python code related to the current Exercise Sheet and show it to the instructor
  - solving Challenge or Supplementary exercises (in addition to the main exercises) will give you bonus points
- 50%: final test during the last practical session
  - work on a given problem: answer some theoretical questions and solve some implementation tasks
  - you are allowed to use all resources available (course notes, personal notes, etc.)

What is optimization?

⋆ given an objective function $x \mapsto f(x)$, find the value(s) of x which give the smallest value of f!

⋆ x may be subjected to some constraints

⋆ often the minimizer x^* may not be found explicitly: numerical simulations are needed in this context

⋆ numerical optimization algorithms produce a sequence (x_n) defined iteratively using the values of f and possibly its derivatives.

⋆ various questions arise concerning the sequence of iterates:

- the convergence of the sequence (x_n) to a minimizer of f
- the speed of convergence

Basic examples

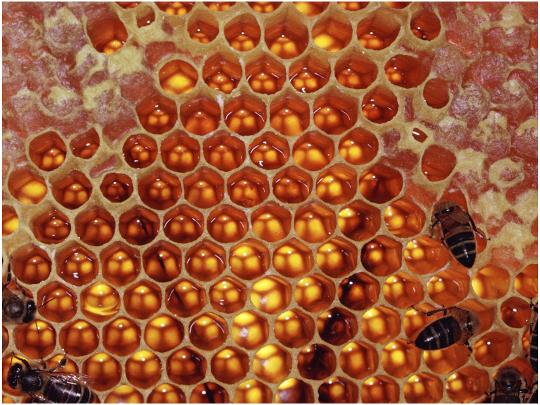
1. Minimize $\frac{1}{2}x^T Ax - b^T x$ where $A \in \mathcal{M}_{m\times n}, x \in \mathbb{R}^n, b \in \mathbb{R}^m$ with $m > n$.

2. Minimize $c \cdot x$ where $c, x \in \mathbb{R}^n$, $x \geq 0$, $Ax \leq b$ (linear programming problem)

3. Model fitting: Given a set of data points (x_i, y_i), $1 \leq i \leq N$ find a function F such that $F(x_i) \approx y_i$.

4. Neural networks: tune machine learning algorithms in order to fit existing data in an optimal way.

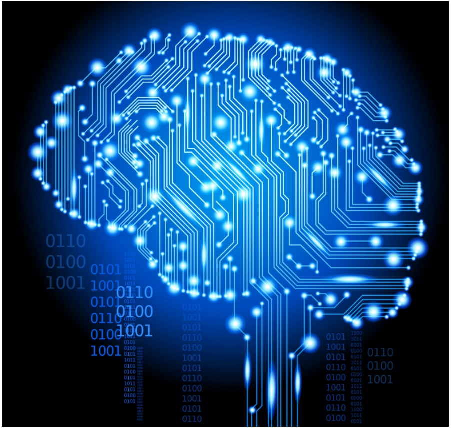
- Honeycombs are optimal in terms of construction cost (mathematical understanding came only recently: Thomas C. Hales (1999))



Examples in Nature

- Soap bubbles tend to minimize the surface area while keeping a fixed volume

- finance, deep learning: process existing information in order to take the best decisions (photo `rostigrabench.ch`)



- Optimal design of structures: reduce the weight while maintaining the desired mechanical properties

Motivation...

- for practical applications, optimization algorithms are used: analytic solutions are not available for complex optimization problems
- the user should formulate an optimization problem starting from the given data or models
- once a function which associates a real value to a certain set of parameters is known, optimization algorithms can be used to search for the minimum
- the methods of optimization are vast
  - gradient-free vs gradient based methods
  - higher order methods (Newton)
- the choice of the method depends on the objective function: unimodal functions (nice), highly oscillating functions, non-smooth functions, etc.
- often some constraints need to be enforced, which complicate the theoretical and numerical aspects of optimization problems

Objective of the course

$\star$ present the theory and practice of the basic optimization algorithms
$\star$ underline possible advantages and pitfalls of the optimization algorithms studied: there is no universal algorithm!

Contents of the course

1. General aspects in optimization
2. Optimization in dimension 1
    - Methods of order zero (without derivatives)
    - Methods of order one and two (using derivatives)
3. Optimization in higher dimensions
    - Gradient descent methods
    - Newton methods
    - quasi-Newton methods
4. Constrained optimization
    - Lagrange multipliers
    - a quick glimpse of linear programming (emphasis on practical issues)

Optimization: general aspects

- The discrete case
- Continuous optimization

General optimization problem

In the following: $\mathcal{A}$ is a non-void set, J is a real function defined on $\mathcal{A}$.

Canonical formulation

Let $J : \mathcal{A} \to \mathbb{R}$ be a real function. We wish to solve the problem

$$\min_{x \in \mathcal{A}} J(x)$$

Question: what about maximization problems?

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$$\min_{x \in \mathcal{A}} J(x)$$

Remark: Note that maximization problems are also included in this framework

$$\max_{x \in \mathcal{A}} J(x) = -\left(\min_{x \in \mathcal{A}} -J(x)\right).$$

Remark 2: The rigorous way is to write inf instead of min when we don't know that a solution exists in $\mathcal{A}$.

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Questions:

- how do we deal with optimization problems in terms of $\mathcal{A}$? (discrete vs continuous case)
- when do we have a solution? what are the conditions for $\mathcal{A}$ and J?

Optimization: general aspects

- The discrete case
- Continuous optimization

$\mathcal{A}$ is finite

$\mathcal{A} = \{x_1, x_2, ..., x_N\}$ so J takes the values

$$\{J(x_1), J(x_2), ..., J(x_N)\}.$$

Questions:

- what about existence of solutions?
- if a solution exists, how do you find it?

$\mathcal{A}$ is finite

$\mathcal{A} = \{x_1, x_2, ..., x_N\}$ so J takes the values

$$\{J(x_1), J(x_2), ..., J(x_N)\}.$$

- if $\mathcal{A}$ is finite, we always have existence of solutions!
- the difficulty of finding the optimal value among $J(x_i)$ depends on multiple factors:
  - how big is N?
  - how fast can you compute $J(x_i)$?
  - is there some underlying structure which can help us get to the solution faster?

Example 1: Optimal assignment problem

Let's say we have the following situation:

	Person 1	Person 2	Person 3
Job 1	100€	120€	80€
Job 2	150€	110€	120€
Job 3	90€	80€	110€

Questions:

1. What is the optimal assignment: Job $i \longrightarrow$ Person j?

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1. What is the optimal assignment: Job $i \longrightarrow$ Person j?
2. What is the cost of the naïve implementation in terms of the number of persons?

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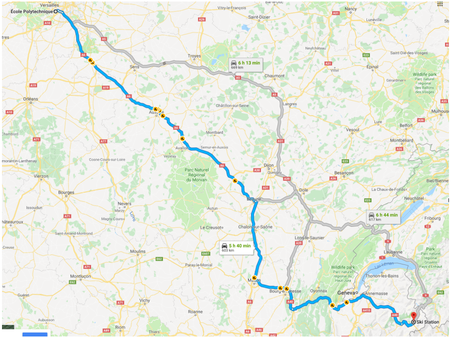
Questions:

1. What is the optimal assignment: Job $i \longrightarrow$ Person j?
2. What is the cost of the naïve implementation in terms of the number of persons? Answer: $O(n!)$
3. Is there a better algorithm? Yes: Hungarian algorithm with complexity $O(n^3)$.

   Reference: link

Dijkstra's algorithm: intelligently find the optimal path going through the branches of your graph



Reference: link

Conclusion on the discrete part

- Discrete optimization problem: finite number of configurations $\longrightarrow$ existence of solutions
- That does not mean that we can always find the optimal solution in reasonable computation time
- We will not talk about discrete optimization in the rest of the course.

Optimization: general aspects

- The discrete case
- Continuous optimization

$\mathcal{A}$ is an infinite subset of $\mathbb{R}^n$

Again, we wish to study the problem

$$\inf_{x\in\mathcal{A}} J(x)$$

Question: Under what classical hypotheses on $\mathcal{A}$ and J can we conclude that the above problem has a solution?

Again, we wish to study the problem

$$\inf_{x\in\mathcal{A}} J(x)$$

Answer

If $\mathcal{A}$ is compact and J is continuous then the infimum is reached for some $x_0 \in \mathcal{A}$:

$$\text{there exists } x_0 \in \mathcal{A} \text{ such that } J(x_0) = \min_{x\in\mathcal{A}} J(x)$$

Examples and counterexamples

1. $\mathcal{A} = \{\frac{1}{n} : n \in \mathbb{N}^*\},\ J(x) = x$
   Issue: If $\mathcal{A}$ is disconnected, how do we choose between its different connected components???
   In the rest of the course, in the one dimensional and higher dimensional case, we always assume $\mathcal{A}$ is connected
2. $\mathcal{A} = (0,1],\ f(x) = x^2$
3. $\mathcal{A} = [0,1],\ f(x) = \begin{cases} -1/x & x > 0 \\ 0 & x = 0 \end{cases}$

Assumptions

In the following we assume that the function we minimize J is regular of class C^k ($k \geq 1$) and the set $\mathcal{A}$ is the closure of an open and connected set (unless otherwise stated)

⋆ **Advantage w.r.t. discrete case:** we use information given by the values of the function J and its derivatives in order to decide how to improve the value of $J(x)$.
⋆ We can advance with increments which are arbitrarily small in order to decrease J: this is not possible if $\mathcal{A}$ is not open and connected

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 $f(x^*) \leq f(x)$ 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 $f(x^*) \geq f(x)$ for every $x \in (x^* - \varepsilon, x^* + \varepsilon)$
3. x^* is a global minimum of f on K if $f(x^*) \leq f(x)$ for every $x \in K$
4. x^* is a global maximum of f on K if $f(x^*) \geq f(x)$ 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...

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

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

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:

$$f'(x^*) = 0 \text{ and } f''(x^*) > 0 \implies x^* \text{ is a local minimum of } f.$$

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

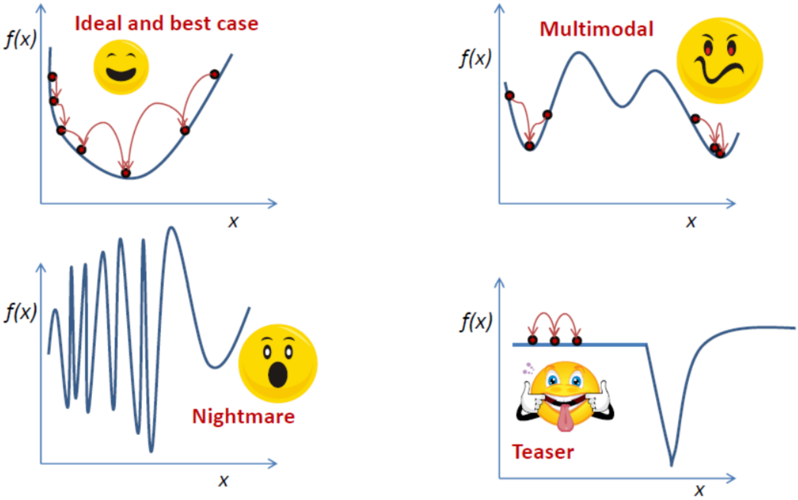
Example of optimization algorithm

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)

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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$\star$ 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: $f(x^-) \leq f(x^+) \Rightarrow$ 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: $\lim_{i\to\infty} (r_{i+1}/r_i) = 0$
- 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

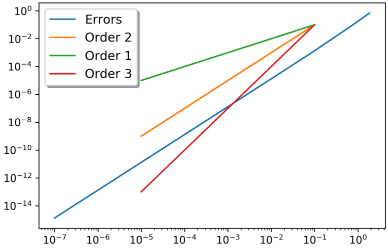
For the convergence of order p we have $r_{i+1} \approx C r_i^p$.

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

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

$\star$ 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.

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

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

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

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

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

$\star$ this is the best we can do in a given number of iterations
[J. Kiefer, *Sequential minimax search for a maximum*]

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What algorithm do you use to compute F_n given n?

Fun fact - computing Fibonacci numbers

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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:

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Complexity: $O(\log n)$

⋆ Exponentiation is very fast if done properly: search for "exponentiation by squaring" or "fast exponentiation" if you are interested
⋆ 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 $F_n \approx \frac{1}{\sqrt{5}}\lambda^{n+1}$

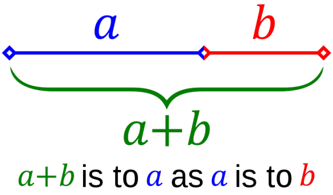
$\star$ in NumPy you will quickly go beyond the 16 digit precision: there is no need to be extremely efficient...

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*

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

$\star$ $|S_N| = \lambda^{-N}|b_0 - a_0|$: 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

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 !!!