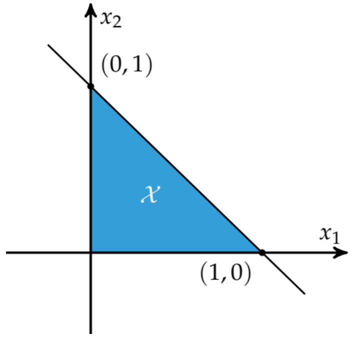
Tecnológico Nacional de México

Instituto Tecnológico de Orizaba/Celaya

Modern Computing Algorithms for Process Optimization with Julia Programming. Part I



“3 -Bracketing”

By:

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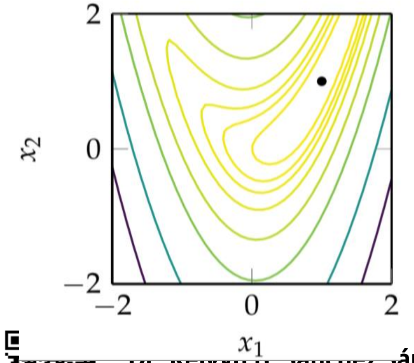
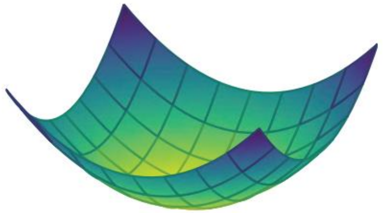
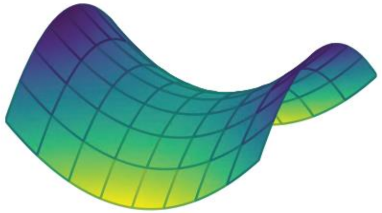
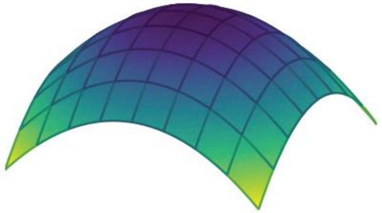
Postdoctoral Researcher/I.T. Celaya









Bracketing

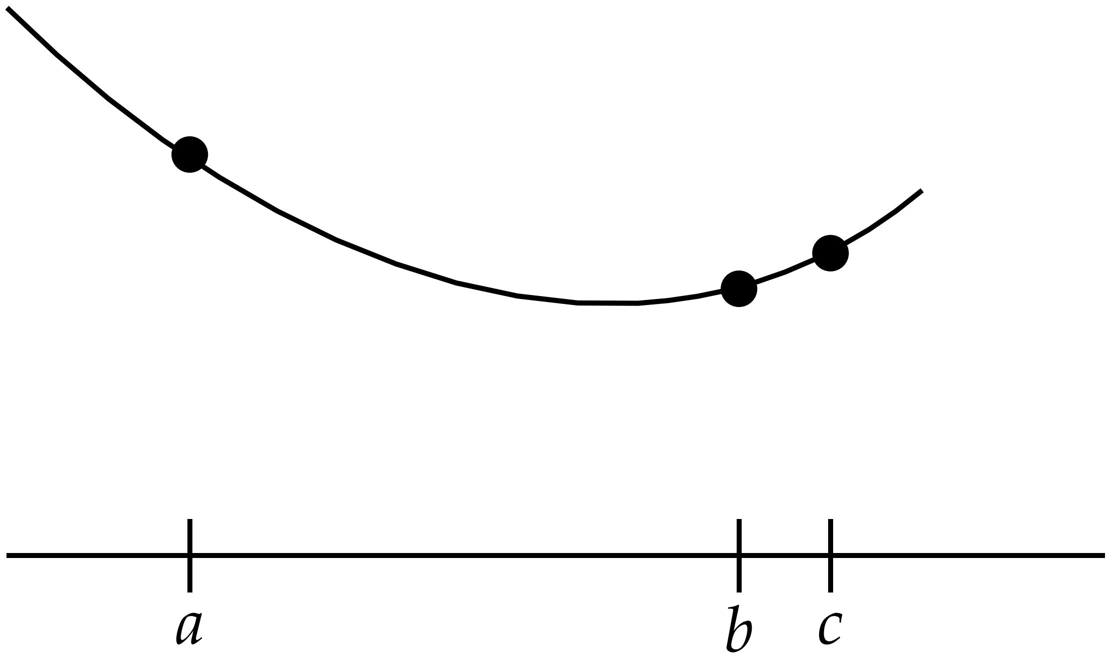
- Identifying an interval containing a local minimum and then successively shrinking that interval

Unimodality

- There exists a unique optimizer $\mathbf{x}^*$ such that f is monotonically decreasing for $\mathbf{x} \leq \mathbf{x}^*$ and monotonically increasing for $\mathbf{x} \geq \mathbf{x}^*$

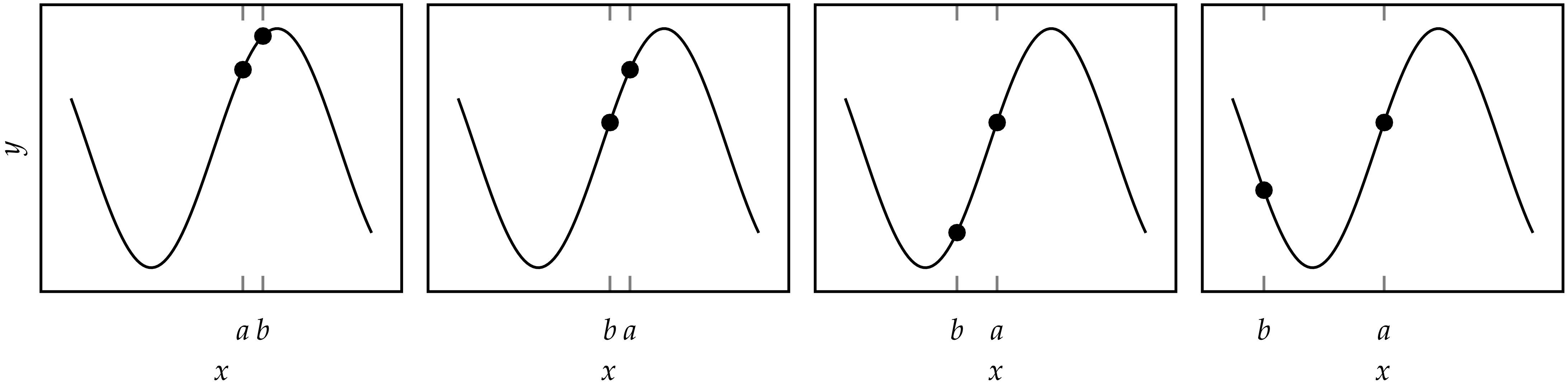
Finding an Initial Bracket

- Given a unimodal function, the global minimum is guaranteed to be inside the interval [a,c] if $f(a) > f(b) < f(c)$



Finding an Initial Bracket

- Example bracketing sequence



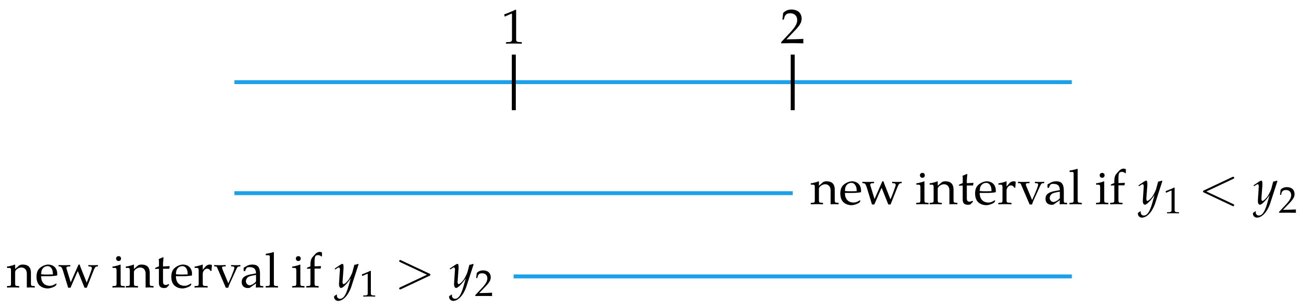
See example 3.1.ipynb

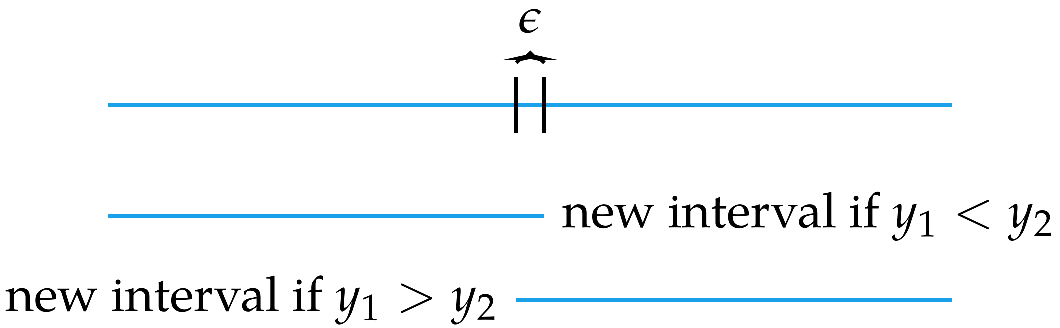
Fibonacci Search

- When function evaluations are limited, the Fibonacci Search algorithm is guaranteed to maximally shrink the bracketed interval

Fibonacci Search

- When restricted to two function evaluations, compare





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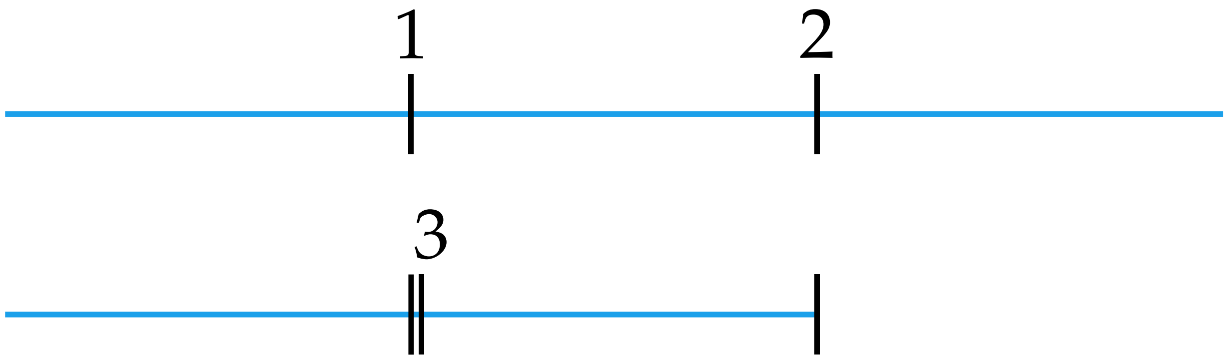
Fibonacci Search

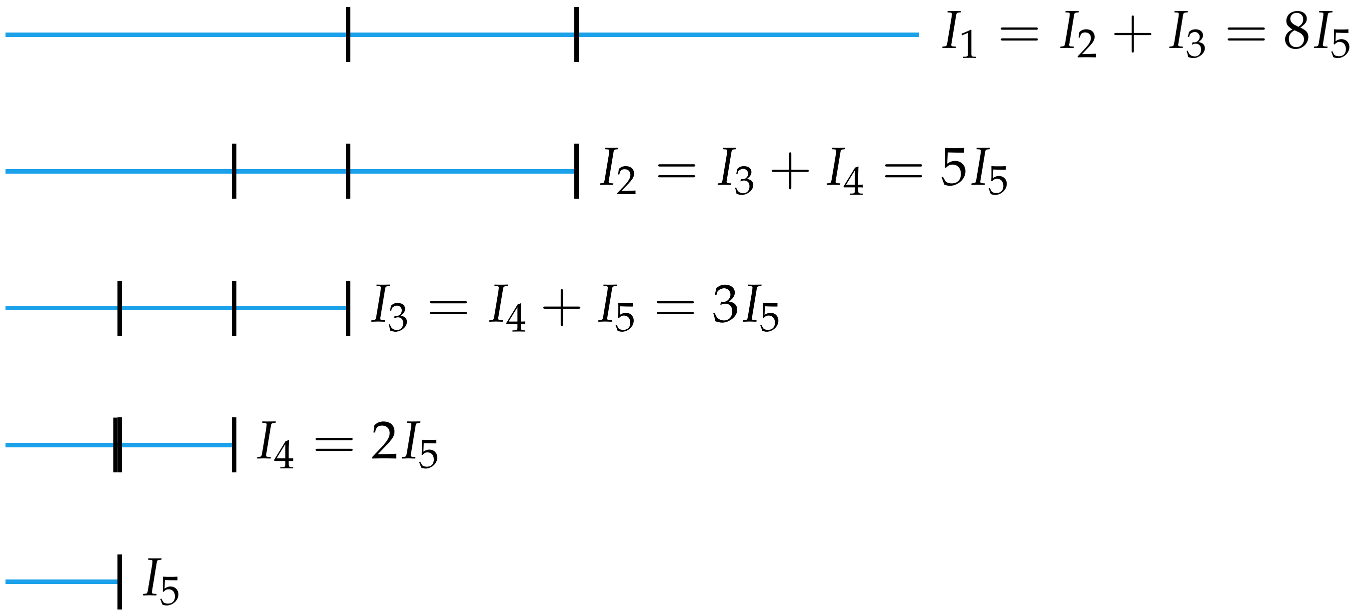
- When restricted to three function evaluations



Fibonacci Search

- When restricted to n function evaluations

$$F_n = \begin{cases} 1 & \text{if } n \leq 2 \\ F_{n-1} + F_{n-2} & \text{otherwise} \end{cases}$$



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Fibonacci Search

- Binet's formula defines a Fibonacci number analytically where ϕ is the Golden Ratio, ϕ=(1+$\sqrt{5})/2 \approx 1.61803$

$$F_n = \frac{\varphi^n - (1-\varphi)^n}{\sqrt{5}},$$

- The ratio between successive Fibonacci numbers is

$$\frac{F_n}{F_{n-1}} = \varphi \frac{1 - s^{n+1}}{1 - s^n}$$

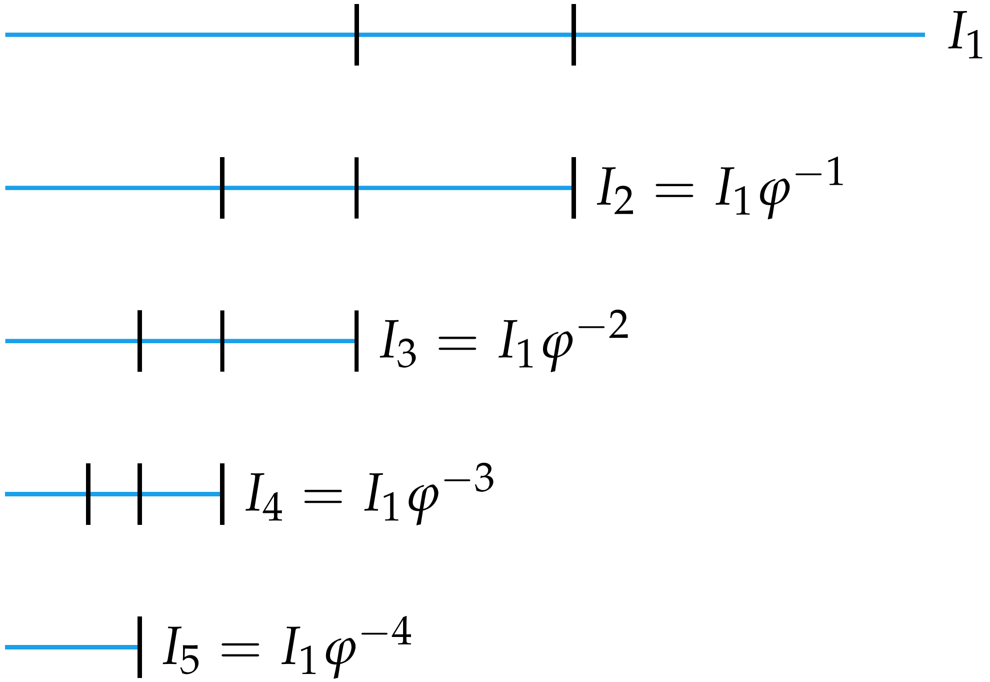
where $s = \frac{1-\sqrt{5}}{1+\sqrt{5}} \approx -0.382$

See example 3.2.ipynb

Golden Section Search

- In the limit of large *N*, the ratio of successive Fibonacci numbers approaches the Golden Ratio, so φ can be used to perform approximate Fibonacci search

$$\lim_{n \to \infty} \frac{F_n}{F_{n-1}} = \varphi$$



See example 3.3.ipynb

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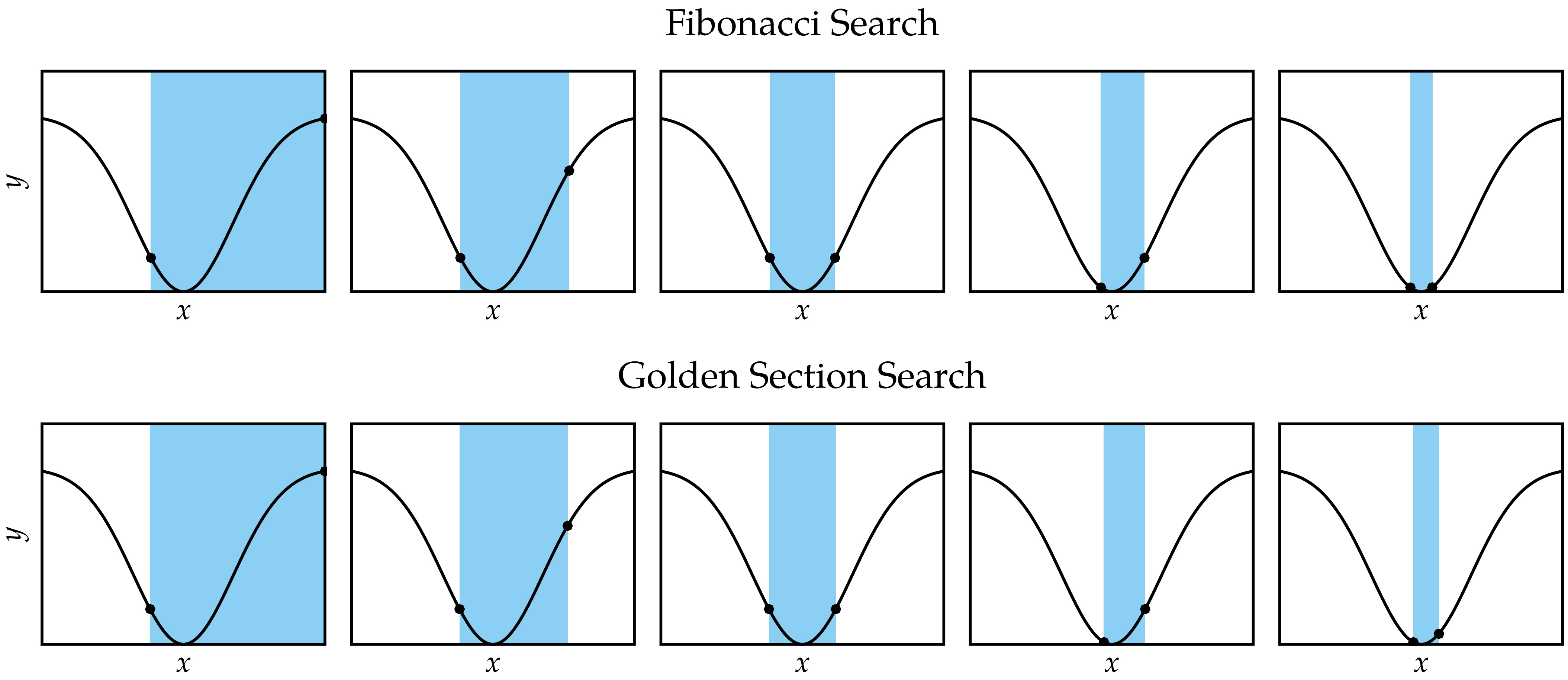
Fibonacci/Golden Section Search Comparison



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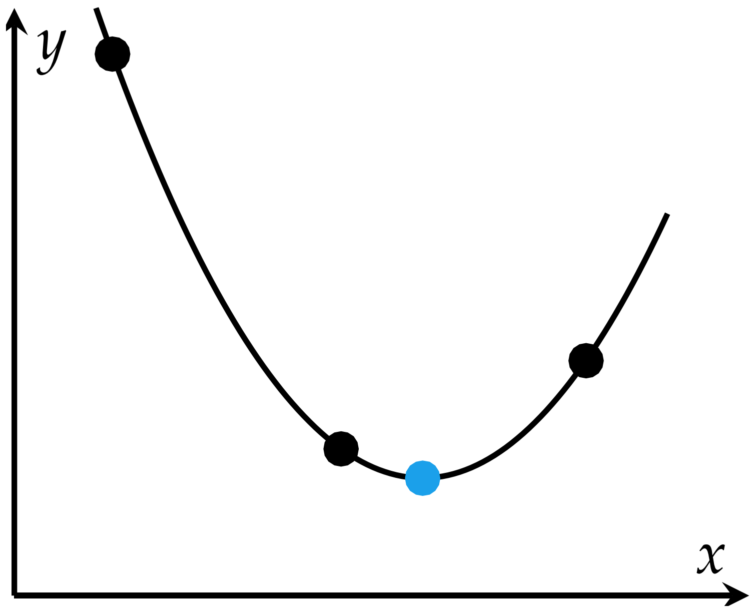
Quadratic Fit Search

- Leverages ability to analytically minimize quadratic functions
- Iteratively fits quadratic function to three bracketing points



Quadratic Fit Search

$$q(x) = p_1 + p_2 x + p_3 x^2$$
$$y_a = p_1 + p_2 a + p_3 a^2$$
$$y_b = p_1 + p_2 b + p_3 b^2$$
$$y_c = p_1 + p_2 c + p_3 c^2$$

$$\begin{bmatrix} y_a \\ y_b \\ y_c \end{bmatrix} = \begin{bmatrix} 1 & a & a^2 \\ 1 & b & b^2 \\ 1 & c & c^2 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

$$\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} 1 & a & a^2 \\ 1 & b & b^2 \\ 1 & c & c^2 \end{bmatrix}^{-1} \begin{bmatrix} y_a \\ y_b \\ y_c \end{bmatrix}$$

Quadratic Fit Search

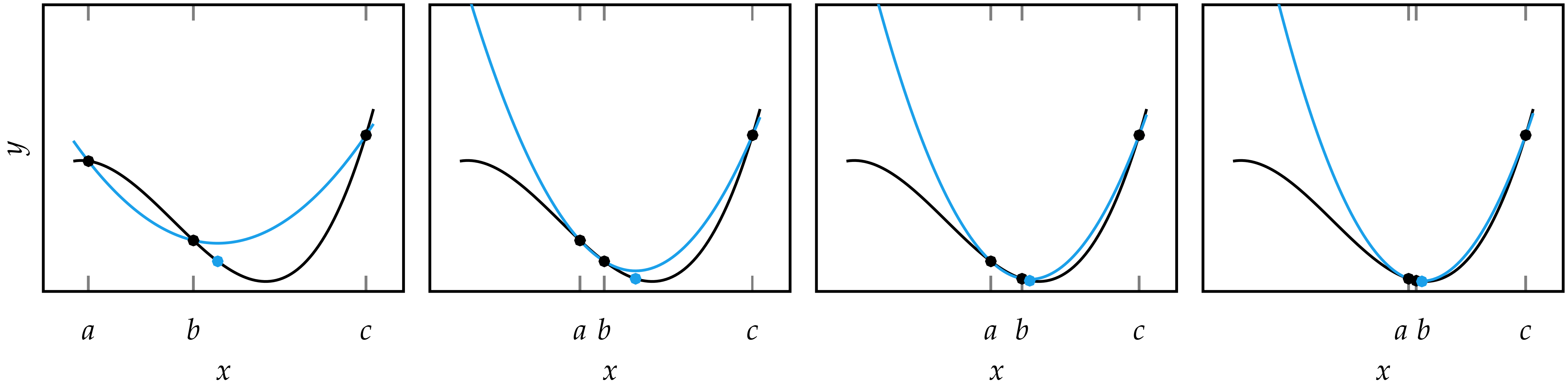
$$q(x) = y_a \frac{(x-b)(x-c)}{(a-b)(a-c)} + y_b \frac{(x-a)(x-c)}{(b-a)(b-c)} + y_c \frac{(x-a)(x-b)}{(c-a)(c-b)}$$

$$x^* = \frac{1}{2} \frac{y_a(b^2-c^2) + y_b(c^2-a^2) + y_c(a^2-b^2)}{y_a(b-c) + y_b(c-a) + y_c(a-b)}$$

See example 3.4.ipynb

Quadratic Fit Search

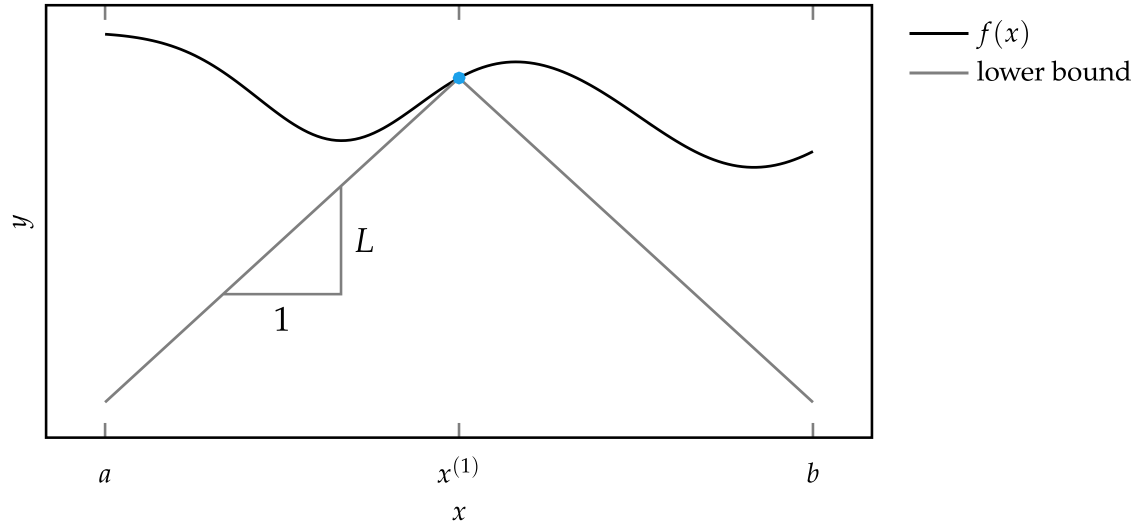
- If a function is locally nearly quadratic, the minimum can be found after several steps

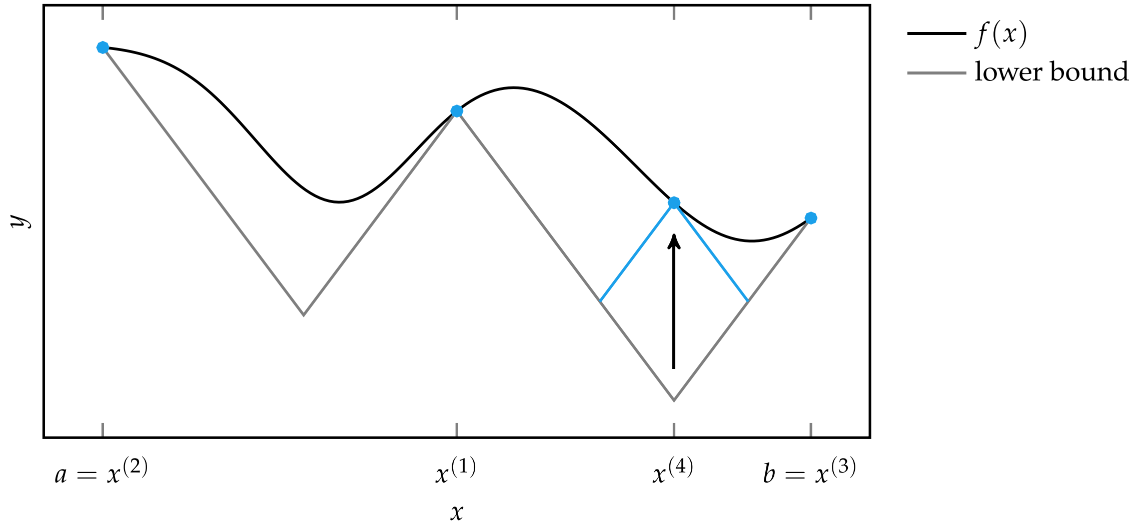


See example 3.5.ipynb

Shubert-Piyavskii Method

- Guaranteed to find the global minimum of any bounded function
- Requires the function be Lipschitz continuous





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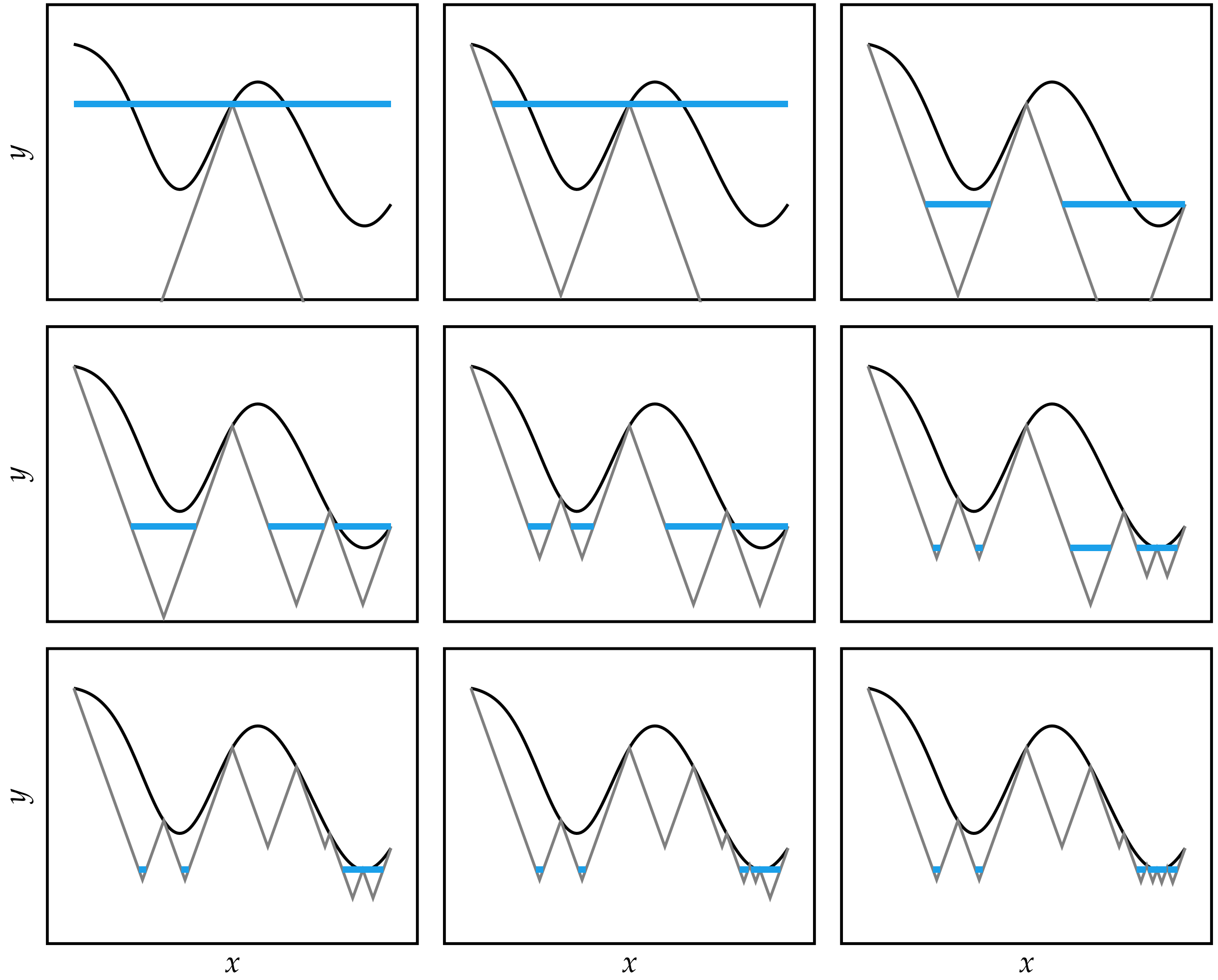
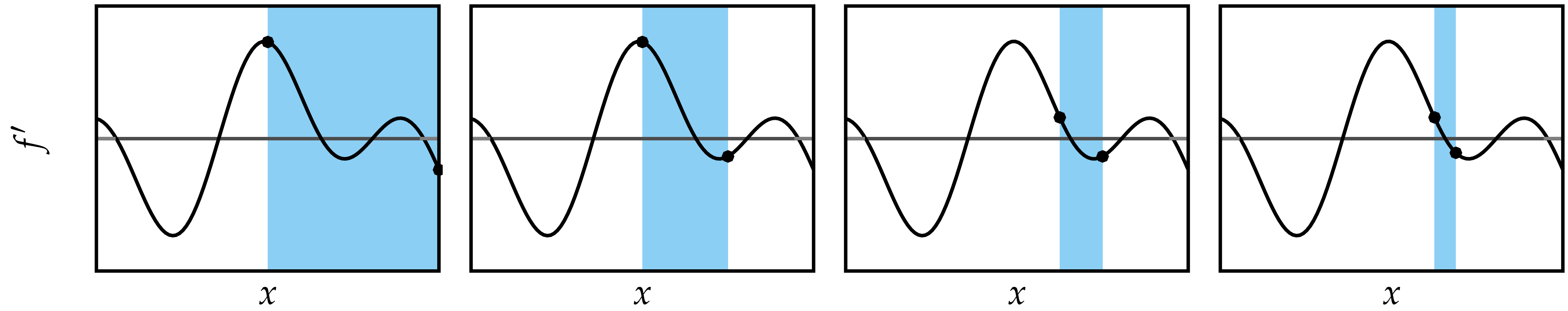
See example 3.6 & 3.7.ipynb

Shubert-Piyavskii Method



Bisection Method

- Used in root-finding methods
- When applied to $f'(x)$, can be used to find minimum



See example 3.8.ipynb

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Summary

- Many optimization methods shrink a bracketing interval, including Fibonacci search, golden section search, and quadratic fit search
- The Shubert-Piyavskii method outputs a set of bracketed intervals containing the global minima, given the Lipschitz constant
- Root-finding methods like the bisection method can be used to find where the derivative of a function is zero