AI505

Optimization

Bracketing

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Outline

Solutions and Recognizing Them for Smooth Functions

Definition

A point $\boldsymbol{x}^*$ is a global minimizer if $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x}$.

Definition

A point $\boldsymbol{x}^*$ is a local minimizer if there is a neighborhood N of $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x})$ for all $\boldsymbol{x} \in N$.

Solutions and Recognizing Them for Smooth Functions

Theorem (Taylor's Theorem)

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ *is continuously differentiable and that* $\boldsymbol{p} \in \mathbb{R}^n$*. Then we have that*

$$f(\boldsymbol{x} + \boldsymbol{p}) = f(\boldsymbol{x}) + \nabla f(\boldsymbol{x} + t\boldsymbol{p})^T \boldsymbol{p},$$

for some $t \in (0, 1)$*. Moreover, if* f *is twice continuously differentiable, we have that*

$$\nabla f(\boldsymbol{x} + \boldsymbol{p}) = \nabla f(\boldsymbol{x}) + \int_0^1 \nabla^2 f(\boldsymbol{x} + t\boldsymbol{p})\boldsymbol{p} dt,$$

and that

$$f(\boldsymbol{x} + \boldsymbol{p}) = f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \boldsymbol{p} + \frac{1}{2}\boldsymbol{p}^T \nabla^2 f(\boldsymbol{x} + t\boldsymbol{p})\boldsymbol{p},$$

for some $t \in (0, 1)$*.*

Solutions and Recognizing Them for Smooth Functions

Theorem (First-Order Necessary Conditions)

If $\boldsymbol{x}^*$ is a local minimizer and f is continuously differentiable in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$.

Definition

We call $\boldsymbol{x}^*$ a stationary point if $\nabla f(\boldsymbol{x}^*) = 0$.

Theorem (Second-Order Necessary Conditions)

If $\boldsymbol{x}^*$ is a local minimizer of f and $\nabla^2 f$ exists and is continuous in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite.

Theorem (Second-Order Sufficient Conditions)

Suppose that $\nabla^2 f$ is continuous in an open neighborhood of $\boldsymbol{x}^*$ and that $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive definite. Then $\boldsymbol{x}^*$ is a strict local minimizer of f.

Theorem

When f is convex, any local minimizer $\boldsymbol{x}^*$ is a global minimizer of f. If in addition f is differentiable, then any stationary point $\boldsymbol{x}^*$ is a global minimizer of f.

Unconstrained Optimization of Smooth Functions

Two main strategies for finding local minima of smooth functions are:

- Line search methods (gradient descent and its variants)
- Trust region methods

A component of both strategies is the ability to find a local minimum of a one-dimensional function, which is the topic of this lecture.

Bracketing: A derivative-free method to identify an interval containing a local minimum and then successively shrinking that interval

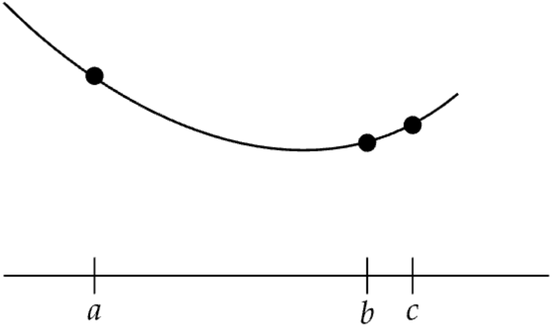
Unimodality

The algorithms in this class assume **unimodality**:

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

Finding an Initial Bracket

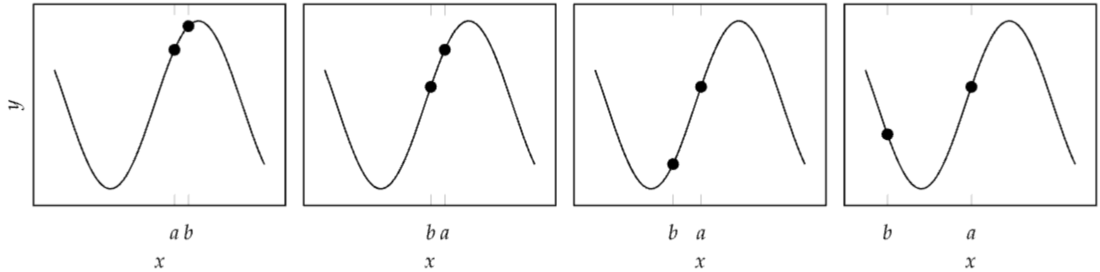
Given a unimodal function, the global minimum is guaranteed to be inside the interval $[a, c]$ if we can find three points $a < b < c$ such that $f(a) > f(b) < f(c)$




```
function bracket_minimum(f, x=0; s=1e-2, k=2.0)
    a, ya = x, f(x)
    b, yb = a + s, f(a + s)
    if yb > ya
        a, b = b, a
        ya, yb = yb, ya
        s = -s
    end
    while true
        c, yc = b + s, f(b + s)
        if yc > yb
            return a < c ? (a, c) : (c, a)
        end
        a, ya, b, yb = b, yb, c, yc
        s *= k
    end
end
```

Finding an Initial Bracket

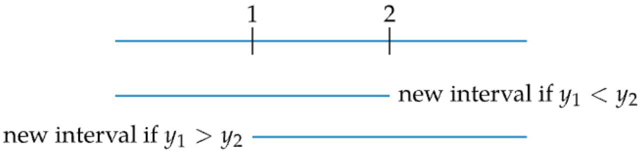
Example of `bracket_minimum` on a function



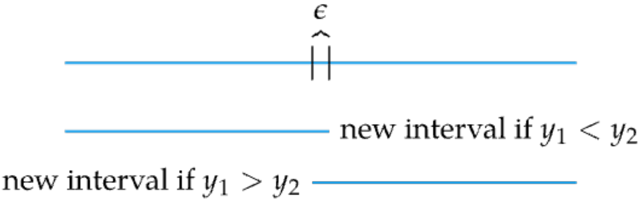
reverses direction between the first and second iteration and expands until a minimum is bracketed in the fourth iteration.

For unimodal functions, when function evaluations are limited, what is the maximal shrinckage we can achieve?

When restricted to only 2 function evaluations (queries) the most we can guarantee to shrink our interval is by just under a factor of 2.

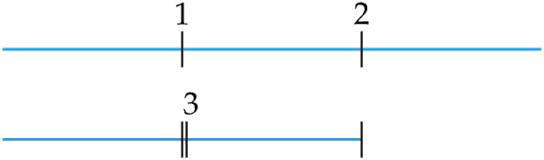


yeilds a factor of 3.



for $\epsilon \to 0$ yields a factor of just less than 2

When restricted to only 3 function evaluations (queries) the most we can guarantee to shrink our interval is by a factor of 3.

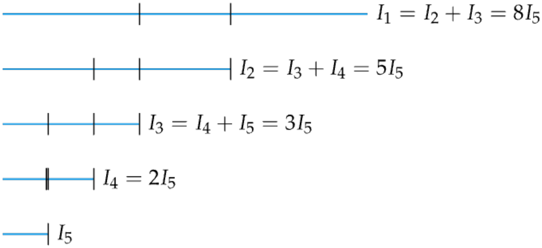


Fibonacci Search

When restricted to n functions evaluations following the previous strategy, we are guaranteed to shrink our interval by a factor of F_{n+1}.

Fibonacci numbers: sum of previous two,
$1, 1, 2, 3, 5, 8, 13, \dots$

$$F_n = \begin{cases} 0 & \text{if } n = 0 \\ 1 & \text{if } n = 1, 2 \\ F_{n-1} + F_{n-2} & \text{otherwise} \end{cases}$$



The length of every interval constructed can be expressed in terms of the final interval times a Fibonacci number.
- final, smallest interval has length I_n,
- second smallest interval has length $I_{n-1} = F_3 I_n$
- third smallest interval has length $I_{n-2} = F_4 I_n$,
and so forth.

Fibonacci Search Algorithm

For a unimodal function f in the interval $[a, b]$, we want to shrink the interval within n iterations. (At each iteration we want to shrink by a factor ϕ).

$$b_{k+1} - a_{k+1} = \frac{F_{n-k+1}}{F_{n-k+2}}(b_k - a_k)$$

Therefore:

$$\begin{aligned} b_n - a_n &= \frac{F_2}{F_3}(b_{n-1} - a_{n-1}) \\ &= \frac{F_2}{F_3}\frac{F_3}{F_4}\cdots\frac{F_n}{F_{n+1}}(b_1 - a_1) \\ &= \frac{1}{F_{n+1}}(b_1 - a_1) \end{aligned}$$

Closed-form expression (Binet's formula):

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

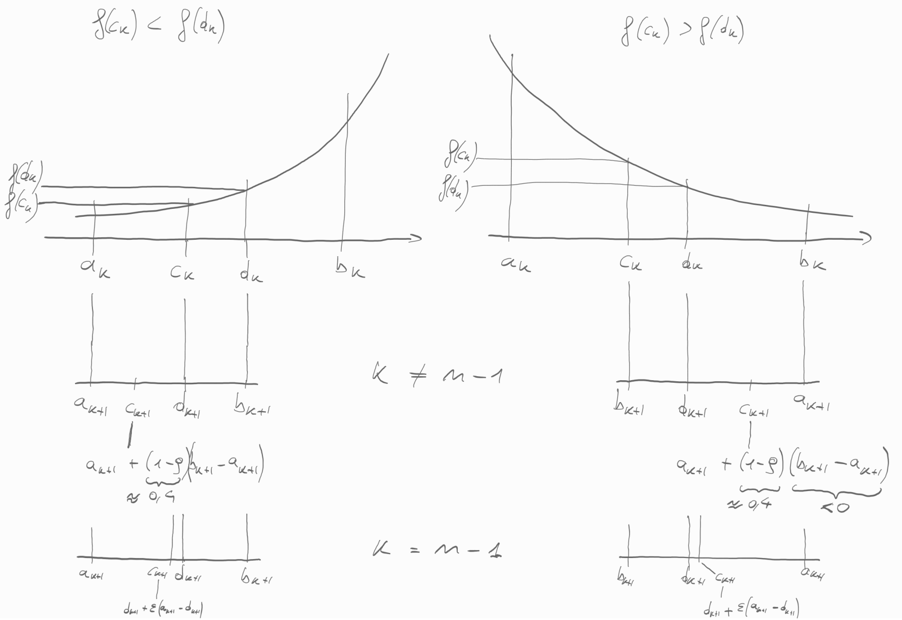
$\phi = (1+\sqrt{5})/2 \approx 1.61803$ is the golden ratio.

$$\frac{F_{n+1}}{F_n} = \phi\frac{1 - s^{n+1}}{1 - s^n}, \quad s = (1-\sqrt{5})(1+\sqrt{5}) \approx -0.38$$

Suppose we have a unimodal function f in the interval $[a, b]$ and a tolerance $\epsilon = 0.01$. Let $k = 1$.

$$\frac{F_n}{F_{n+1}} = \rho_n = \frac{1 - s^n}{\phi(1 - s^{n+1})} \approx 0.6$$

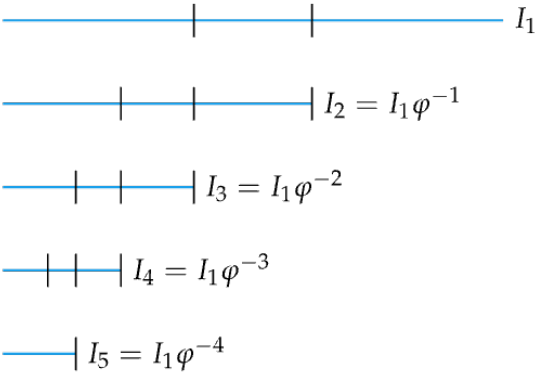
1. $d_k = a_k + \frac{F_{n-k+1}}{F_{n-k+2}}(b_k - a_k)$
2. if $k \neq n - 1$:
$$c_k = a_k + \left(1 - \frac{F_{n-k+1}}{F_{n-k+2}}\right)(b_k - a_k)$$
   otherwise: $c_k = d_k + \epsilon(a_k - d_k)$
3. if $f(c_k) < f(d_k)$: $\quad b_{k+1} = d_k, \quad d_{k+1} = c_k, \quad a_{k+1} = a_k$
   otherwise: $a_{k+1} = b_k, \quad b_{k+1} = c_k, \quad d_{k+1} = d_k$
4. $k = k + 1$, if $k = n$ go to step 5, else go to step 2
5. return (a_k, b_k) if $(a_k < b_k)$ else (b_k, a_k)



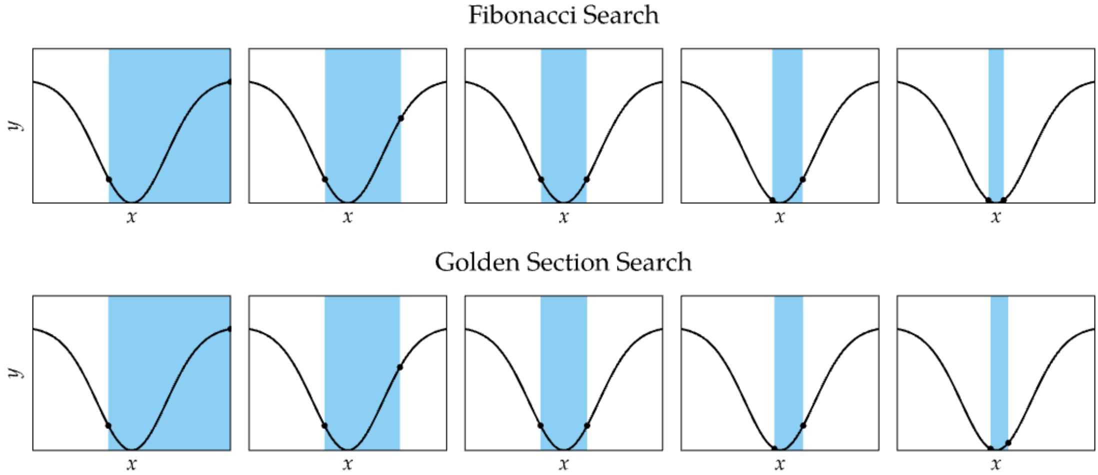
f(c_k) < f(d_k)
f(c_k) > f(d_k)
f(d_k)
f(c_k)
a_k
c_k
d_k
b_k
a_k
c_k
d_k
b_k
f(c_k)
f(d_k)
a_{k+1}
c_{k+1}
d_{k+1}
b_{k+1}
k ≠ n − 1
b_{k+1}
d_{k+1}
c_{k+1}
a_{k+1}
a_{k+1} + (1 − ρ)(b_{k+1} − a_{k+1})
≈ 0,4
a_{k+1} + (1 − ρ)(b_{k+1} − a_{k+1})
≈ 0,4
< 0
k = n − 1
a_{k+1}
c_{k+1}
d_{k+1}
b_{k+1}
d_{k+1} + ε(a_{k+1} − d_{k+1})
b_{k+1}
d_{k+1}
c_{k+1}
a_{k+1}
d_{k+1} + ε(a_{k+1} − d_{k+1})

Golden Section Search

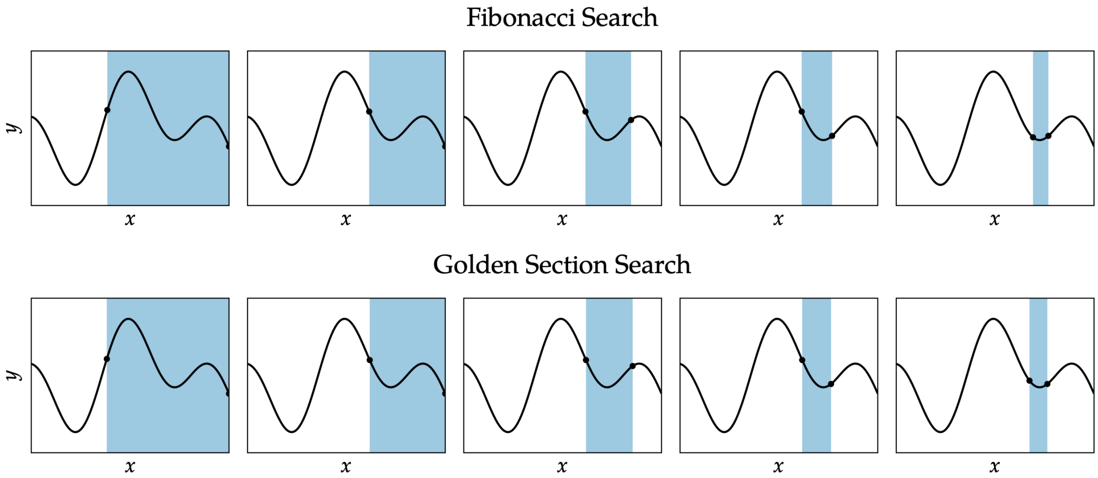
$$\lim_{n\to\infty} \frac{F_{n+1}}{F_n} = \lim_{n\to\infty} \frac{1}{\rho_n} = \lim_{n\to\infty} \phi \frac{1-s^{n+1}}{1-s^n} = \phi \approx 1.61803 \qquad \frac{1}{\phi} \approx 0.618$$



Comparison

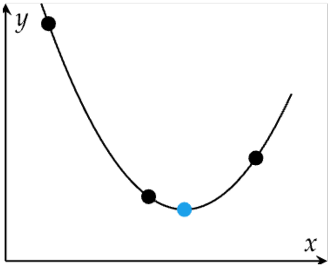


Comparison



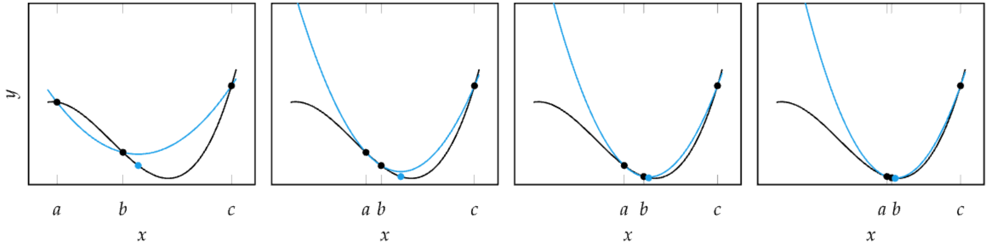
Quadratic Fit Search

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



Quadratic Fit Search

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



Maintain a bracketing interval $[a, c]$ with $a < b < c$ and $f(a) > f(b) < f(c)$.

```
if x > b
  if yx > yb
    c, yc = x, yx
  else
    a, ya, b, yb = b, yb, x, yx
```

```
elif x < b
  if yx > yb
    a, ya = x, yx
  else
    c, yc, b, yb = b, yb, x, yx
```

Using Linear Algebra

- We assume that the variable y is related to $x \in \mathbb{R}$ quadratically, so for some constants b_0, b_1, b_2:

$$y = b_0 + b_1 x + b_2 x^2$$

- Given the set of 3 points $(y_1, x_1,), \ldots, (y_3, x_3)$ in the ideal case, we have that $y_i = b_0 + b_1 x_i + b_2 x_i^2$, for all $i = 1, 2, 3$. In matrix form:

$$\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

This can be written as $A\boldsymbol{z} = \boldsymbol{y}$ to emphasize that $\boldsymbol{z}$ are our unknowns and A and $\boldsymbol{y}$ are given.

In Python

In polynomial regression, the $m \times (n+1)$ matrix A is called a **Vandermonde matrix** (a matrix with entries $a_{ij} = x_i^{n+1-j}$, $j = 1..n+1$).
NumPy's `np.vander()` is a convenient tool for quickly constructing a Vandermonde matrix, given the values $x_i, i = 1..m$, and the number of desired columns $(n+1)$.

```
>>> print(np.vander([2, 3, 5], 2))
[[2 1]                              # [[2**1, 2**0]
 [3 1]                              #  [3**1, 3**0]
 [5 1]]                             #  [5**1, 5**0]]

>>> print(np.vander([2, 3, 5, 4], 3))
[[ 4  2  1]                         # [[2**2, 2**1, 2**0]
 [ 9  3  1]                         #  [3**2, 3**1, 3**0]
 [25  5  1]                         #  [5**2, 5**1, 5**0]
 [16  4  1]]                        #  [4**2, 4**1, 4**0]
```

In Python

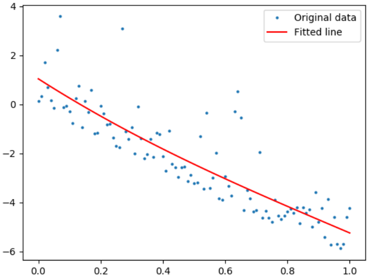
```
A = np.vander(x,4)

coeff = np.linalg.solve(A,y) ## Error!! Why?

B = A.T @ A
z = np.linalg.inv(B) @ A.T @ y

coeff = np.linalg.lstsq(A, y)[0]
np.allclose(z,coeff)

f=np.poly1d(coeff)
plt.plot(x, y, 'o', label='Original data', ↪
    ↪markersize=2)
plt.plot(x, f(x), 'r', label='Fitted line')
plt.legend()
plt.show()
```



However, for three points the system $Az = y$ is solvable, also in closed form!

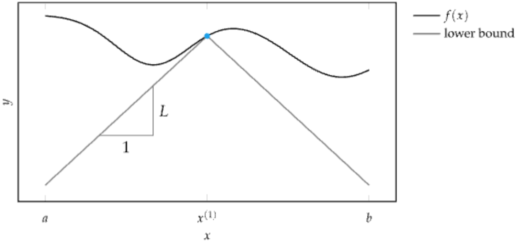
Shubert-Piyavskii Method

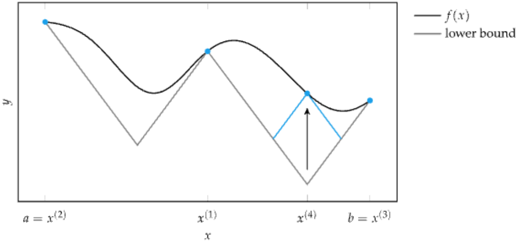
- The Shubert-Piyavskii method is guaranteed to find the global minimum of any bounded function

- but requires that the function be Lipschitz continuous

- A function is **Lipschitz continuous** if there is an upper bound on the magnitude of its derivative. A function f is Lipschitz continuous on $[a, b]$ if there exists an $\ell > 0$ such that:

$$|f(x) - f(y)| \leq \ell |x - y|, \quad \forall x, y \in [a, b]$$





The Algorithm

Given a valid Lipschitz constant ℓ and an initial interval $[a, b]$:

Initialize:
Sample the midpoint, $x^{(1)} = (a + b)/2$.
Construct a sawtooth lower bound using lines of slope $\pm\ell$ from $x^{(1)}$. These lines will always lie below f if ℓ is a valid Lipschitz constant

Iterate:
Upper vertices in the sawtooth correspond to sampled points. Lower vertices correspond to intersections between the Lipschitz lines originating from each sampled point.
Further iterations find the minimum point in the sawtooth $(x^{(i)}, y^{(i)})$, evaluate the function at that $x^{(i)}$ value, $f(x^{(i)})$, and then use the result to update the sawtooth.

Terminate:

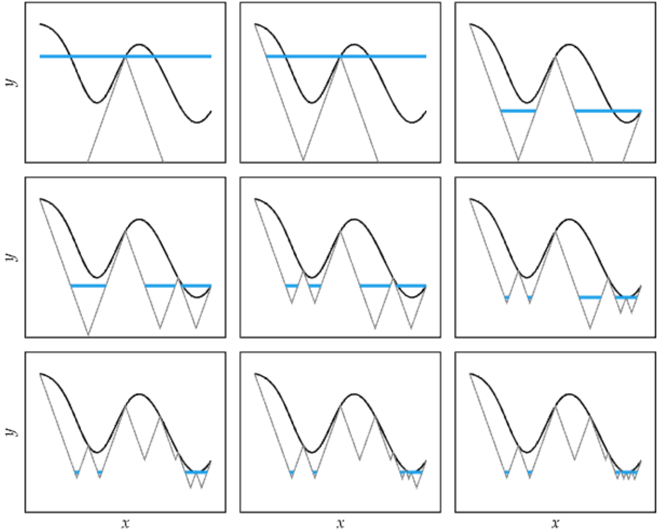
when: $|y^{(i)} - f(x^{(i)})| < \epsilon$.

For every peak, an uncertainty region (blue segments) can be computed according to:

$$\left[x^{(i)} - \frac{1}{\ell}\left(y_{\min} - y^{(i)}\right),\right.$$
$$\left. x^{(i)} + \frac{1}{\ell}\left(y_{\min} - y^{(i)}\right)\right]$$

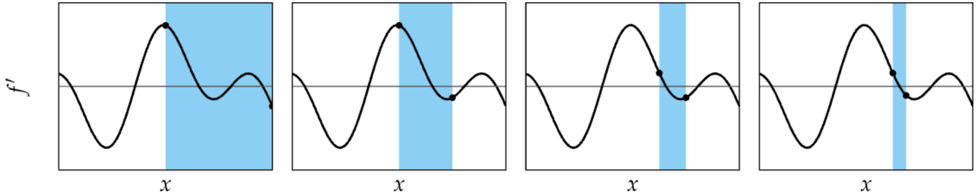
$\left(x^{(i)}, y^{(i)}\right)$ sawtooth lower vertex

$\left(x_{\min}, y_{\min}\right)$ minimum sawtooth upper vertex



Bisection Method

- **Intermediate value theorem**: If f is continuous on $[a, b]$, and there is some $y \in [f(a), f(b)]$, then there exists at least one $x \in [a, b]$, such that $f(x) = y$.
- Used in root-finding methods
- When applied to $f'(x)$, can be used to find minimum of f
- if $\text{sign}(f'(a)) \neq \text{sign}(f'(b))$, or equivalently, $f'(a)f'(b) \leq 0$ then $[a, b]$ is guaranteed to contain a zero.



Bisection Method

- Cut the bracketed region $[a, b]$ in half with every iteration
- Evaluate the midpoint $(a + b)/2$
- form a new bracket from the midpoint and whichever side that continues to bracket a zero.
- Terminate after a fixed number of iterations.
- Guaranteed to converge within ϵ of x^* within $\lg_2(|b - a|/\epsilon)$

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