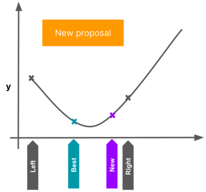
Optimization in Machine Learning

Univariate optimization
Golden ratio



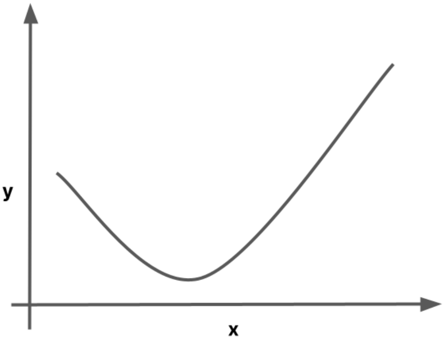
Learning goals

- Simple nesting procedure
- Golden ratio

UNIVARIATE OPTIMIZATION

Let $f : \mathbb{R} \to \mathbb{R}$.

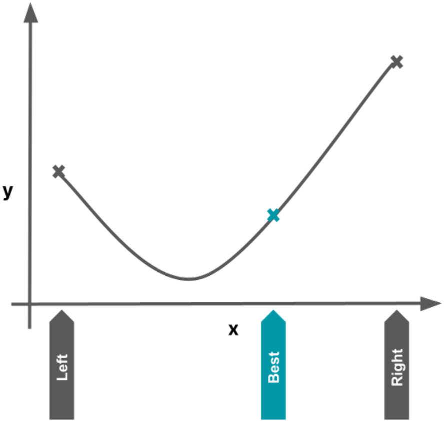
Goal: Iteratively improve eval points. Assume function is unimodal. Will not rely on gradients, so this also works for black-box problems.



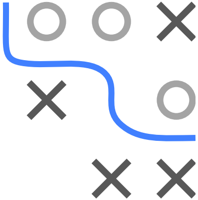
SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

Always maintain three points: left, right, and current best.

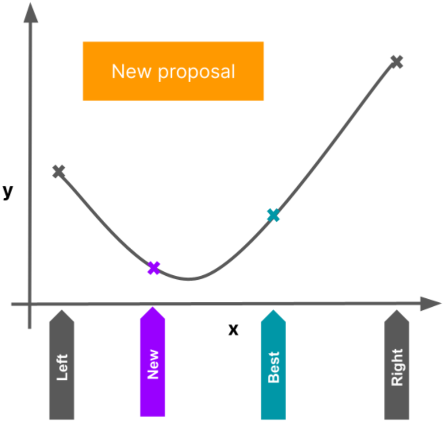


SIMPLE NESTING PROCEDURE



Let $f : \mathbb{R} \to \mathbb{R}$.

Propose random point in interval.

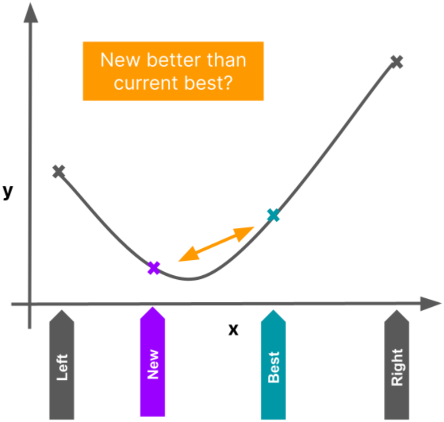


NB: Later we will define the optimal choice for a new proposal.

SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

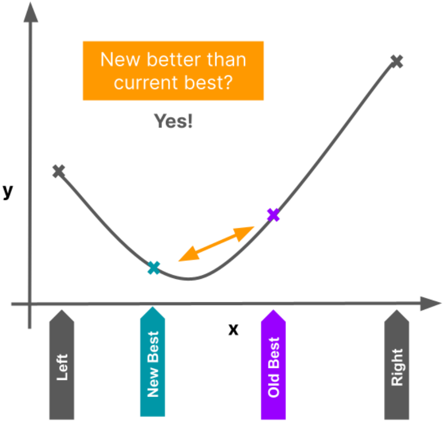
Compare proposal against current best.

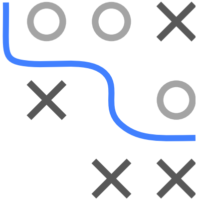


SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

If it is better: proposal becomes current best.

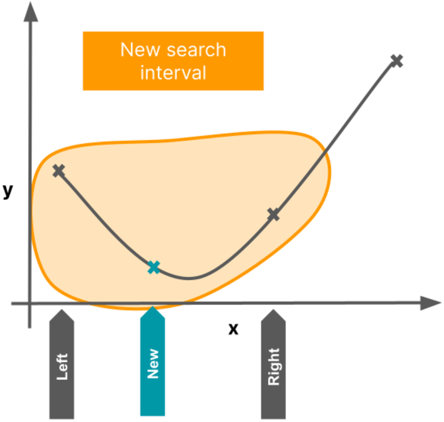


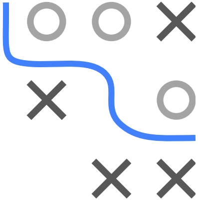


SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

New search interval: around current best.

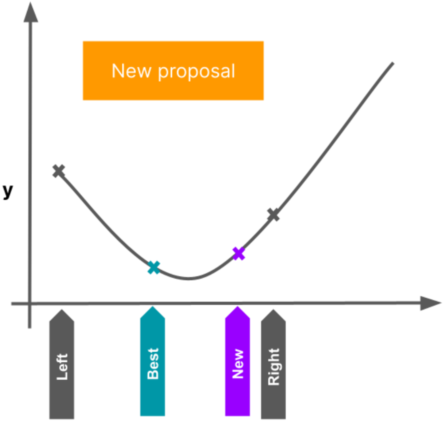


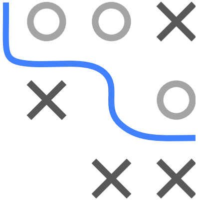


SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

Propose a random point.





SIMPLE NESTING PROCEDURE

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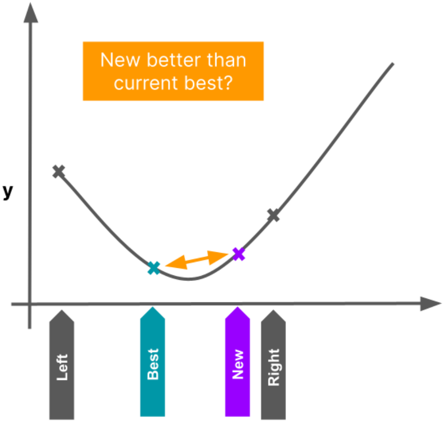
Compare proposal against current best.



SIMPLE NESTING PROCEDURE

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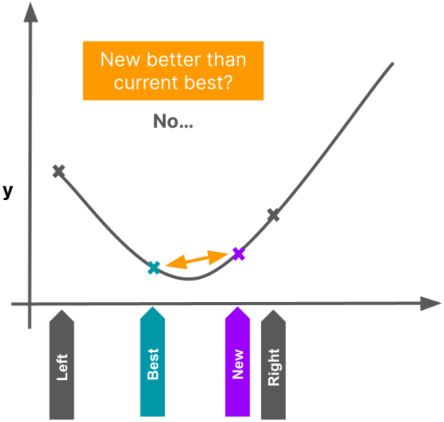
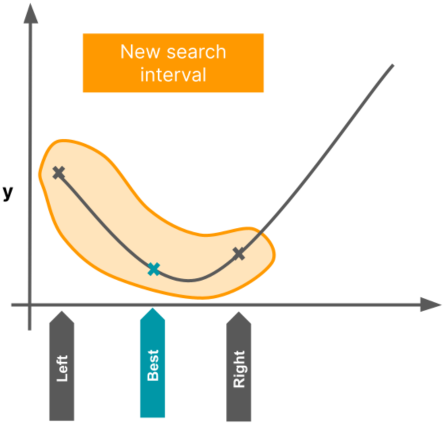
If it is better: proposal becomes current best.



SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

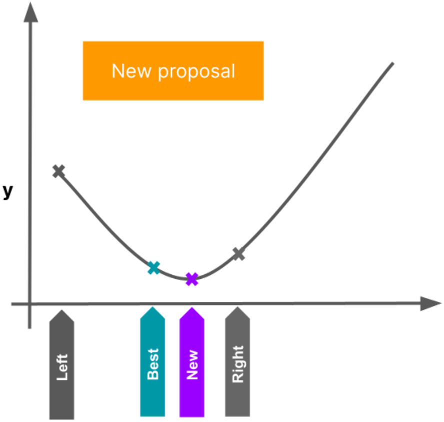
New search interval: around current best.



SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

Propose a random point.



SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.

Compare proposal against current best.

SIMPLE NESTING PROCEDURE

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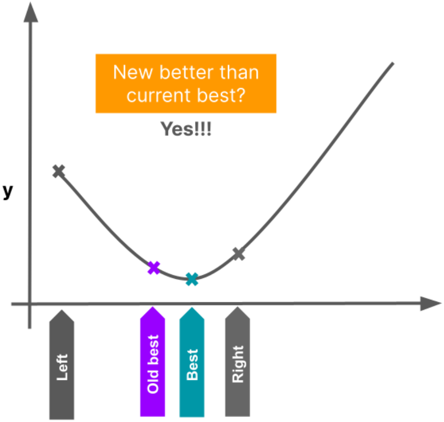
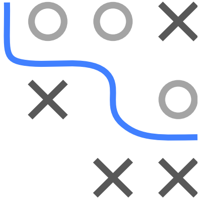
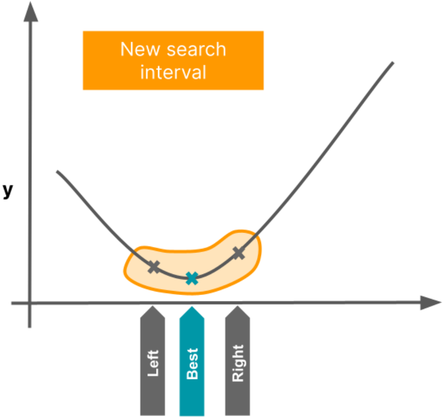




SIMPLE NESTING PROCEDURE

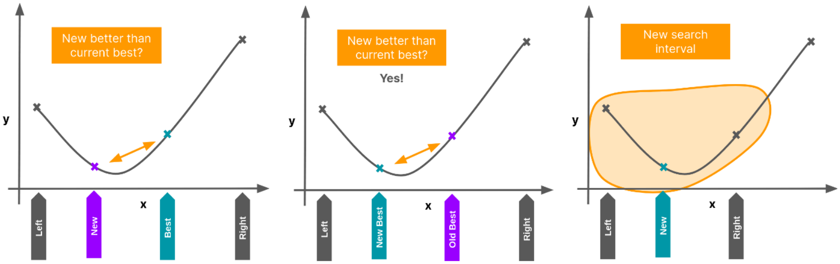
Let $f : \mathbb{R} \to \mathbb{R}$.

New search interval: around current best.



SIMPLE NESTING PROCEDURE

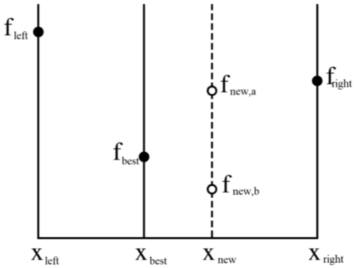
- **Initialization**: Search interval $(x^{\text{left}}, x^{\text{right}})$, $x^{\text{left}} < x^{\text{right}}$
- Choose x^{best} randomly.
- For $t = 0, 1, 2, \ldots$
  - Choose x^{new} randomly in $[x^{\text{left}}, x^{\text{right}}]$
  - If $f(x^{\text{new}}) < f(x^{\text{best}})$:
    - $x^{\text{best}} \leftarrow x^{\text{new}}$
  - New interval: Points around x^{best}



GOLDEN RATIO

Key question: How can x^{new} be chosen better than randomly?

- **Insight 1:** Always in bigger subinterval to maximize reduction.
- **Insight 2:** x^{new} symmetrically to x^{best} for uniform reduction.

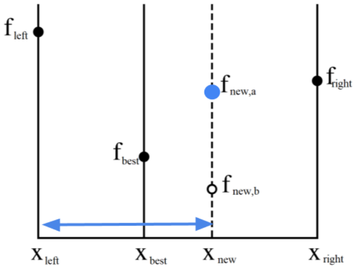


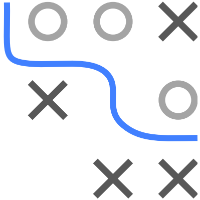
Consider two hypothetical outcomes x^{new}: $f_{new,a}$ and $f_{new,b}$.

GOLDEN RATIO / 2

If $f_{new,a}$ is the outcome, x_{best} stays best and we search around x_{best} :

$$[x_{left}, x_{new}]$$

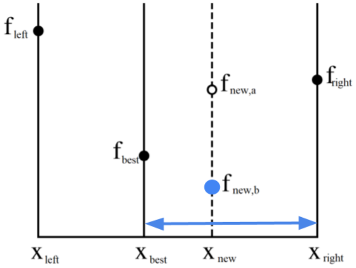


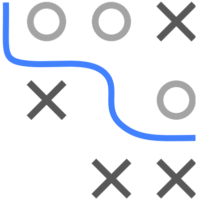


GOLDEN RATIO / 3

If $f_{new,b}$ is outcome, x_{new} becomes best point and search around x_{new} :

$$[x_{best}, x_{right}]$$

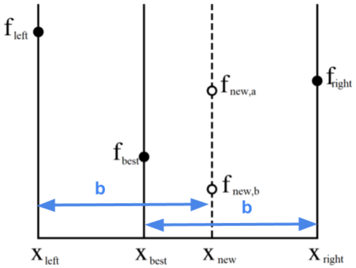




GOLDEN RATIO / 4

For uniform reduction, require the two potential intervals equal sized:

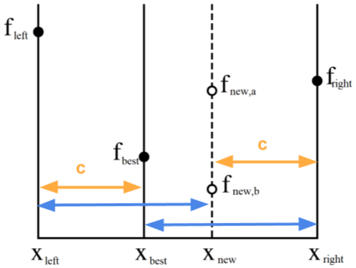
$$b := x_{right} - x_{best} = x_{new} - x_{left}$$

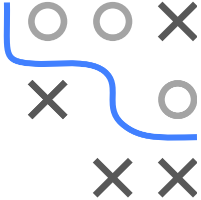


GOLDEN RATIO / 5

One iteration ahead: require again the intervals to be of same size.

$$c := x_{best} - x_{left} = x_{right} - x_{new}$$

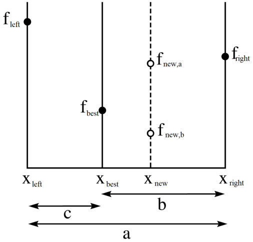


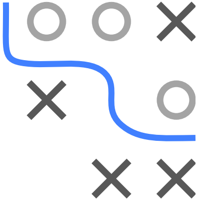


GOLDEN RATIO / 6

To summarize, we require:

$$
\begin{aligned}
a &= x^{right} - x^{left}, \\
b &= x_{right} - x_{best} = x_{new} - x_{left} \\
c &= x_{best} - x_{left} = x_{right} - x_{new}
\end{aligned}
$$





GOLDEN RATIO / 7

- We require the same percentage improvement in each iteration
- For φ reduction factor of interval sizes (a to b, and b to c)

$$\varphi := \frac{b}{a} = \frac{c}{b}$$

$$\varphi^2 = \frac{b}{a} \cdot \frac{c}{b} = \frac{c}{a}$$

- Divide $a = b + c$ by a:

$$\begin{aligned}
\frac{a}{a} &= \frac{b}{a} + \frac{c}{a} \\
1 &= \varphi + \varphi^2 \\
0 &= \varphi^2 + \varphi - 1
\end{aligned}$$

- Unique positive solution is $\varphi = \frac{\sqrt{5}-1}{2} \approx 0.618$.

GOLDEN RATIO / 8

- With x^{new} we always go φ percentage points into the interval.
- Given x^{left} and x^{right} it follows

$$
\begin{aligned}
x^{best} &= x^{right} - \varphi(x^{right} - x^{left}) \\
&= x^{left} + (1 - \varphi)(x^{right} - x^{left})
\end{aligned}
$$

and due to symmetry

$$
\begin{aligned}
x^{new} &= x^{left} + \varphi(x^{right} - x^{left}) \\
&= x^{right} - (1 - \varphi)(x^{right} - x^{left}).
\end{aligned}
$$

GOLDEN RATIO / 9

Termination criterion:

- A reasonable choice is the absolute error, i.e. the width of the last interval:

$$|x^{best} - x^{new}| < \tau$$

- In practice, more complicated termination criteria are usually applied, for example in *Numerical Recipes in C, 2017*

$$|x^{right} - x^{left}| \leq \tau(|x^{best}| + |x^{new}|)$$

  is proposed as a termination criterion.