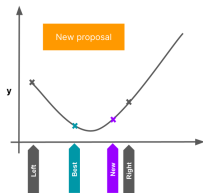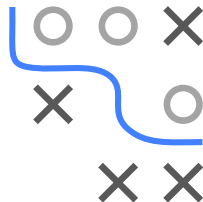# Optimization in Machine Learning
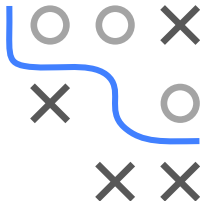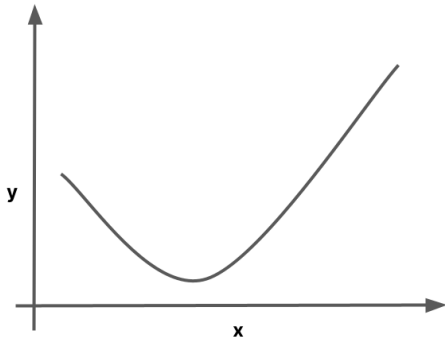
Univariate optimization
Golden ratio

Learning goals

- Simple nesting procedure
- Golden ratio

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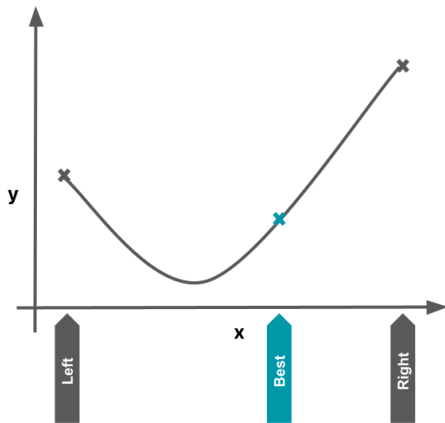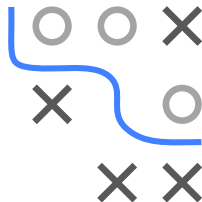
Let $f : \mathbb{R} \to \mathbb{R}$.

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

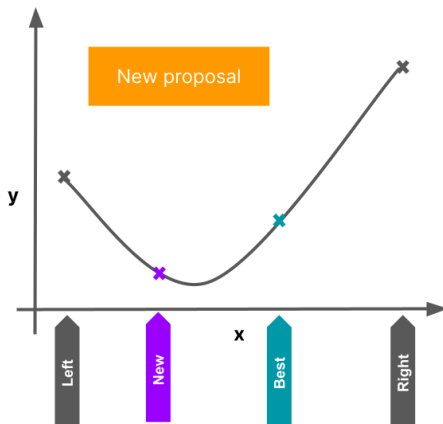# SIMPLE NESTING PROCEDURE

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

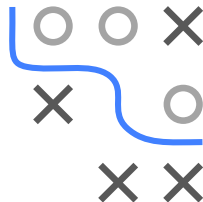Always maintain three points: left, right, and current best.

SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.
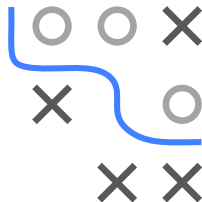
Propose random point in interval.

New proposal

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.

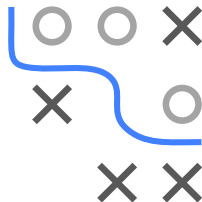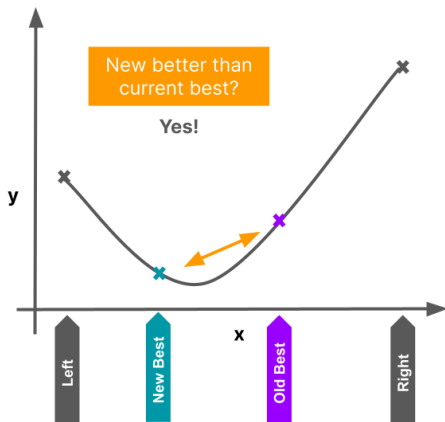# SIMPLE NESTING PROCEDURE

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

Compare proposal against current best.

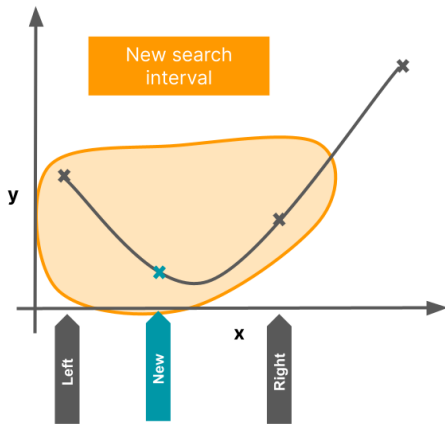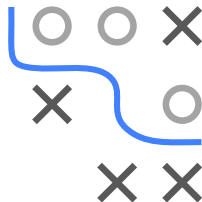# SIMPLE NESTING PROCEDURE

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

If it is better: proposal becomes current best.

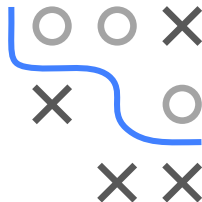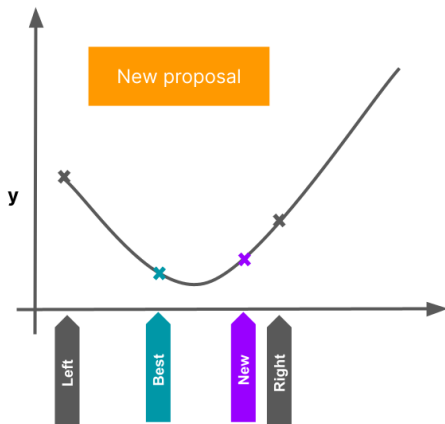# SIMPLE NESTING PROCEDURE

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

New search interval: around current best.

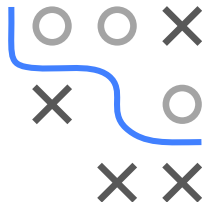# SIMPLE NESTING PROCEDURE

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

Propose a random point.

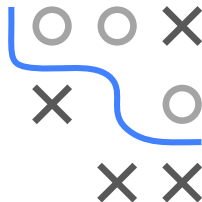# SIMPLE NESTING PROCEDURE

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

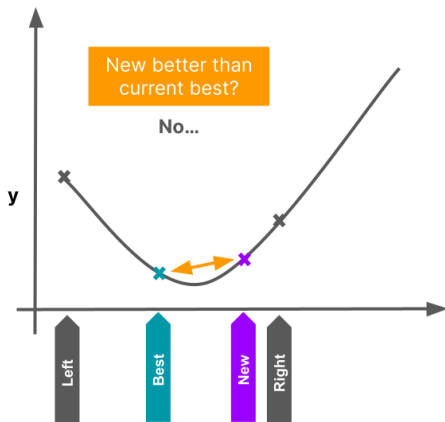Compare proposal against current best.

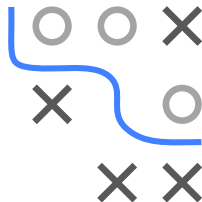# SIMPLE NESTING PROCEDURE

Let $f : \mathbb{R} \to \mathbb{R}$.
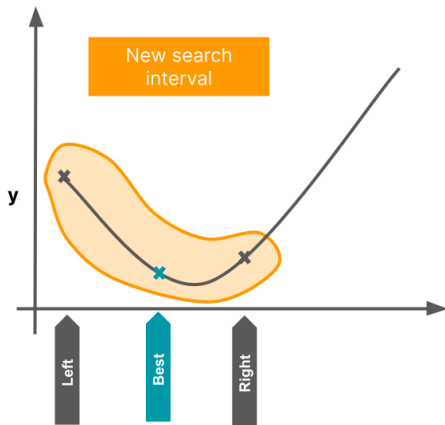
If it is better: proposal becomes current best.

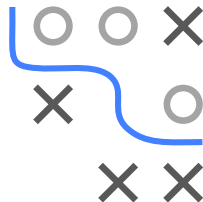# SIMPLE NESTING PROCEDURE

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

New search interval: around current best.
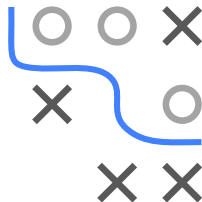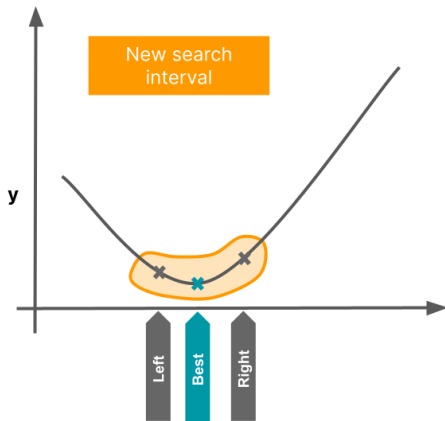
SIMPLE NESTING PROCEDURE

- **Initialization**: Search interval $(x^{\text{left}}, x^{\text{right}})$, $x^{\text{left}} < x^{\text{right}}$
- Choose x^{best} randomly.
- For $t = 0, 1, 2, ...$
  - 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}
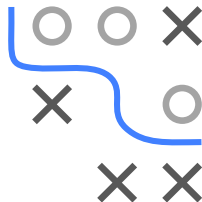
GOLDEN RATIO

Key question: How can x^{new} be chosen better than randomly?
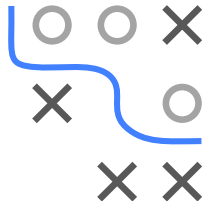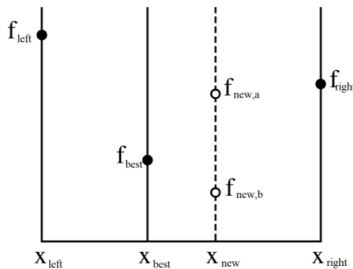
- **Insight 1:** Always in bigger subinterval to maximize reduction.
- **Insight 2:** x^{new} symmetrically to x^{best} for uniform reduction.
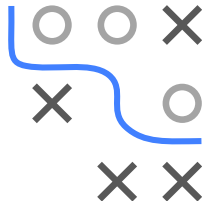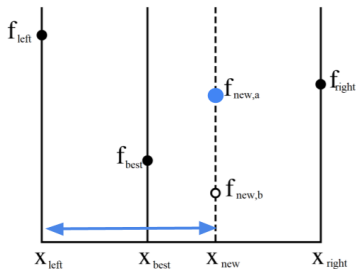

Consider two hypothetical outcomes x^{new}: $f_{new,a}$ and $f_{new,b}$.

GOLDEN RATIO / 2

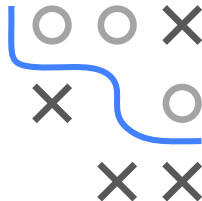If $f_{new,a}$ is the outcome, x_{best} stays best and we search around x_{best} :

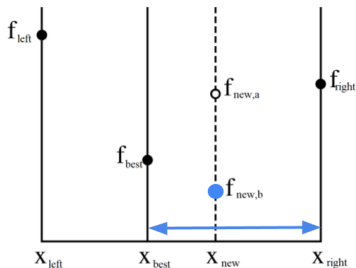$$[x_{left}, x_{new}]$$

GOLDEN RATIO / 3

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

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

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

$$b := x_{right} - x_{best} = x_{new} - x_{left}$$
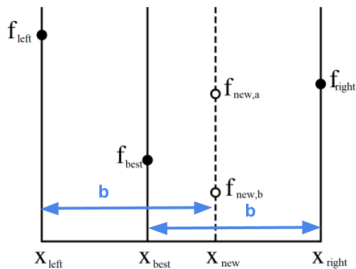
One iteration ahead: require again the intervals to be of same size.
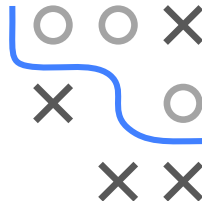
$$c := x_{best} - x_{left} = x_{right} - x_{new}$$
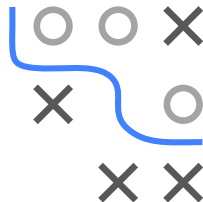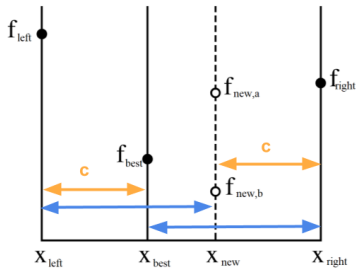
To summarize, we require:

$$a = x^{right} - x^{left},$$
$$b = x_{right} - x_{best} = x_{new} - x_{left}$$
$$c = x_{best} - x_{left} = x_{right} - x_{new}$$
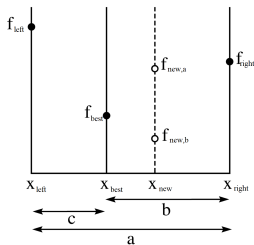
- We require the same percentage improvement in each iteration
- For φ reduction factor of interval sizes (a to b, and b to c)

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

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

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

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

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

GOLDEN RATIO / 8

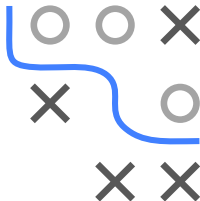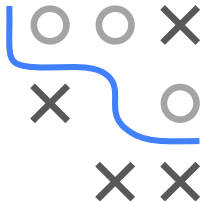- With x^{new} we always go φ percentage points into the interval.
- Given x^{left} and x^{right} it follows

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

and due to symmetry

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

GOLDEN RATIO

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.