

1. General Structure of the Algorithm

This method conducts an iterative search over a parameter space that may contain **continuous**, **integer**, and **categorical** variables. Its main components are:

1. Elite Selection

A set of the best-performing trials (based on the objective function) is selected at each iteration. These are the “elites.”

2. Noise Perturbation

New candidate solutions are generated by perturbing the parameters of these elite trials with a noise term that adapts over time.

3. Noise Annealing

The noise level is decreased as the number of iterations increases, often using a cosine-annealing schedule. This ensures broader exploration at the beginning and more focused exploitation later on.

4. Categorical Handling

Categorical parameters are internally represented via one-hot encoding. A softmax function (with a temperature parameter) is used to stochastically choose among possible categories based on the (perturbed) mean of elite vectors.

5. Integer Handling

Integer parameters are sampled as continuous values and then probabilistically rounded to the nearest integers.

Let:

- N be the total number of iterations (trials).
- t be the index of the current iteration, with $0 \leq t < N$.
- $p_t = \frac{t}{N}$ be the **progress ratio**.

2. Number of Elite Trials n_{elite}

At each iteration t , the number of elite trials selected to guide the next sample can be defined by a function that depends on the progress ratio p_t . One commonly used form is:

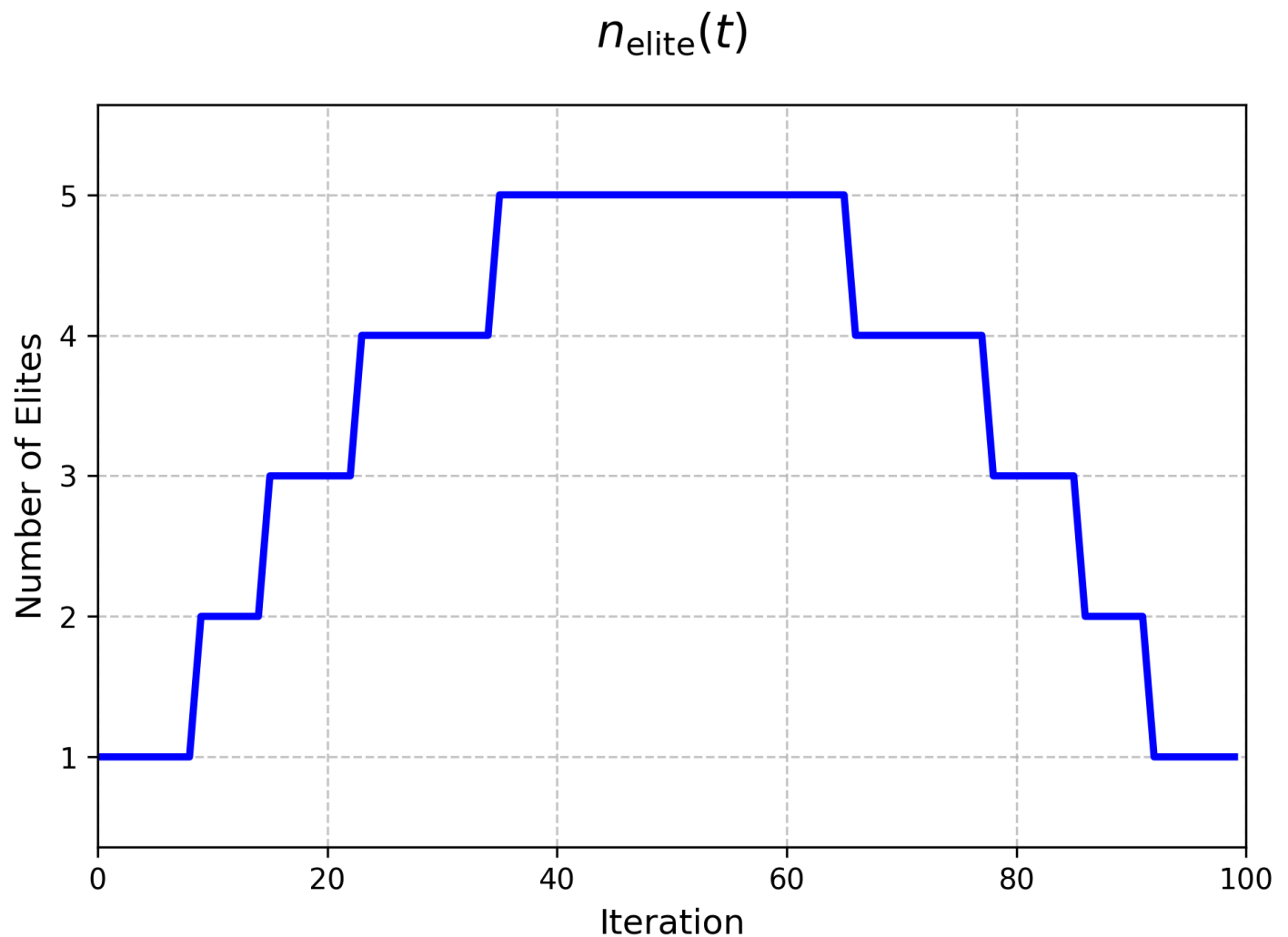
$$n_{\text{elite}}(t) = \max\left(1, \text{round}\left(\alpha \sqrt{N} \cdot p_t \cdot (1 - p_t)\right)\right),$$

where:

- α is a constant (for example, $\alpha = 2$) that scales according to the total number of trials N .
- The factor $p_t (1 - p_t)$ creates a bell-shaped curve over $t \in [0, N]$, reaching its maximum around $t \approx \frac{N}{2}$.
- The use of $\max(1, \dots)$ ensures that at least one trial is always considered elite.

Visualizing $n_{\text{elite}}(t)$

If desired, a plot of $n_{\text{elite}}(t)$ against t can show how the number of elite trials starts near 0 or 1 at $t = 0$, grows to a maximum in the middle iterations, and then decreases again near $t = N$.



3. Noise Scheduling with Cosine Annealing

Let η_{init} be the **initial noise** (e.g., 0.2) and $\eta_{\text{final}} = \frac{1}{N}$ be the **final noise** (or another chosen small value). At iteration t , define a **cosine annealing** factor:

$$\text{cos_anneal}(t) = 0.5 (1 + \cos(\pi p_t)),$$

where $p_t = \frac{t}{N}$.

Then, the noise level $\eta(t)$ can be updated as:

$$\eta(t) = \eta_{\text{final}} + (\eta_{\text{init}} - \eta_{\text{final}}) \text{cos_anneal}(t).$$

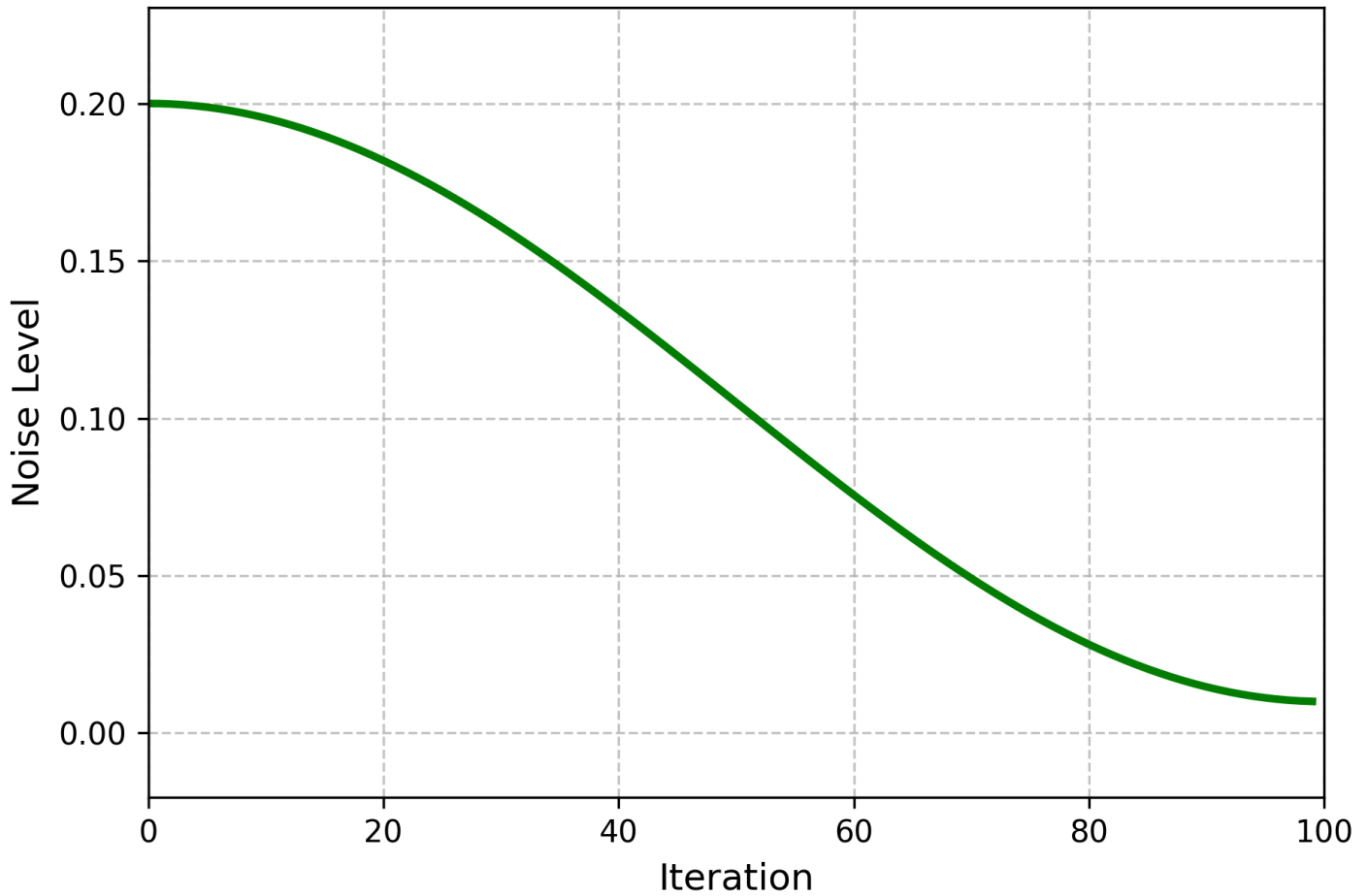
- When t is close to 0, $p_t = 0$, so $\cos(\pi p_t) = 1$ and $\eta(t) \approx \eta_{\text{init}}$.
- Near $t = N$, $\cos(\pi p_t) = -1$, so $\eta(t) \approx \eta_{\text{final}}$.

Hence, the noise transitions gradually from a larger initial value down to a smaller final value.

Visualizing $\eta(t)$

A plot of $\eta(t)$ across iterations t typically shows a smooth curve descending from η_{init} at $t = 0$ to η_{final} at $t = N$.

$$\eta(t)$$



4. Continuous and Integer Parameters

4.1. Continuous Variables

For a continuous variable x in the range $[\text{low}, \text{high}]$, new samples may first be drawn randomly (uniformly or log-uniformly) during early iterations. Once enough iterations have passed, the algorithm exploits the elite solutions:

1. **Select an Elite Value**

One of the elite trials (in terms of objective value) is chosen at random. Let its parameter be x_{elite} .

2. **Add Noise**

Draw a random value $\delta \sim \mathcal{N}(0, \sigma)$, where σ depends on $\eta(t)$ and possibly the range $\text{high} - \text{low}$. A typical approach is:

$$x_{\text{new}} = x_{\text{elite}} + \delta \cdot (\text{high} - \text{low}) \cdot \eta(t).$$

3. Reflect at Boundaries

If x_{new} goes below low or above high, it is reflected back into the valid range, for instance by:

$$\text{while } x_{\text{new}} < \text{low or } x_{\text{new}} > \text{high: } \begin{cases} x_{\text{new}} = \text{high} - (x_{\text{new}} - \text{high})/2 & \text{if } x_{\text{new}} > \text{high}, \\ x_{\text{new}} = \text{low} + (\text{low} - x_{\text{new}})/2 & \text{if } x_{\text{new}} < \text{low}. \end{cases}$$

4.2. Integer Variables

To handle an integer parameter in $\{\text{low}, \dots, \text{high}\}$, one can:

1. Sample a **continuous** value as above, obtaining v .
2. Let $\lfloor v \rfloor$ be the floor of v and $f = v - \lfloor v \rfloor$ be its fractional part.
3. Draw u from a uniform distribution $U(0, 1)$.
4. If $u < f$, set the integer value to $\lceil v \rceil$. Otherwise, set it to $\lfloor v \rfloor$.

Thus, a value close to 10.7 is more likely to become 11 than 10, while a value close to 10.2 is more likely to become 10 than 11.

5. Categorical Parameters: One-Hot and Softmax

Categorical parameters are represented as **one-hot vectors**. Suppose there are k possible categories c_1, c_2, \dots, c_k . Each trial stores a vector of length k , e.g., $[1, 0, 0]$ if category c_1 is chosen, $[0, 1, 0]$ if c_2 is chosen, etc.

5.1. Averaging and Noise

Let $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{n_{\text{elite}}}$ be the one-hot vectors of the best $n_{\text{elite}}(t)$ trials. Compute the component-wise mean:

$$\bar{\mathbf{v}} = \frac{1}{n_{\text{elite}}(t)} \sum_{i=1}^{n_{\text{elite}}(t)} \mathbf{v}_i.$$

Then add Gaussian noise \mathbf{z} with scale $\eta(t)$, typically ensuring the result stays within $[0, 1]$ by reflection if necessary.

5.2. Temperature and Softmax

A temperature parameter $T_{\text{cat}}(t)$ is introduced to control how sharply categories are chosen. One approach is to define

$$T_{\text{cat}}(t) = \frac{1}{\eta_{\text{final}} + (1 - \eta_{\text{final}}) \cos_anneal(t)},$$

where

$$\cos_anneal(t) = 0.5 (1 + \cos(\pi p_t)).$$

After adding noise to $\bar{\mathbf{v}}$, each component m_j represents the “score” for category j . These scores are converted to probabilities $\{\pi_1, \dots, \pi_k\}$ via a softmax scaled by $T_{\text{cat}}(t)$:

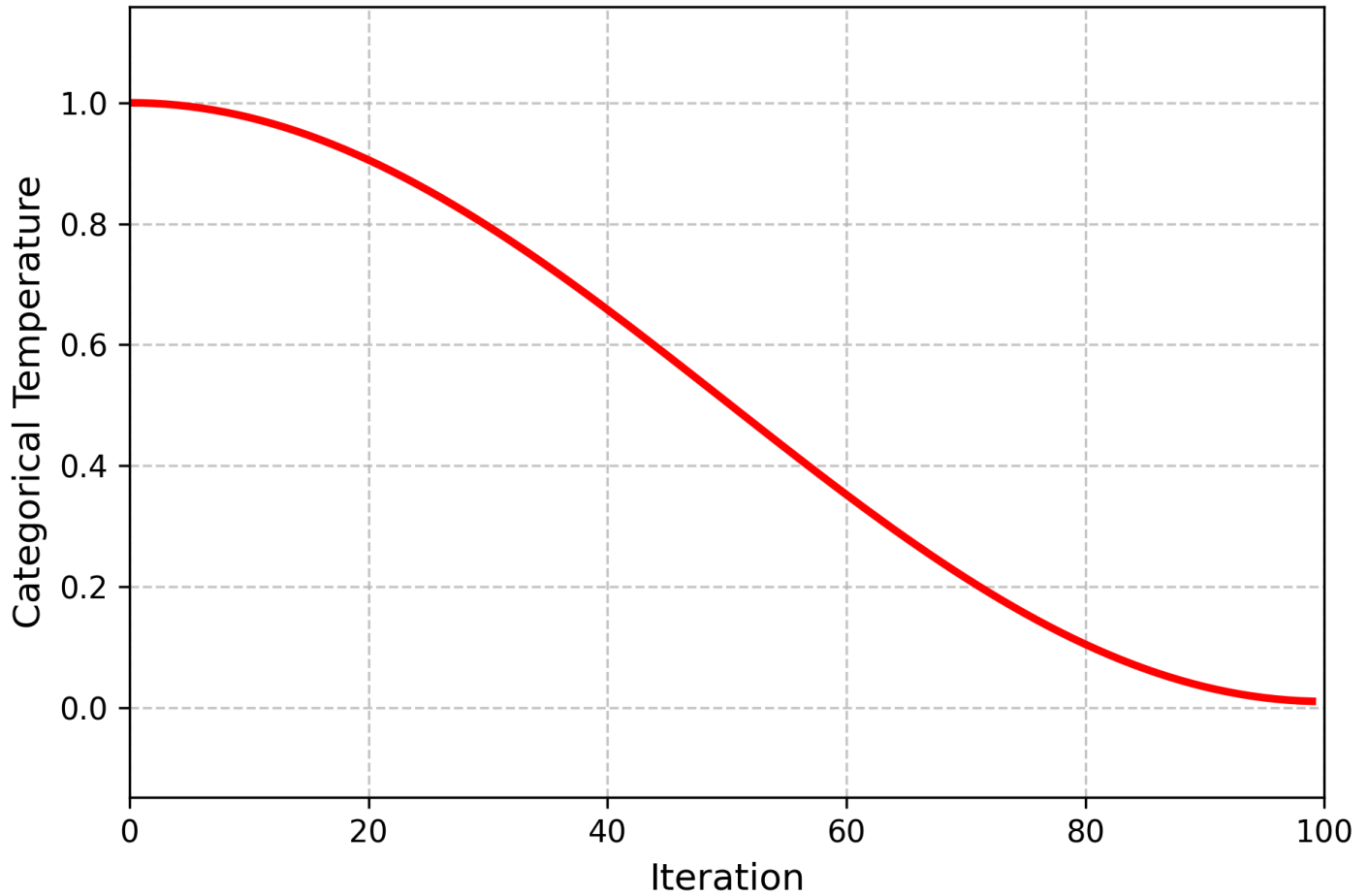
$$\pi_j = \frac{\exp(m_j T_{\text{cat}}(t))}{\sum_{r=1}^k \exp(m_r T_{\text{cat}}(t))}, \quad j = 1, \dots, k.$$

Finally, a category c_j is sampled with probability π_j , and the corresponding one-hot vector is set to $[0, \dots, 1, \dots, 0]$ with 1 at position j .

Visualizing $T_{\text{cat}}(t)$

If desired, a plot of $T_{\text{cat}}(t)$ against t can show how the categorical temperature starts high at $t = 0$, allowing broad exploration, then gradually decreases, focusing more on the best categories over time.

$$T_{\text{cat}}(t)$$



6. Iterative Procedure

Let:

- N be the total number of iterations (trials).
- $n_{\text{init_points}}$ be the number of initial trials that are sampled purely at random (commonly $\text{round}(\sqrt{N})$ if not specified).
- t be the index of the current iteration, with $0 \leq t < N$.
- $p_t = \frac{t}{N}$ be the **progress ratio**.

At **each iteration** t (from 0 up to $N - 1$):

If $t < n_{\text{init_points}}$:

- **Randomly sample** all parameters (continuous, integer, and categorical) within their valid ranges.

- Skip steps 2, 3, and 4 below (since no elite-based adaptation is used yet).

Otherwise ($t \geq n_{\text{init_points}}$):

1. Compute Progress:

$$p_t = \frac{t}{N}.$$

2. Determine Elite Count:

$$n_{\text{elite}}(t) = \max\left(1, \text{round}\left(\alpha \sqrt{N} \cdot p_t (1 - p_t)\right)\right),$$

3. Update Noise (Cosine Annealing):

$$\eta(t) = \eta_{\text{final}} + (\eta_{\text{init}} - \eta_{\text{final}}) \times 0.5 (1 + \cos(\pi p_t)).$$

4. Handle Parameters:

- **Continuous:** Select an elite value, add $\mathcal{N}(0, \sigma)$ noise scaled by $\eta(t)$ and reflect if out of bounds.
- **Integer:** Same as continuous, but use *probabilistic rounding* (fractional part decides rounding up/down).
- **Categorical:** Form an average one-hot vector from the elites, add noise, apply a temperature-based softmax, then pick a category.

5. Evaluate Objective:

- Pass the newly sampled parameter set to the objective function for a score.

6. Update Ranking:

- Keep track of the best $n_{\text{elite}}(t)$ trials (“elites”) for the next iteration.

This process repeats until $t = N$. Early in the search ($t < n_{\text{init_points}}$), the algorithm explores broadly by drawing random samples. Once $t \geq n_{\text{init_points}}$, it transitions to the adaptive phase: higher noise in the beginning encourages wide exploration, whereas lower noise in later iterations focuses the search around the most promising solutions found so far.

Additional Notes

- **Reflections at Boundaries**

Ensuring that samples do not remain outside a valid range often involves a “mirror” or “reflect” step.

- **Log-Scale Sampling**

If a parameter is specified as log-scaled $\in [\text{low}, \text{high}]$, sampling can be done in log-space, i.e., $\exp(\text{Uniform}(\log(\text{low}), \log(\text{high})))$.

- **Temperature**

When $\eta(t)$ becomes small, $T_{\text{cat}}(t)$ becomes large, so the softmax distribution becomes more “peaked” around the best categories discovered.