0.1 Theoretical guarantee of convergence

Here we establish theoretical guarantees for the convergence of our probabilistic generative model, RoboLDA, *when combined with an evolutionary algorithm.* We first demonstrate that RoboLDA asymptotically converges to global optima, and then show that RoboLDA exhibits linear convergence in terms of the average convergence rate. These results serve as evidence that RoboLDA can effectively approximate the global distribution of high-performing morphological designs.

0.1.1 Asymptotic convergence to optimal solutions

Let θ_τ denote the parameters of RoboLDA in generation τ, and let $p_{\theta_\tau}(x;t) = \int p_{\theta_\tau}(H_t|t) \cdot p_{\theta_\tau}(x|H_t)\mathrm{d}H_t$ denote the robot design distribution of task t learned by VAE. Define the entire robot design space as $\mathcal{X}$, and any specific design within this space as x. Also denote the task set as $\mathcal{T}$. Note that given the highly non-convex and multi-modal nature of VSR fitness landscape, we do not assume that the optimal robot design for each task t is unique. Instead, we allow for multiple globally optimal designs, collectively denoted as $\mathcal{A}(t)$. Denote the distribution of elite samples (i.e. robots selected from the morphology-fitness pool to fit the VAE model) for task t in generation τ as $C_\tau(x;t)$. The updating process of RoboLDA can thus be approximated by a weighted average between the previous distribution and the elite distribution: $p_\tau(x;t) = (1-\alpha_\tau)p_{\tau-1}(x;t) + \alpha_\tau C_\tau(x;t)$, for $x \in \mathcal{X}$ and $t \in \mathcal{T}$ (also known as *smoothed updating*). We now show that RoboLDA asymptotically converges to the optimal solutions under mild conditions.

Theorem 1 (Asymptotic Convergence of RoboLDA) Consider the evolutionary process of RoboLDA as a stochastic process, with its state represented as $(p_\tau(t), X_\tau(t)) \quad (\forall t \in \mathcal{T})$. Here $p_\tau(t)$ denotes the distribution defined by the generative process of VAE for task t in generation τ, and $X_\tau(t)$ stands for the set of elite solutions of task t in generation τ (i.e. the support of $C_\tau(x;t)$). Assume the aforementioned sequence α_t satisfies:

$$\alpha_\tau \leq 1 - \frac{\log(\tau+1)}{\log(\tau+2)}, \quad (\tau \geq T) \tag{1}$$

for some $T > 0$, and

$$\sum_{\tau=1}^{\infty} \alpha_\tau = \infty. \tag{2}$$

It then follows that
(a) $X_\tau(t)$ converges to $X^*(t)$ with probability one as $\tau \to \infty$, where $X^*(t)$ represents an arbitrary set of robot designs that include at least one optimal solution of task t.
(b) $p_\tau(t)$ converges to $p^*(t)$ as $\tau \to \infty$, where $p^*(x;t)$ is an *optimal distribution* that assigns non-zero probability only to optimal designs[1]. In other words, the distribution learned by RoboLDA would eventually degenerate onto optimal solutions.

[1]Since all optimal solutions have the same performance, we do not discriminate p^*'s with different probability allocation on $\mathcal{A}$, but rather treat them equally as *optimal distributions*.

proof of Theorem 1: The theorem is proved for $\forall t \in \mathcal{T}$, and we omit t from now on for brevity. Consider the probability that the optimal solutions are never obtained:

$$
\begin{aligned}
&P\{X^* \text{ is never obtained }\}\\
&= \prod_{\tau=0}^{\infty} P\{X^* \text{ not obtained in generation } \tau | X^* \text{ not obtained before generation } \tau\}.
\end{aligned} \tag{3}
$$

We can calculate a lower bound of $p_{\theta_\tau}(x)$, which corresponds to the case when x didn't show up as an elite sample through all previous generations:

$$
\begin{aligned}
p_{\theta_\tau}(x) &\geq \left[\prod_{i=0}^{\tau}(1-\alpha_i)\right] p_{\theta_0}(x) \geq \left[\prod_{t=0}^{T-1}(1-\alpha_i)\right]\left[\prod_{i=T}^{\tau}\frac{\log(i+1)}{\log(i+2)}\right] p_{\theta_0}(x)\\
&= \left[\prod_{i=0}^{T-1}(1-\alpha_i)\right] p_{\theta_0}(x)\frac{\log(T+1)}{\log(\tau+2)} = \frac{\text{const}}{\log(\tau+2)},
\end{aligned} \tag{4}
$$

where the second inequality follows from Equation (1). Hence, the probability of VAE generating any of $\mathcal{A}$ in generation τ is greater or equal to $|\mathcal{A}| \cdot \text{const}/\log(\tau+2)$. Note that this lower bound holds for arbitrary scenarios that could happen before generation τ, and therefore we have

$$
\begin{aligned}
&P\{X^* \text{ is not obtained in generation } \tau | X^* \text{ wasn't obtained before generation } \tau\}\\
&\leq \left[1 - \frac{|\mathcal{A}| \cdot \text{const}}{\log(\tau+2)}\right]^N,
\end{aligned} \tag{5}
$$

where N denotes the population size, and the inequality holds because individuals in the population are generated independently. Hence, the probability in Equation (3) is upper bounded by

$$
\prod_{\tau=0}^{T-1} 1 \cdot \prod_{\tau=T}^{\infty}\left[1 - \frac{|\mathcal{A}| \cdot \text{const}}{\log(\tau+2)}\right]^N = \prod_{\tau=T}^{\infty}\left[1 - \frac{|\mathcal{A}| \cdot \text{const}}{\log(\tau+2)}\right]^N.
$$

Further taking logarithm of the right-hand side, we have that

$$
N\sum_{\tau=T}^{\infty}\log\left[1 - \frac{|\mathcal{A}| \cdot \text{const}}{\log(\tau+2)}\right] \leq -N\sum_{\tau=T}^{\infty}\left(\frac{|\mathcal{A}| \cdot \text{const}}{\log(\tau+2)}\right) = -\infty,
$$

where the inequality follows from the fact that $\log(x) < x - 1$ for all $x \in (0,1)$, and the identity holds because $\sum_\tau(\log(\tau+1))^{-1} = \infty$. Consequently, $P\{X^* \text{ is never obtained}\} = 0$. Note that once one or more optimal solutions are obtained, they will remain in elite samples thereafter, and therefore X_τ converges to X^* almost surely as $\tau \to \infty$.

So far, we proved that at least one of the optimal solutions will be obtained with probability 1 as the number of generations tends to infinity. Let us denote by τ^* the generation in which X^* is attained for the first time. Now, consider the probability of any x that does not belong to $\mathcal{A}$ in generation $\tau^*+\Delta\tau$. To this end, notice that for any non-optimal x, due to the selection pressure favoring high-performing robot designs, once one or more optimal solutions are attained, there should exist $d < 1$ such that $C_{\tau+1}(x) \leq d \cdot p_\tau(x)$. Hence, for any $x \notin \mathcal{A}$ and $\tau \geq \tau^*$, we have

$$p_{\tau+1}(x) = (1-\alpha_{\tau+1})p_\tau(x) + \alpha_{\tau+1}C_{\tau+1}(x) \leq (1-\alpha_{\tau+1}+d\alpha_{\tau+1})p_\tau(x), \quad \forall x \notin \mathcal{A}. \tag{6}$$

Hence, for any x that does not belong to the optimal solutions, we have

$$p_{\tau^*+\Delta\tau}(x) \leq \left[\prod_{\tau=\tau^*+1}^{\tau^*+\Delta\tau}(1-\alpha_\tau + d\cdot\alpha_\tau)\right]\cdot p_{\tau^*}(x).$$

Since $\log\prod_{\tau=0}^{\infty}(1-(1-d)\cdot\alpha_\tau) = \sum_{\tau=0}^{\infty}\log(1-(1-d)\cdot\alpha_\tau) < -(1-d)\cdot\sum_{\tau=0}^{\infty}\alpha_\tau = -\infty$, where "$<$" follows again from the fact that $\log(x) < x-1$ for $\forall x \in (0,1)$, and the second identity is due to (2), we know that $\prod_{\tau=0}^{\infty}(1-(1-d)\cdot\alpha_\tau) = 0$. As a consequence,

$$\lim_{\Delta\tau\to\infty} p_{\tau^*+\Delta\tau}(x) \leq \left[\prod_{\tau=\tau^*+1}^{\infty}(1-(1-d)\cdot\alpha_\tau)\right]\cdot p_{\tau^*}(x) = 0, \quad \text{for } \forall x \notin \mathcal{A},$$

which means that the probability of any non-optimal design would tend to zero, and thus $p_\tau(x)$ converges to p^*. With this, we complete the proof of **Theorem 1**. □

0.1.2 Linear convergence w.r.t ACR

Before delving into the analysis of ACR, we first provide its formal definition, originally proposed in [1].

Definition 1 (Average Convergence Rate, ACR) Consider the maximization problem:

$$\max f(\mathbf{x}), \quad \mathbf{x} = (x_1, \cdots, x_d) \in \mathcal{S} \subset \mathbb{R}^d,$$

where $f(\cdot)$ is the objective function, $\mathcal{S}$ is the domain of feasible solutions, and f^* denotes the maximal value of f. Let X_τ be the population at generation τ, with its fitness defined as $f(X_\tau) := \max\{f(x)|x \in X_\tau\}$, and its discrepancy with f^* as $e(X_\tau) := f^* - f(X_\tau)$. The *average convergence rate* (ACR) for τ consecutive generations of an evolutionary algorithm, starting from the initial population, is then defined as:

$$ACR_\tau := 1 - \left(\frac{e_\tau}{e_0}\right)^{1/\tau} = 1 - \left(\prod_{k=1}^{\tau} CR_k\right)^{1/\tau}, \quad \tau \in \mathbb{Z}^+,$$

where $e_\tau := \mathbb{E}[e(X_\tau)]$ and $CR_k := e_k/e_{k-1}$.

From **Definition 1**, we see that a larger ACR indicates faster convergence. $ACR = 1$ means the optimal solution has been found, while $ACR < 0$ suggests a decline in performance compared to X_0. *Linear convergence*, defined as $\lim_{\tau\to+\infty} ACR_\tau = C > 0$, is considered a desirable convergence rate.

Definition 2 (ρ-promising region) The *ρ-promising region* of a population X is defined as $S(X,\rho) := \{Y \subset \mathcal{S} | e(Y) < \rho e(X)\}$, i.e., all the populations that improve upon X by a factor of ρ. With $\rho = 1$, $S(X,\rho)$ is simply referred to as a promising region.

Theorem 2 (Linear Convergence of RoboLDA *w.r.t.* ACR) For each specific task $t \in \mathcal{T}$, let $P^{(\kappa)}(X(t); Y(t))$ denote the probability of transitioning from population $X(t)$ to population $Y(t)$ over κ generations during evolution. Assume RoboLDA satisfies

$$C_\rho := \inf\{P^{(\kappa)}(X(t); S(X(t),\rho)); X(t) \neq X^*(t)\} > 0$$

for some $0 < \rho < 1$ and positive integer κ. This assumption implies that the probability of transitioning from a non-optimal population to one of its ρ-promising region over κ generations is bounded below by a positive value. Then, we have that $\lim_{\tau\to\infty} ACR_\tau \geq C > 0$, i.e., RoboLDA achieves linear convergence.

Proof of Theorem 2: First, it is easy to see that $S(X_k,\rho) \subset S(X_k,1)$ for any $0 < \rho < 1$, and for any $Y \in S(X_k,\rho)$, we have $f(Y) - f(X_k) > (1-\rho)(f^* - f(X_k))$. Therefore, for κ consecutive generations, we have:

$$\begin{aligned}
&e(X_k) - e(X_{k+\kappa}) \\
&= \sum_{Y \in S(X_k,1)} (f(Y) - f(X_k))P^{(\kappa)}(X_k; Y) \\
&> \sum_{Y \in S(X_k,\rho)} (1-\rho)(f^* - f(X_k))P^{(\kappa)}(X_k; Y) \\
&\geq (1-\rho)C_\rho e(X_k),
\end{aligned} \tag{7}$$

where the identity is due to the fact that we treat the elite samples as our population, and hence for $Y \notin S(X_k,1)$, either $P^{(\kappa)}(X_k; Y) = 0$ or $f(Y) - f(X_k) = 0$.

Then,

$$\frac{\Delta^{(\kappa)} e_k}{e_k} = \frac{\mathbb{E}[e(X_k) - e(X_{k+\kappa})]}{\mathbb{E}[e(X_k)]} > (1-\rho)C_\rho.$$

Consequently, it holds that

$$\begin{aligned}
\lim_{\tau\to+\infty} ACR_\tau &= \lim_{\tau\to+\infty} \left[1 - \left(\prod_{k=1}^{\tau} \frac{e_k}{e_{k-1}}\right)^{1/\tau}\right] \\
&> 1 - [1 - (1-\rho)\cdot C_\rho] = (1-\rho)C_\rho > 0,
\end{aligned} \tag{8}$$

which completes the proof of **Theorem 2**. □

References

[1] Chen, Y., He, J.: Average convergence rate of evolutionary algorithms in continuous optimization. Information Sciences **562**, 200–219 (2021)