MorphVAE: Advancing Morphological Design of Voxel-Based Soft Robots with Variational Autoencoders

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Abstract

Soft robot design is an intricate field with unique challenges due to its complex and vast search space. In the past literature, evolutionary computation algorithms, including novel probabilistic generative models (PGMs), have shown potential in this realm. However, these methods are sample inefficient and predominantly focus on rigid robots in locomotion tasks, which limit their performance and application in robot design automation. In this work, we propose MorphVAE, an innovative PGM that incorporates a multi-task training scheme and a meticulously crafted sampling technique termed "continuous natural selection", aimed at bolstering sample efficiency. This method empowers us to gain insights from assessed samples across diverse tasks and temporal evolutionary stages, while simultaneously maintaining a delicate balance between optimization efficiency and biodiversity. Through extensive experiments in various locomotion and manipulation tasks, we substantiate the efficiency of MorphVAE in generating high-performing and diverse designs, surpassing the performance of competitive baselines.

1 Introduction

Voxel-Based Soft Robots (VSRs), which are made up of elastic blocks that expand or contract with many degrees of freedom, were first introduced in Hiller and Lipson (2011) and attracted the attention from both the academia and the industry due to their great flexibility and resemblance to natural organisms. A considerable number of works have studied the design automation of VSRs, mostly with traditional Evolutionary Algorithms (EAs) that feature biologically inspired meta-heuristics (Cheney, Bongard, and Lipson 2015; Bhatia et al. 2021; Medvet et al. 2021). However, the substantial combinatorial search space of VSRs poses a big challenge to EAs and limits their performance; Generative encoding, on the other hand, has demonstrated promise as a solution (Cheney et al. 2014; Corucci et al. 2018; Hu et al. 2022). Nonetheless, the potential of probabilistic generative models, extensively applied in modeling complex geometries (Gómez-Bombarelli et al. 2018; Joy et al. 2020; Xu et al. 2023), remains largely untapped in the realm of soft robot design. Probabilistic generative models, albeit requiring additional computational expense for training, hold particular appeal to robot design automation, including their inherent multimodality, rapid execution speed and the capability to statistically deduce patterns from diverse samples, which we deem well worth further leveraging.

In this paper, we capitalize on the remarkable potential of generative models to unlock shared insights from diverse multimodal resources. Our investigation into the distribution of robot designs across seemingly disparate tasks reveals a remarkable pattern: many designs cluster closely, hinting at shared sub-structures that traverse task boundaries. Driven by this revelation, we propose **MorphVAE**, which, to the best of our knowledge, stands as the pioneering method for task-specific and free-form soft robot design. Unlike existing approaches, MorphVAE makes full use of probabilistic generative models to deduce favorable morphological structures from evaluated robot designs across different tasks and the evolutionary timeline. Its training adopts a bootstrapping manner, eliminating reliance on conventional EAs.

To be more specific, our methodology employs the Variational Autoencoder (VAE; Kingma and Welling (2013)), a prominent probabilistic generative model, to establish a mapping from tasks to their distributions of high-performing robot designs. We introduce a novel sampling technique named *continuous natural selection*, gradually pushing the generator towards higher-performing designs, and apply a temperature parameter to flexibly control the strength of selection pressure. Additionally, we propose a technique named *exploration-exploitation rebalancing* to promote broader search ranges and diverse robot designs. In summary, our work makes the following contributions:

1. We observe, through pilot experiments, that high-performing robot designs overlap across different tasks, and adopt a multi-task training approach so that knowledge could be shared across task boundaries.
2. We propose MorphVAE, featuring a novel sampling technique termed *continuous natural selection*, which unprecedentedly tackles free-form robot design automation with probabilistic generative models that are trained in a completely bootstrapping manner. Such an approach al-

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lows for exceptional flexibility between high efficiency and high diversity during evolution.

3. Through extensive experiments involving various locomotion and manipulation tasks, we demonstrate the advantage of MorphVAE in aiding robots with the emergence of favorable structures and yielding diversified robot designs.

2 Related Work

2.1 Robot co-design

Inspired by the philosophy of embodied cognition (Pfeifer and Bongard 2006; Pfeifer, Iida, and Lungarella 2014), co-designing the structure and controller of robots has become a concensus in Robotics. So far, the most widely used paradigm for robot co-design is bi-level optimization (Bhatia et al. 2021), involving control optimization in the inner loop that optimizes a controller for each robot and evaluates its fitness, and design optimization in the outer loop that evolves robots according to their fitness. A wide range of powerful reinforcement learning algorithms could be leveraged in the inner loop, while the choices for design optimization could be roughly divided into the following categories.

Evolutionary Algorithms. Evolutionary Algorithms (EAs) have long been the *de facto* choice in robot design automation, which maintain a population of robot designs and carry out elitism selection and stochastic operations in search of better ones. Among plenty of research, Leger (2012) pioneered the application of EAs to the design of rigid robots; Wang et al. (2019) proposed Neural Graph Evolution that performs evolutionary search in the graph space of rigid-robot designs. However, many genetic encodings in EAs do not scale to the large search spaces of soft robots (Cheney et al. 2014). To this end, researchers recently began to explore the benefit of generative encoding over direct encoding in robot design automation (Cheney et al. 2014; Ha, Agrawal, and Song 2021). However, these works assume a one-on-one mapping from tasks to morphologies, ignoring the multimodal nature of design automation.

Probabilistic Generative Models. Over the last decade, probabilistic generative models, such as Variational Autoencoder (VAE; Kingma and Welling (2013)), Generative Adversarial Network (GAN; Goodfellow et al. (2020)) and Diffusion Model (DM; Ho, Jain, and Abbeel (2020)), have witnessed widespread application in generating images or intricate structures like molecular geometries (Gómez-Bombarelli et al. 2018; Joy et al. 2020; Xu et al. 2023). These models hold paticular appeal to robot design due to their inherent multimodality, rapid execution speed, and their capability to statistically deduce patterns from diverse samples. Nonetheless, their integration into robot design automation remains relatively limited. Existing efforts have primarily concentrated on rigid robots, optimizing fixed-topology design parameters through inter-generation optimization (as opposed to free-form optimization), or mapping robot designs into continuous latent spaces for subsequent optimization using traditional EAs (Spielberg et al. 2019, 2021; Hu et al. 2022; Hu, Whitman, and Choset 2023). Consequently, we contend that the potential of probabilistic generative models in the design automation of soft robot has yet to be fully harnessed.

2.2 Diversity in robot design automation

Diversity of living creatures (i.e. *biodiversity*) is how nature makes life robust to disruptive changes in the environment. Likewise, a long-term goal of Robotics is to build robots that are able to operate reliably in hazardous and dynamic environments (Buchanan et al. 2020). In real-life application, diversified alternatives would be necessary when "first-choice" designs fail and cannot be replaced immediately. However, traditional EAs do not guarantee diversity; on the contrary, they tend to end up with similar solutions for a given task (Miras, Ferrante, and Eiben 2020). To this end, more and more works propose novel techniques in pursuit of diversity (Gupta et al. 2021; Medvet et al. 2021; Hu et al. 2022). Specifically, Hu et al. (2022) verified the intrinsic potential of probabilistic generative models in proposing diverse robots, which we further dig into in this work.

3 MorphVAE

This section commences with an exposition of our pivotal observation concerning shared structures that traverse task boundaries. Then we detail the architecture of MorphVAE and present a training procedure customized for capturing shared knowledge across tasks and evaluated designs. Finally, we introduce two distinct variants of MorphVAE to demonstrate its flexibility in satisfying various purposes.

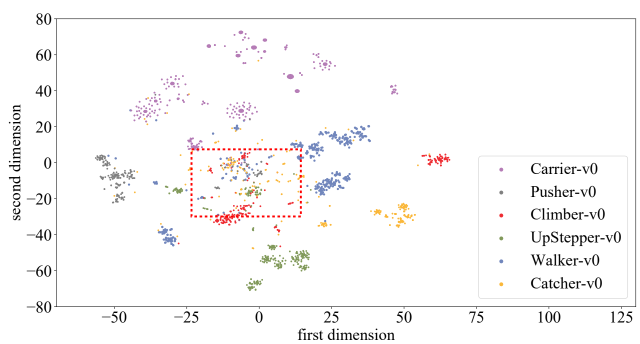


Figure 1: Overlapping of robot designs in multiple tasks

3.1 Shared structures across tasks

We choose Evolution Gym (Bhatia et al. 2021) as simulation environment. In Evolution Gym, the building blocks of voxel-based soft robots include rigid and soft voxels, horizontal and vertical actuators and empty voxel. These components collectively form the 2-D matrix structure of a soft robot. In pilot experiments, we explored multiple existing EAs, including the Genetic Algorithm (GA), Bayesian Optimization (BO) and Compositional Pattern Producing Network evolved with Neural Evolution of Augmenting Topologies (CPPN-NEAT), to independently evolve robot designs

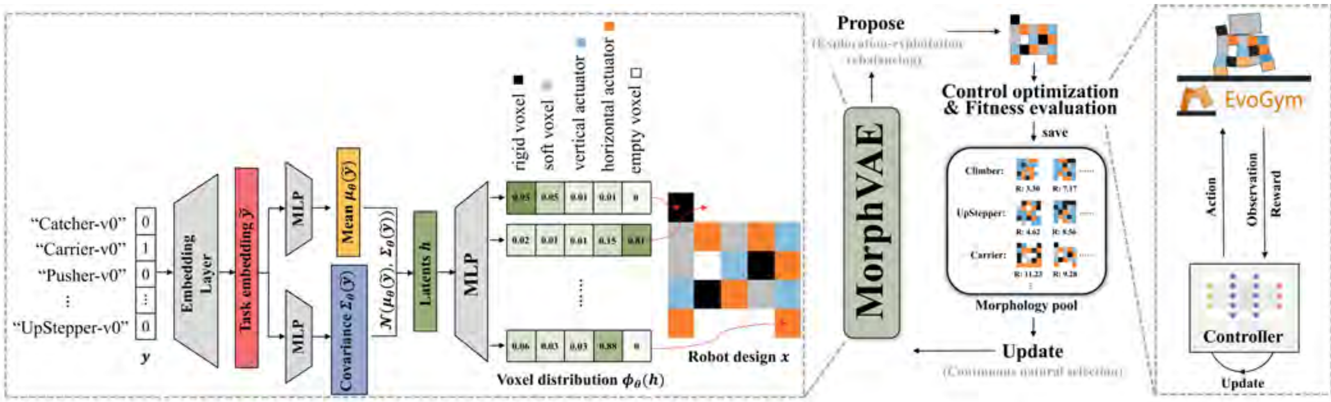


Figure 2: Model architecture and training procedure of MorphVAE. The left dashed box illustrates generative process of MorphVAE, spanning from one-hot tasks encoding to robot design proposals. The circular-flow diagram in the middle outlines the training procedure of MorphVAE. The right dashed box depicts detailed process of a robot to interact with the simulation task, optimize its controller, and ultimately derive its fitness evaluation.

for six tasks in Evolution Gym, conducting 1000 evaluations for each method in each task. Then the top 10% of designs (300 for each task) were selected based on fitness, and using t-SNE algorithm (Van der Maaten and Hinton 2008), their high-performing designs were mapped into a two-dimensional space. As can be seen from Figure 1, robot designs of locomotion and manipulation tasks are generally separate from each other, with exceptions such as the overlap of Catcher with three locomotion tasks, as well as with Pusher (illustrated by the red bounding box), indicating that there exist shared sub-structures among various tasks.

Motivated by this observation, we propose MorphVAE, a novel variational autoencoder for optimizing morphological design of VSRs. MorphVAE integrates a multi-task optimization scheme and employs a unique continuous natural selection method during training. In this manner, design experience (i.e. evaluated robot samples) could be fully leveraged not only longitudinally (i.e. across generations), but also horizontally (i.e. across different tasks), so that sample efficiency would be dramatically improved.

3.2 Model architecture of MorphVAE

The model architecture of MorphVAE consists of two parts, namely the generative process and approximate posterior.

The generative process. The generative process, as illustrated in the left dashed box of Figure 2, is responsible for proposing robot morphology. It consists of a 3-layered hierarchy, i.e., task $\rightarrow$ latent $\rightarrow$ voxel. The generative process takes the type of task, denoted as y, as input and is thus conditional on y. y follows a multinomial distribution and is transformed into an embedding vector denoted as $\tilde{y}$. Each task corresponds to a unique trainable embedding vector that captures its characteristics. Then, $\tilde{y}$ is fed into two sets of Multi-Layered Perceptrons (MLPs) and transformed into a mean vector and a diagonal variance-covariance matrix, which are denoted as $\mu_\theta(\tilde{y})$ and $\Sigma_\theta(\tilde{y})$ respectively, and θ collectively stands for the parameters in the generative process. After that, we sample from the multivariate Gaussian distribution $\mathcal{N}(\mu_\theta(\tilde{y}), \Sigma_\theta(\tilde{y}))$ which yields the latents h. Finally, h is fed into another MLP, denoted as ϕ_θ, to compute the voxel distribution which is made up of a multinomial distribution over all voxel material types per entry of the voxel matrix. For example, for a 5×5 robot, the voxel distribution consists of 25 multinomial distributions, each of which takes 5 possible values namely rigid voxel, soft voxel, vertical actuator, horizontal actuator and empty voxel. Sampling from the voxel distribution leads to a specific robot design denoted as x. The generative process described above is concisely represented as follows.

$$\tilde{y} = \text{Embed}_\theta(y); \quad h \sim \mathcal{N}(\mu_\theta(\tilde{y}), \Sigma_\theta(\tilde{y})); \quad x \sim \phi_\theta(h).$$

The approximate posterior. The true posterior of latents is approximated in order to construct a variational lower bound (typically addressed as the evidence lower bound, ELBO) which is easier to optimize than the original likelihood function. The resulting ELBO is written as

$$\begin{aligned} &E_{y\sim\mathcal{Y}} E_{x\sim\mathcal{X}_y}[E_{h\sim q_\phi(h|x,y)} \log p_\theta(x|h)] \\ &\quad - D_{\text{KL}}(p_\theta(h|y)||q_\phi(h|x,y)), \end{aligned} \tag{1}$$

where $\mathcal{Y}$ denotes a uniform distribution over all tasks, $\mathcal{X}_y$ denotes the distribution of advantageous morphology corresponding to task y, which would be detailed in Section 3.3, p_θ stands for the generative process, and $q_\phi(h|x,y)$ denotes the aforementioned approximate posterior. Please refer to our appendix on Github for more details.

3.3 Training of MorphVAE

Continuous natural selection. In order to customize the training of VAE for robot design automation, we innovatively propose a special training procedure that we term *continuous natural selection*. The procedure mainly features a morphology pool and stepwise updates of parameters. Firstly, note that we follow the popular paradigm of robot co-design as described in Section 2.1, i.e. a two-level optimization problem. Specifically, for the inner loop we adopt the Proximal Policy Optimization (PPO; Schulman et al. (2017)) algorithm for optimizing the controller of a given robot design and returning the cumulated reward (also known as fitness) it obtains, while the outer loop evolves the population of robot designs according to their fitness, and this is where MorphVAE fits in.

In each generation, we generate a population of robot designs with MorphVAE, optimize their controllers and evaluate their fitness. Then we put these designs and corresponding fitness scores into the morphology pool. After that, we sample robots from the morphology pool with replacement according to probabilities positively correlated with fitness (as shown in (2)), and carry out one step of Stochastic Gradient Ascent towards maximizing the ELBO defined in (1) based on the sampled robots. The *sampling and updating* step is carried out multiple times in each generation, and the number of steps linearly increases with the number of generation to prevent premature convergence. Note that better-performing robots have higher probabilities of being chosen, and this yields a robot distribution that favors better designs in each generation. Hence, the generator in VAE is gradually improved in a *bootstrapping* manner. Also note that instead of subjectively setting a threshold and splitting robot designs into good ones and bad ones, we adjust the probability of each robot design showing up in our sample *continuously* according to their fitness. This prevents favorable designs from being omitted or unfavorable ones from sneaking in, and allows us to more fully leverage all the robot designs we have evaluated. This process can be thought of as a continuous and thus more flexible version of natural selection, and is summarized in Algorithm 1. Specifically, the probability of each robot in the pool being chosen is calculated as:

$$P(x_i^h \text{ being chosen}) = \frac{\exp[\tau \cdot f_i^h]}{\sum_{k=1}^{K} \exp[\tau \cdot f_k^h]}, h = 1, \cdots, H, \tag{2}$$

where x_i^h denotes the i-th robot of task h, f_i^h denotes the fitness of x_i^h, H is the total number of tasks, K is the total number of robots corresponding to task h in the pool, and τ is a temperature parameter controlling the strength of selection pressure. With a higher τ, we more exclusively favor best-performing robots, while with a lower τ, we spare some of our attention for slightly worse-performing robots as well. We would verify later in our experiments that τ provides us with great convenience in balancing between optimization efficiency and biodiversity.

Exploration-exploitation rebalancing. In order to further boost diversity in robot designs, we propose a technique called *exploration-exploitation rebalancing*. To be more specific, since the VAE is fitted repeatedly with robot samples drawn from the morphology pool, it might become too conservative and produce morphologies that greatly resemble existing ones in later generations. In this work, we term a morphology with no less than $s\%$ same voxels with at least one existing morphology as a sample of "exploitation", or otherwise a sample of "exploration". In each generation, we query the VAE model repeatedly until a pre-specified number of "exploration" samples have been generated. In this manner, our VAE model is encouraged to adventurously try

Algorithm 1: Continuous natural selection

Input: A morphology pool (including both evaluated robot designs and their fitnesses, denoted as $\mathcal{M}$) of size K for each task; The number of morphologies, denoted as N, to draw from the pool for each task; The temperature parameter τ.
Output: A sample of N high-performing robot designs for each task, denoted as $\mathcal{S}$.
Calculate the probability of each robot design in $\mathcal{M}$ showing up in the sample according to (2), and denote it as p_i^h.
Initialize $\mathcal{S} = \Phi$.
for $h = 1, 2, \cdots, H$ **do**
  for $n = 1, 2, \cdots, N$ **do**
    Sample a robot design of task h from $\mathcal{M}$ according to p_i^h; Append it to $\mathcal{S}$.
Return: $\mathcal{S}$.

out diverse robot designs and prevented from too desperately exploiting favorable robot designs in the morphology pool. In our experiments, we set s as 75, and schedule the proportion of "exploration" samples in each generation to linearly decrease from 50% to zero. The overall training procedure of MorphVAE is illustrated in the right half of Figure 2, and summarized in Algorithm 2.

4 Experiments

4.1 Experimental setup

Our experiments are based on six tasks in Evolution Gym (Bhatia et al. 2021), among which three are locomotion tasks (Walker-v0, Climber-v0, UpStepper-v0) and three are manipulation tasks (Catcher-v0, Carrier-v0, Pusher-v0); Please refer to our appendix on Github for a detailed introduction to these tasks. Following the standard practice in the literature (Cheney, Clune, and Lipson 2014; Marzougui, Biondina, and wyffels 2022; Mertan and Cheney 2023), we limit our robot designs to a 5×5 bounding box to keep the search space tractable. We employ the PPO algorithm (Schulman et al. 2017) as mentioned in Section 3.3 for controller optimization and robot evaluation, where both the actor and critic are modeled as a fully-connected neural network with 2 hidden layers, each consisting of 64 hidden units, and Tanh as the non-linear activation function. We report comparison results with competitive baselines as well as between different variants of our method. For every method in each task, we carry out a maximum of 1000 robot design evaluations to allow for thorough morph evolution. All the experimental results are averaged across three independent runs. Our experiments are conducted on four servers, each equipped with an Intel Xeon Silver 4214 CPU @ 2.20GHz and 4 NVIDIA Titan RTX GPUs, running Ubuntu 22.04. Our codes, together with an appendix including hyperparameters and additional analysis of experimental results, are available on Github (https://github.com/WoodySJR/MorphVAE).

Algorithm 2: The training procedure of MorphVAE

Input: Parameters of MorphVAE - number of tasks H, morphology size w (default=5), numbers of hidden layers and hidden units in MLP, schedule for the number of updates per generation m_t, number of robot samples per update n_t, temperature parameter τ in (2), threshold for morphology similarity s and the proportion of "exploration" samples β_t as mentioned in Section 3.3, learning rate α, number of generations T, and population size P.

Output: Optimized parameters in VAE, evolved robot designs and their controllers.

Initialize VAE model according to given parameters;

for $t = 1, 2, \cdots, T$ **do**

  Step 1: proposing robot designs

  Repeatedly query the VAE model until $P \times \beta_t$ exploration samples (i.e. have fewer than $s \times w^2$ same voxels with all existing designs) have been generated for each task;

  Step 2: evaluating robot designs

  Optimize controllers of robot designs in the current population; Store these designs, along with their fitness, into the morphology pool;

  Step 3: updating VAE parameters

  for $i = 1, 2, \cdots, m_t$ **do**

    Sample $H \times n_t$ robot designs (n_t for each task), denoted as $\mathcal{S}$, from the morphology pool through continuous natural selection as defined in Algorithm 1.

    Do one step of Stochastic Gradient Ascent towards maximizing the ELBO defined in (1), based on $\mathcal{S}$.

Return: VAE parameters and the morphology pool (including $H \times T \times P$ robot designs, together with their fitness and controllers.)

4.2 MorphVAE for high-performance and biodiversity

In order to demonstrate the great flexibility afforded by MorphVAE, we propose two variants that focus on the efficiency of finding advantageous robot designs and the diversity of robot designs, respectively. The former variant is denoted as **MorphVAE-H**(igh performance), where the temperature parameter τ in (2) is set as 1.5. The latter variant is denoted as **MorphVAE-B**(iodiversity), where τ is set as 0.7 and exploration-exploitation rebalancing is utilized for a wider range of design search.

4.3 Baselines

We first benchmark our method against the following competitive baselines.

- **CPPN-NEAT:** Compositional Pattern Producing Network (CPPN), originally used for generating high-resolution geometric patterns, is one of the predominant approaches to soft robot design in existing literature (Cheney, Clune, and Lipson 2014; Cheney et al. 2014; Corucci et al. 2018; Bhatia et al. 2021). It takes the spacial coordinates of a robot voxel as input, and outputs the corresponding voxel type. We obtain a robot by querying the CPPN of all spacial coordinates in a voxel matrix. NeuroEvolution of Augmenting Topologies (NEAT) is used to optimize the architectures and weights of CPPNs with mutation, crossover and selection operators.
- **Bayesian Optimization (BO):** Bayesian Optimization (Kushner 1964; Močkus 1975) is commonly used to optimize functions that are expensive to evaluate. In this work, we use the Gaussian Process as the surrogate model of the objective function (i.e. the mapping from robot design to fitness), and use the expected improvement as the acquisition function.
- **Genetic Algorithm (GA)**: GA (Zbigniew 1996) is inspired by "the survival of the fittest" in nature. It selects the best-performing robots in each generation as survivors and randomly mutate their voxel types to produce offspring. The $\mu + \lambda$ generational model is used where parents and their children are merged together.

The implementation of CPPN-NEAT, BO and GA strictly follows Bhatia et al. (2021). We introduce two more state-of-the-art methods to further demonstrate the advantages of MorphVAE in generating both high-performing and diverse robot designs:

- **Speciated Evolver (SE)**: SE has been proven by Medvet et al. (2021) to be a superior algorithm for optimizing VSRs in locomotion tasks, in terms of both the traveling distance and diversity. It is a modification of GA that in each generation first clusters robots into several species with k-means algorithm and then carries out natural selection per species, thus encouraging the diversity of robot designs.
- **roboGAN**: roboGAN has been proven by Hu et al. (2022) to be superior over conventional GA for optimizing design parameters with fixed topologies. In each generation, roboGAN treats robot designs proposed by the generator as negative samples. Subsequently, these designs undergo several iterations of GA evolution to yield positive samples, progressively guiding the generator towards higher-performing regions.

To allow for fair comparison and thorough morph evolution, we set the number of robot evaluations to 1000 for each method in each task. With a population size of 25, it results in 40 generations for CPPN-NEAT, BO and MorphVAE; The numbers of generations for GA and SE are 63 and 46 respectively, due to their reservation of parents in subsequent generations whose controllers need not be optimized. As for roboGAN, we set the population size as 20 and the number of GA steps in each generation as 4 with a survival rate of 0.5, leading to 50 evaluations per generation and a total of 20 generations. Notably, both roboGAN and MorphVAE incorporate a multi-task training approach. We additionally drew comparisons with two more baselines which leverage Action Inheritance (Liu et al. 2023) and Random Forest (Sun et al. 2020) respectively, but relegate the results to our appendix on Github due to space limit.

4.4 Evaluation metrics

We employ three metrics to facilitate a comprehensive comparison among different methods.

- **Maximal fitness:** The fitness of the best-performing robot, given the number of evaluations. This is widely used in the literature of robot design to evaluate the efficiency of optimization, as the primary emphasis in most cases is on achieving optimal design.
- **Fitness distribution:** The distribution of fitnesses yielded throughout evolution, depicted with boxplots, characterizes overall performance of robot designs generated by an algorithm, and provides distributional information that complements the single-dimensional summaries and facilitates more comprehensive comparisons.
- **Diversity:** The diversity metric assesses a population's capacity to adapt to dynamic environments. It has been a longstanding evaluation criterion in previous literature to gauge the effectiveness of robot design algorithms (Medvet et al. 2021; Pigozzi et al. 2023). See our appendix on Github for more details about how we measure diversity.

4.5 Comparison study

In this section, we present and interpret the results of our comparison study according to the metrics in Section 4.4.

Maximal fitness. The comparisons of maximal fitness are demonstrated in Figure 3. It can be seen that MorphVAE-H significantly outperforms the other competitors in the first four of the six tasks and shows competitive performance in the last two (i.e. Walker-v0 and Catcher-v0), in terms of the efficiency of finding high-performing robot designs. Specifically, in tasks Carrier-v0 and Pusher-v0, MorphVAE-H outperforms the other competitors in both the speed of convergence and fitness of the optimal design. In addition, while MorphVAE-B shows similar or slightly poorer performance than MorphVAE-H, it still outperforms the other competitors with obvious advantages. In tasks Climber-v0 and UpStepper-v0, the advantage of MorphVAE-H is even more obvious. In Walker-v0 and Catcher-v0, MorphVAE shows competitive speed of convergence to a certain level of maximal fitness, after which it has difficulty further improving compared with other algorithms.

The results could be explained as follows. For challenging tasks, such as Climber-v0 and UpStepper-v0, specific advantageous sub-structures are essential for a robot's success. For instance, successful climbers, such as the four robots on the left-hand side of Figure 4, demand horizontal actuators both in its upper and lower body parts, leading to alternate force bearing points against the pipe wall, and meanwhile requires vertical actuators in the middle to pull the whole body upwards. Any departure from such specific structures, such as the four robots on the right in Figure 4, would very likely lead to an unqualified climber that hovers at the bottom of the pipe all the way. This necessitates an algorithm that can effectively learn from past evaluations and deduce discernible patterns from them. This is precisely where MorphVAE comes into play. It adopts a multi-task training approach and assimilates knowledge from a diverse range of task-specific morphological pools, thereby significantly enhancing sample efficiency.

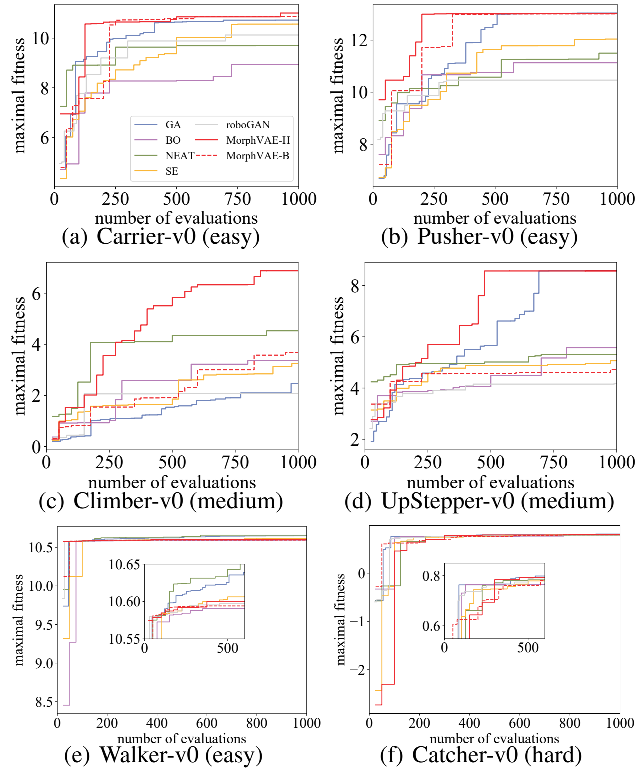


Figure 3: Performance comparison of maximal fitness

In the context of less demanding tasks such as Carrier-v0 and Pusher-v0, functional sub-structures are easier to evolve, resulting in a diminished advantage for MorphVAE. On the other hand, for tasks Walker-v0 and Catcher-v0, the former is too simple that neutral designs suffice for a controller to excel and the latter is considerably hard that few trials meet the requirements. Consequently, fitness evaluations in these two tasks offer less explicit directions toward high-performing designs, leaving room for other competitive algorithms, especially GA which mutates upon single survivors and searches for delicate structures that lead to marginal improvements, to achieve superior performance. Besides, the strikingly unsatisfactory performance of roboGAN is possibly due to its low sample efficiency, as it requires multiple steps of GA to obtain positive samples and employs evaluated robot designs only once during evolution.

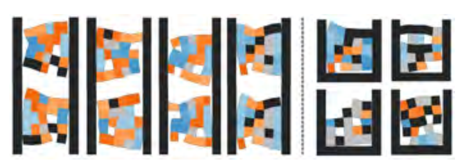
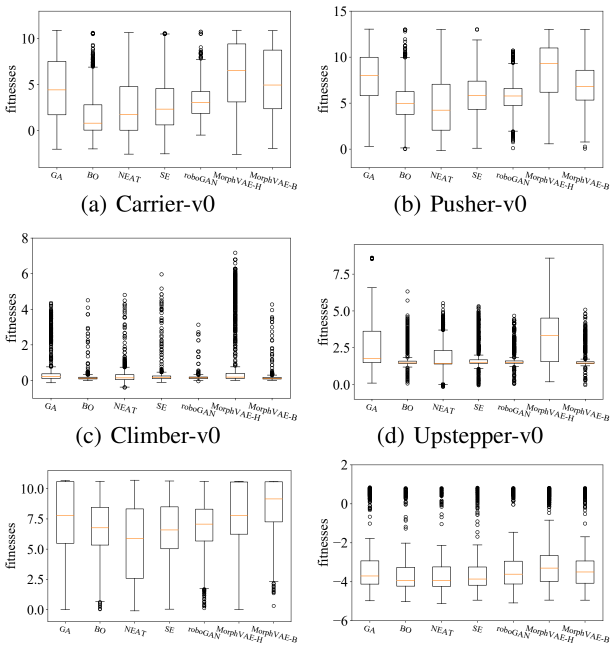


Figure 4: Qualified (left) and unqualified (right) climbers

Fitness distribution. The distribution of robot fitnesses obtained by different algorithms throughout the course of evolution are shown as boxplots in Figure 5. Overall, we find the fitness distributions of MorphVAE-H locate higher than baselines in all tasks, with greater quartiles or more outliers at the top. That is, in addition to the optimal robot designs, MorphVAE-H reveals obvious superiority in terms of overall performance as well; See results of the Wilcoxon Rank Sum test that statistically justify the significance of such superiority in our appendix on Github. Meanwhile, although MorphVAE-B features a larger extent of exploration in design search, it still achieves superior or at least comparable results to its counterparts. Furthermore, we investigate into different algorithms' consistency in generating high-performing robot designs during evolution, which could be relevant in practical deployment, and discover the distinct advantage of MorphVAE in this respect as well; The results are included in our appendix on Github.



(a) Carrier-v0 (b) Pusher-v0

(c) Climber-v0 (d) Upstepper-v0

(e) Walker-v0 (f) Catcher-v0

Figure 5: Boxplots of fitness obtained by different methods

Diversity. Here we evaluate the diversity of robot designs, and demonstrate the advantage of MorphVAE-B in this respect. As it would be meaningless to look into the diversity of poor robot designs, we first put together the robot designs obtained by all methods and select top $k\%$ percent for comparision. As illustrated in Figure 6, while MorphVAE-B does not consistently come in first, its performance in maintaining diversity is much more stable than other baselines.

By averaging the ranks across six tasks for different methods, we have rankings [5.83, 2.67, 3.83, 4.67, 3.0, **2.17**, 5.83] for $k = 10$ and [5.0, 2.17, 4.17, 5.17, 4.5, **1.83**, 5.17] for $k = 5$, in the order of GA, BO, NEAT, SE, roboGAN, MorphVAE-B and MorphVAE-H. The results indicate that MorphVAE-B outperforms other baselines on average in terms of robot diversity. Note that roboGAN achieves comparable or higher diversity than MorphVAE in quite a few cases, substantiating the intrinsic potential of probabilistic generative models in this respect; Nonetheless, roboGAN fails to produce well-performing robot designs altogether in many other cases. It is also worth noting that BO reveals a remarkable potential to promote diversity as well, which is largely due to the fact that its acquisition function manages to strike a balance between exploration and exploitation.

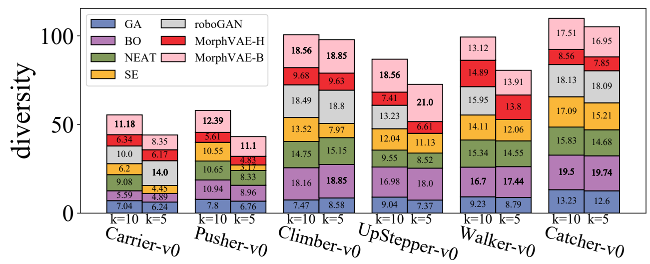


Figure 6: Performance comparison of diversity. In some cases such as roboGAN in Pusher-v0, the algorithm fails to produce more than one robot design that could enter top k percent and thus diversity is not available.

Combining results in Section 4.5, we confirm that MorphVAE has a greater edge in tasks that more exclusively require specific morphological structures, and that it has great flexibility to adapt to different purposes (i.e. optimization efficiency or diversity) and achieve leading performance.

5 Conclusions

In this work, we propose MorphVAE, a novel approach to free-form soft-robot design automation that leverages probabilistic generative models. Our approach stems from the observation drawn from pilot experiments that high-performing robot designs across different tasks exhibit substantial overlap. To harness this insight, we adopt a multi-task training scheme to promote knowledge sharing between tasks. We also propose a novel sampling technique termed *continuous natural selection* to customize the training of VAE for robot design automation, which not only improves the generator in a bootstrapping manner without any reliance on existing EAs, but also affords us great flexibility between optimization efficiency and diversity. The combined impact of multi-task training and continuous natural selection allows us to exploit evaluated robot designs both across generations and tasks, significantly improving sample efficiency. Furthermore, We present a sampling method, termed *exploration-exploitation rebalancing* to further enlarge the range of morphology search in MorphVAE and yield more diverse morphologies. Through extensive experiments encompassing manipulation and locomotion tasks, we demonstrate the efficacy of MorphVAE in efficiently optimizing and consistently proposing high-performing and diversified designs. However, we notice the slightly poorer performance of MorphVAE in extremely simple and hard tasks, and suppose that using controllers with adaptive complexity could relieve this problem; We leave this for our future work.

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References

Bhatia, J.; Jackson, H.; Tian, Y.; Xu, J.; and Matusik, W. 2021. Evolution gym: A large-scale benchmark for evolving soft robots. *Advances in Neural Information Processing Systems*, 34: 2201–2214.

Buchanan, E.; Le Goff, L. K.; Li, W.; Hart, E.; Eiben, A. E.; De Carlo, M.; Winfield, A. F.; Hale, M. F.; Woolley, R.; Angus, M.; et al. 2020. Bootstrapping artificial evolution to design robots for autonomous fabrication. *Robotics*, 9(4): 106.

Cheney, N.; Bongard, J.; and Lipson, H. 2015. Evolving soft robots in tight spaces. In *Proceedings of the 2015 annual conference on Genetic and Evolutionary Computation*, 935–942.

Cheney, N.; Clune, J.; and Lipson, H. 2014. Evolved electrophysiological soft robots. In *Artificial life conference proceedings*, 222–229. MIT Press One Rogers Street, Cambridge, MA 02142-1209, USA journals-info . . . .

Cheney, N.; MacCurdy, R.; Clune, J.; and Lipson, H. 2014. Unshackling evolution: evolving soft robots with multiple materials and a powerful generative encoding. *ACM SIGEVOlution*, 7(1): 11–23.

Corucci, F.; Cheney, N.; Giorgio-Serchi, F.; Bongard, J.; and Laschi, C. 2018. Evolving soft locomotion in aquatic and terrestrial environments: effects of material properties and environmental transitions. *Soft robotics*, 5(4): 475–495.

Gómez-Bombarelli, R.; Wei, J. N.; Duvenaud, D.; Hernández-Lobato, J. M.; Sánchez-Lengeling, B.; Sheberla, D.; Aguilera-Iparraguirre, J.; Hirzel, T. D.; Adams, R. P.; and Aspuru-Guzik, A. 2018. Automatic chemical design using a data-driven continuous representation of molecules. *ACS central science*, 4(2): 268–276.

Goodfellow, I.; Pouget-Abadie, J.; Mirza, M.; Xu, B.; Warde-Farley, D.; Ozair, S.; Courville, A.; and Bengio, Y. 2020. Generative adversarial networks. *Communications of the ACM*, 63(11): 139–144.

Gupta, A.; Savarese, S.; Ganguli, S.; and Fei-Fei, L. 2021. Embodied intelligence via learning and evolution. *Nature communications*, 12(1): 5721.

Ha, H.; Agrawal, S.; and Song, S. 2021. Fit2Form: 3D generative model for robot gripper form design. In *Conference on Robot Learning*, 176–187. PMLR.

Hiller, J.; and Lipson, H. 2011. Automatic design and manufacture of soft robots. *IEEE Transactions on Robotics*, 28(2): 457–466.

Ho, J.; Jain, A.; and Abbeel, P. 2020. Denoising diffusion probabilistic models. *Advances in neural information processing systems*, 33: 6840–6851.

Hu, J.; Whitman, J.; and Choset, H. 2023. GLSO: Grammar-guided Latent Space Optimization for Sample-efficient Robot Design Automation. In *Conference on Robot Learning*, 1321–1331. PMLR.

Hu, J.; Whitman, J.; Travers, M.; and Choset, H. 2022. Modular robot design optimization with generative adversarial networks. In *2022 International Conference on Robotics and Automation (ICRA)*, 4282–4288. IEEE.

Joy, T.; Schmon, S. M.; Torr, P. H.; Siddharth, N.; and Rainforth, T. 2020. Capturing label characteristics in vaes. *arXiv preprint arXiv:2006.10102*.

Kingma, D. P.; and Welling, M. 2013. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*.

Kushner, H. 1964. A New Method of Locating the Maximum Point of an Arbitrary Multipeak Curve in the Presence of Noise. *Journal of Basic Engineering*, 86(1): 97–106.

Leger, C. 2012. *Darwin2K: An evolutionary approach to automated design for robotics*, volume 574. Springer Science & Business Media.

Liu, S.; Yao, W.; Wang, H.; Peng, W.; and Yang, Y. 2023. Rapidly Evolving Soft Robots via Action Inheritance. *IEEE Transactions on Evolutionary Computation*, 1–1.

Marzougui, D.; Biondina, M.; and wyffels, F. 2022. A comparative analysis on genome pleiotropy for evolved soft robots. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, 136–139.

Medvet, E.; Bartoli, A.; Pigozzi, F.; and Rochelli, M. 2021. Biodiversity in evolved voxel-based soft robots. In *Proceedings of the Genetic and Evolutionary Computation Conference*, 129–137.

Mertan, A.; and Cheney, N. 2023. Modular Controllers Facilitate the Co-Optimization of Morphology and Control in Soft Robots. *arXiv preprint arXiv:2306.09358*.

Miras, K.; Ferrante, E.; and Eiben, A. E. 2020. Environmental influences on evolvable robots. *PloS one*, 15(5): e0233848.

Močkus, J. 1975. On Bayesian methods for seeking the extremum. In *Optimization Techniques IFIP Technical Conference: Novosibirsk, July 1–7, 1974*, 400–404. Springer.

Pfeifer, R.; and Bongard, J. 2006. *How the body shapes the way we think: a new view of intelligence*. MIT press.

Pfeifer, R.; Iida, F.; and Lungarella, M. 2014. Cognition from the bottom up: on biological inspiration, body morphology, and soft materials. *Trends in cognitive sciences*, 18(8): 404–413.

Pigozzi, F.; Medvet, E.; Bartoli, A.; and Rochelli, M. 2023. Factors Impacting Diversity and Effectiveness of Evolved Modular Robots. *ACM Transactions on Evolutionary Learning*, 3(1): 1–33.

Schulman, J.; Wolski, F.; Dhariwal, P.; Radford, A.; and Klimov, O. 2017. Proximal policy optimization algorithms. *arXiv preprint arXiv:1707.06347*.

Spielberg, A.; Amini, A.; Chin, L.; Matusik, W.; and Rus, D. 2021. Co-learning of task and sensor placement for soft robotics. *IEEE Robotics and Automation Letters*, 6(2): 1208–1215.

Spielberg, A.; Zhao, A.; Hu, Y.; Du, T.; Matusik, W.; and Rus, D. 2019. Learning-in-the-loop optimization: End-to-end control and co-design of soft robots through learned deep latent representations. *Advances in Neural Information Processing Systems*, 32.

Sun, Y.; Wang, H.; Xue, B.; Jin, Y.; Yen, G. G.; and Zhang, M. 2020. Surrogate-Assisted Evolutionary Deep Learning Using an End-to-End Random Forest-Based Performance Predictor. *IEEE Transactions on Evolutionary Computation*, 24(2).

Van der Maaten, L.; and Hinton, G. 2008. Visualizing data using t-SNE. *Journal of machine learning research*, 9(11).

Wang, T.; Zhou, Y.; Fidler, S.; and Ba, J. 2019. Neural graph evolution: Towards efficient automatic robot design. *arXiv preprint arXiv:1906.05370*.

Xu, M.; Powers, A. S.; Dror, R. O.; Ermon, S.; and Leskovec, J. 2023. Geometric latent diffusion models for 3d molecule generation. In *International Conference on Machine Learning*, 38592–38610. PMLR.

Zbigniew, M. 1996. Genetic algorithms+ data structures= evolution programs. *Comput Stat*, 372–373.