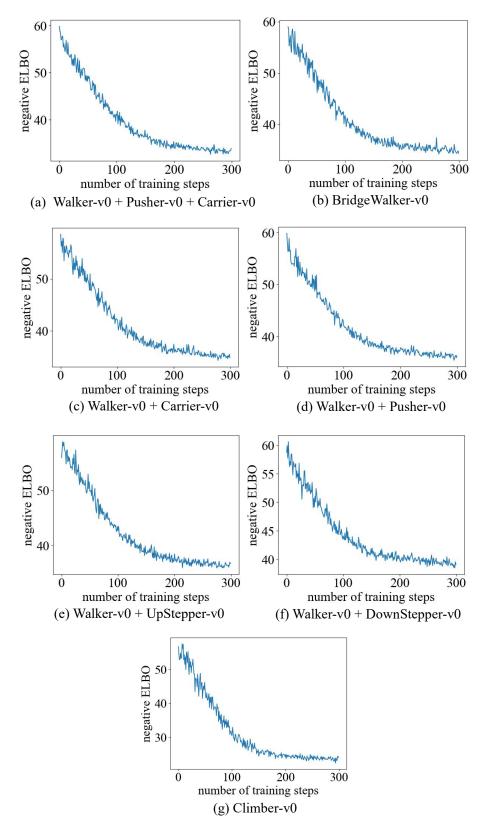
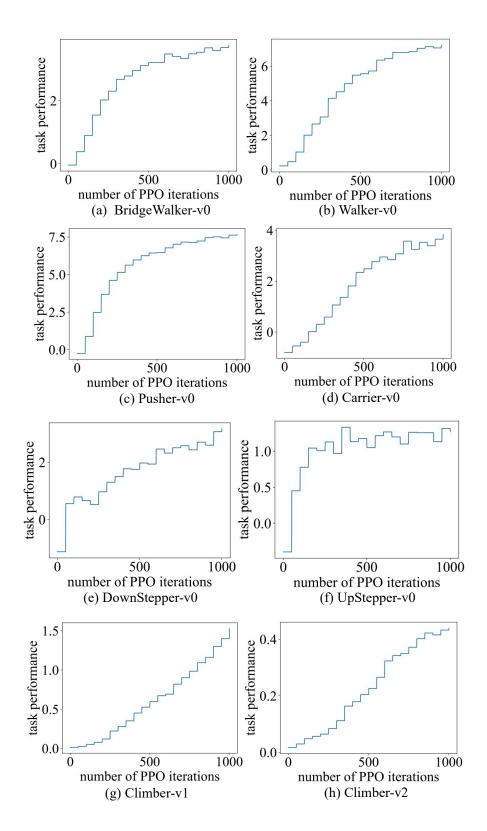
RoboLDA: A Probabilistic Generative Model for Uncovering Embodied Hierarchical Structures within Voxel-based Soft Robot Morphology

Supplementary Material 1: Learning curves of RoboLDA and PPO algorithm



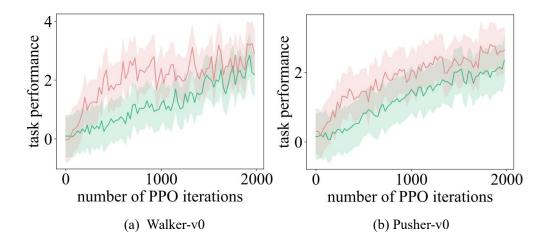
Supplementary Figure 1: Learning curves of RoboLDA. The caption of each subplot represents the corresponding training tasks (listed in Table 1 of the paper).



Supplementary Figure 2: Average learning curves of PPO for evaluating zero-shot fitness in Table 2 of the paper. We have chosen the same parameter setting as in [1] across all baseline algorithms to ensure fair comparison.

Reference:

[1] Bhatia, Jagdeep, et al. "Evolution gym: A large-scale benchmark for evolving soft robots." *Advances in Neural Information Processing Systems* 34 (2021): 2201-2214.

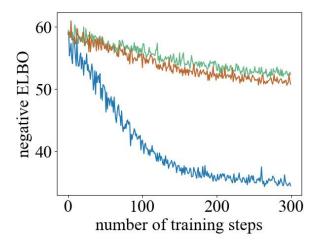


Supplementary Figure 3: Additional control experiments, where the organ structures inferred by RoboLDA are applied to SOLAR[1] (**red**). The results outperform the original version of SOLAR (**green**), validating the generalizability of RoboLDA to other universal controllers beyond MetaMorph.

Reference:

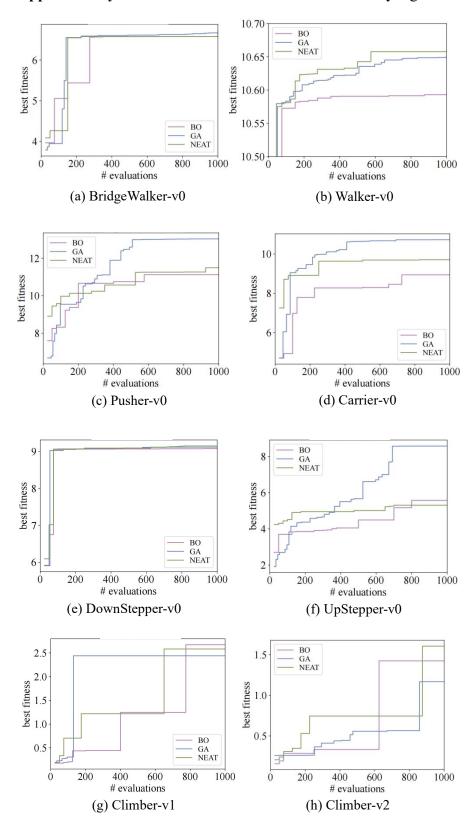
[1] Dong, Heng, et al. "Low-rank modular reinforcement learning via muscle synergy." *Advances in Neural Information Processing Systems* 35 (2022): 19861-19873.

Supplementary Material 3: Justification of using high-performing samples for morphological modeling



Supplementary Figure 4: Influence of sample quality on the training of RoboLDA. **Blue** represents original results reported in the paper (*i.e.*, using top-ranking morphologies), green represents medium-quality morphologies (*i.e.*, those residing between 60% and 90% fitness quantiles), and **brown** represents low-quality morphologies (residing between 30%~60%). The latter two have higher loss curves (poorer goodness of fit), indicating that they lack consistent and distinct hierarchical structures which are more likely to exist in high-performing designs.

Supplementary Material 4: Fitness curves of evolutionary algorithms



Supplementary Figure 5: Fitness curves of evolutionary algorithms (EAs). The horizontal axis represents the number of robot evaluations, while the vertical axis represents the maximal fitness obtained within a given number of evaluations.

Supplementary Material 5:

Similarity analysis between zero-shot designs and training data

Supplementary Table 1: Similarity analysis of zero-shot generated morphologies and training data. Similarity is measured by first calculating the percentage of identical voxels within each pair of zero-shot sample and training sample, and then taking an average.

Task	Similarity
BridgeWalker-v0	46.3%
Walker-v0	53.3%
Pusher-v0	43.7%
Carrier-v0	42.3%
DownStepper-v0	44.9%
UpStepper-v0	37.7%
Climber-v1	85.6%
Climber-v2	83.6%

Supplementary Material 6: Sensitivity analysis of random initialization

Supplementary Table 2: Sensitivity analysis of RoboLDA to random initialization. The results are obtained from three random trials. The variation in Pusher-v0 and Carrier-v0 is higher than others, mainly due to the additional stochasticity introduced by object manipulation. However, their coefficient of variation is only slightly over 0.1, indicating stability across different trials.

Task	Average zero-shot fitness (avg)	Standard Deviation (std)	Coefficient of Variation (std/avg)
BridgeWalker-v0	6.570	0.004	< 0.001
Walker-v0	10.621	0.003	< 0.001
Pusher-v0	11.277	1.213	0.108
Carrier-v0	9.757	1.098	0.113
DownStepper-v0	9.070	0.006	< 0.001
UpStepper-v0	4.316	0.277	0.064
Climber-v1	5.684	0.050	0.009
Climber-v2	1.737	0.027	0.016

Supplementary Material 7:

Additional comparison studies of zero-shot generalization

Table 2 (updated): Comparisons of zero-shot fitness with more baseline algorithms.

Task	RoboLDA	MorphVAE	PreCo	RoboGAN	BO/GA	CPPN
BridgeWalker-v0	6.57	6.12	3.60	3.97	3.94	6.57
Walker-v0	10.65	10.64	-	8.45	9.85	6.42
Pusher-v0	11.42	11.22	-	7.60	7.79	9.67
Carrier-v0	8.47	8.61	-	4.70	5.98	6.58
DownStepper-v0	9.07	9.06	7.10	5.92	6.00	6.21
UpStepper-v0	5.13	3.65	-	2.71	3.08	2.41
Climber-v1	5.78	3.25	-	0.21	0.54	0.25
Climber-v2	1.75	0.73	-	0.27	0.23	0.26
GapJumper-v0	5.81	4.37	4.50	3.65	2.65	3.41

Note: the results of PreCo are derived from the bar chart in [1]; We are currently working on re-implementing PreCo on the remaining tasks, and results will be updated once available. Newly added baseline algorithms and task are marked using red font.

Reference:

[1] Wang, Yuxing, et al. "Preco: Enhancing generalization in co-design of modular soft robots via brain-body pre-training." *Conference on Robot Learning*. PMLR, 2023.

Supplementary Material 8:

Augmenting training data with manually designed samples

Supplementary Table 3: We manually designed 100 BridgeWalkers and use them to augment the training data. The zero-shot fitness in Walker-v0 exhibits a slight decrease. We believe this is because the voxel assembly in VSRs are abstract and counter-intuitive, rendering its design highly demanding for humans. This argument has also been made in [1].

Training data composition	High-performing BridgeWalkers	Higher-performing BridgeWalkers + 100 manual designs
Zero-shot fitness in Walker-v0	10.621 (0.003)	10.609 (0.005)

Reference:

[1] Song, Junru, et al. "LASeR: Towards Diversified and Generalizable Robot Design with Large Language Models." *The Thirteenth International Conference on Learning Representations*.