

## Supplementary material 7: LLM’s interpretation of robot design

In our preliminary experiments, we included explicit LLM reasoning, where the LLM was prompted to explain its design choices (similar to chain-of-thought). However, we observed no significant performances gains by doing so, and therefore opted to remove the reasoning process to speed up evolution and save computational costs. Nevertheless, we would like to clarify that **our approach is capable of affording higher interpretability**. This can readily be achieved by explicitly instructing the LLM to explain its decision-making process, rather than serving as a black box. We provide in **Supplementary figure 7** (on next page) the output generated by GPT-4o-mini after receiving a collection of high-performing Catcher-v0 designs and instructed to generate a new one with higher performance. The explanations provided are insightful and reasonable, revealing the advantageous structures present in high-performing designs. This suggests that LLMs are indeed able to **align specific voxel assembly patterns with high performance**, and **leverage these principles to generate improved offspring solutions**.

The designs provided demonstrate several key principles that contribute to their performance in the Catcher-v0 task, where the goal is to catch and carry a box. Here's a summary of observed design principles:

- 1. Structural Stability:** The bottom row is consistently filled with rigid and soft voxels, which provide a solid foundation and enhance stability when carrying loads. Rigid voxels are typically positioned towards the bottom or at critical structural points to resist deformation under load.
- 2. Effective Use of Actuators:** The designs incorporate both horizontal and vertical actuators strategically. This allows for dynamic adjustments to the robot's shape to better engage with the carried box. The placement of actuators near the center of mass or at junctions of flexible structures facilitates effective load distribution and manipulation.
- 3. Balance of Soft and Rigid Voxels:** A mix of soft and rigid voxels provides the flexibility needed for absorbing shocks while also maintaining structural integrity. Designs often use soft voxels in upper layers to allow for some deformation without compromising overall structure, which can help absorb impacts when catching the box.
- 4. Optimized Catching Mechanism:** Successful designs tend to have a specific configuration that aids in maximizing the area available for catching the box. This often involves using soft voxels around the central area to create a "cushion" effect. The presence of empty voxels strategically placed helps optimize the weight distribution and maneuverability.
- 5. Symmetry and Connectivity:** Many designs exhibit symmetrical features, which can help ensure balanced weight distribution and stability during movement. The connectivity between adjacent voxels supports resilience against shear forces and promotes coordinated movements, particularly important during the catch-and-carry process.
- 6. Adaptability:** The ability to dynamically adjust through the actuators enables the robot to adapt to various scenarios—this is critical when dealing with different box sizes or weights.

Here's a proposed new catcher design aimed at enhancing proficiency in the task:

```
proposed_design = np.array([[3, 4, 0, 2, 1], [1, 4, 3, 1, 3], [3, 2, 4, 3, 4], [4, 1, 2, 3, 1], [0, 1, 2, 1, 2]])
```

#### Design Features:

- 1. Enhanced Stability:** The bottom row consists of two rigid voxels flanking a soft voxel providing a stable base while allowing slight deformation.
- 2. Improved Actuation:** The second row contains two actuators (one vertical and one horizontal), enabling more versatile manipulations and adaptations to different box sizes.
- 3. Strategic Placement of Soft Voxels:** The arrangement of soft voxels in the middle provides cushioning during the catch phase, helping to absorb any sudden movements.
- 4. Central Weight Distribution:** The design emphasizes centralized soft voxels, allowing for effective engagement and support of the box once caught.
- 5. Flexibility and Adaptation:** Additional soft voxels above the actuators ensure adaptability in height and width as needed, improving the ability to secure and carry the box efficiently.

This proposed design aims to leverage the advantages of existing high-performing designs while introducing modifications that could enhance its capacity to perform well in the 'Catcher-v0' task. By emphasizing stability, adaptability, and an effective actuation mechanism, this design could potentially outperform prior iterations.

**Supplementary figure 7.** The LLM-generated output on Catcher-v0. In this example, the LLM is prompted to explain its decision-making process when generating a new robot design.