Model shows evolution had many optimal outcomes to choose from

Is there only one optimal configuration an organism can reach during evolution?

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Is there only one optimal configuration an organism can reach during evolution? Is there a single formula that describes the trajectory towards the optimum? And can we 'derive' it in a purely theoretical fashion?

A team of researchers, including from the Institute of Science and Technology Austria (ISTA), has answers. Their mathematical model forecasts the ideal body plan of a fruit fly's early embryo, suggesting that evolution might have had many optimal options at its disposal.

It is hypothesized that optimization is the secret sauce for many of nature's fascinating phenomena, suggesting the world is driven toward a state of minimal energy, the most efficient output, or the highest fitness. Whether it is pods of whales or collectives of tiny cells, life's building blocks have been selected to self-organize close to peak efficiency.

The development of an animal embryo, from a small cluster of cells to a multicellular organism, might also have been optimized and fine-tuned to an almost perfect system. However, a precise mathematical formula predicting the optimal structure has been elusive until now.

Physicists from the Institute of Science and Technology Austria (ISTA), the Frankfurt Institute for Advanced Studies, and Princeton University now present exactly that: A theoretical model of the fruit fly's early embryonic development, nearly two decades in the making.

With their detailed model, they could theoretically derive and thus predict the optimal 'wiring' of the gene-regulation network that controls the early developmental processes. The results are published in *PNAS*.

Evolution = optimization

Evolution is the driving force for every organism. Given its environment, an organism adapts, survives, and withstands selective pressure. "Adaptation can be seen as an optimization process, or at least as a process that requires optimization of certain traits and functions," explains Thomas Sokolowski, first author of the study.

Compared to physical systems, where optimization typically leads to a final state with the lowest energy, biological systems seem to have multiple optimal solutions for the same problem. For instance, eyes evolved independently in various animals, yet their overall structure is remarkably similar across species.

"Eyes were optimized for the same well-defined objective function, which is maximal uptake of light and its encoding into neural spikes. They are therefore strongly dictated by laws of physics. Nuanced differences between animals may be explained by differences in the side circumstances under which they evolved," Sokolowski continues.

Also, for the development of various embryos, many diverse strategies have evolved. They all share the same outcome: a highly precise and reproducible body plan. While these strategies were likely shaped and improved by evolution to serve specific purposes, it is quite difficult to pinpoint which purpose dominated the optimization process.

"It is increasingly clear how an embryo develops, but it is not clear which mathematical function guides the system to come together," Sokolowski says. "It's like finding a mathematical needle in the biological haystack."

The fruit fly

Drosophila, as biologists refer to it, is a widely studied organism, probably best known for the 1995 Noble Prize-winning work of Eric Wieschaus, Christiane Nüsslein-Volhard, and Edward B. Lewis. They identified the genes that are crucial for the correct development of the fly, in particular, the so-called "gap genes" and morphogen (signaling molecule) gradients that control them.

The gap gene network plays a crucial role during the development of the embryo's head-to-tail axis. This "genetic positioning system" helps individual cells acquire the right fate in the right place, ultimately forming the segmented body of a fruit fly.

The varying activation levels of the gap genes form an incredibly precise "positional code" along this axis, providing each cell with exactly the right information on where they are located within the embryo.

Time flies

Already 20 years ago, work by William Bialek, Gašper Tkačik, Curtis Callan, Aleksandra Walczak, Thomas Gregor, and others suggested that the gap gene network in the fruit fly has been fine-tuned by evolution for providing high positional information with a limited number of signaling molecules, much like providing a precise GPS signal with the smallest number of satellites.

The scientists therefore came up with the key idea of finding a mathematical function to explain this phenomenon.

In the first attempt, Tkačik and colleagues looked at simplified theoretical models that implemented only parts of the regulatory mechanisms of the gap gene network. They gradually increased the model complexity to make it more realistic.

While these "toy" models did not capture all combined characteristics of the gap gene system, they still paved the way toward a full optimization attempt.

"Our early work showed that it was possible to obtain nontrivial and originally unexpected predictions for gene regulatory interactions by optimizing them for maximal information throughput under realistic biophysical and molecular resource constraints," says Tkačik.

Meanwhile, Thomas Sokolowski and colleagues have been studying detailed stochastic models—models that explicitly include randomness—of spatially interacting genes akin to the gap genes.

Sokolowski then joined the Tkačik group at ISTA in 2014, which created a unique opportunity to combine the original optimization approach with detailed spatial-stochastic modeling. Together, the scientists quickly managed to implement a spatial-stochastic model that, on the one hand, was realistic about what happens in the actual fruit fly and, on the other hand, computationally efficient.

Initially being a simplified version with only two genes, the model was extended to the full set of four interacting gap genes and three morphogen gradients, suitable for carrying out fully-featured optimizations of the gap gene system. "Remarkably, the optimal networks we derived closely matched characteristic features of the spatial gene expression profiles observed in the real fruit fly," Tkačik continues.

Many 'optimal' ways

Additionally, the scientists found out that there is more than one optimal way for encoding positional information in the gap network. Different sets of biophysical parameters can lead to the required optimal properties of the system. While being only a tiny subset of all physically possible solutions, the optimal solutions still display a remarkable variety.

"We believe this is not a detriment, but an advantage for evolution, as the same fitness can be potentially reached by many imaginable evolutionary paths," Sokolowski suggests.

"While the evolution that led to Drosophila which we study today followed one particular path, the fact that many alternative routes potentially exist may have facilitated its access to a fit organism." The more options are available, the higher are the chances to select a functional one.

To understand the processes leading to functional body plans in more detail and get a more accurate representation of the actual evolutionary dynamics, the researchers will require additional modeling that goes beyond numerical optimization of parameters.

This will involve taking into account factors such as environmental influences or the mechanisms of natural selection—an intriguing and challenging quest for future research in theoretical biology.

More information: Thomas R. Sokolowski et al, Deriving a genetic regulatory network from an optimization principle, *Proceedings of the National Academy of*

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