A central biological question is how natural organisms are so evolvable (capable of quickly adapting to new environments). A key driver of evolvability is the widespread modularity of biological networks—their organization as functional, sparsely connected subunits—but there is no consensus regarding why modularity itself evolved. While most hypotheses assume indirect selection for evolvability, here we demonstrate that the ubiquitous, direct selection pressure to reduce the cost of connections between network nodes causes the emergence of modular networks. Experiments with selection pressures to maximize network performance and minimize connection costs yield networks that are significantly more modular and more evolvable than control experiments that only select for performance. These results will catalyze research in numerous disciplines, including neuroscience, genetics and harnessing evolution for engineering purposes.

A long-standing open question in biology is how populations are capable of rapidly adapting to novel environments, a trait called evolvability. A major contributor to evolvability is the fact that many biological entities are modular, especially the many biological processes and structures that can be modeled as networks, such as brains, metabolic pathways, gene regulation and protein interactions. Networks are modular if they contain highly connected clusters of nodes that are sparsely connected to nodes in other clusters. Despite its importance and decades of research, there is no agreement on why modularity evolves. Intuitively, modular systems seem more adaptable, a lesson well-known to human engineers because it is easier to rewire a modular network with functional subunits than an entangled, monolithic network. However, because this evolvability only provides a selective advantage over the long-term, such selection is at best indirect and may not be strong enough to explain the level of modularity in the natural world.

Modularity is likely caused by multiple forces acting to various degrees in different contexts and a comprehensive understanding of the evolutionary origins of modularity involves identifying those multiple forces and their relative contributions. The leading hypothesis is that modularity mainly emerges due to rapidly changing environments that have common subproblems, but different overall problems. Computational simulations demonstrate that in such environments (called modularly varying goals: MVG), networks evolve both modularity and evolvability. In contrast, evolution in unchanging environments produces non-modular networks that are slower to adapt to new environments. Follow-up studies support the modularity-generating force of MVG in nature: the modularity of bacterial metabolic networks is correlated with the frequency with which their environments change. It is unknown how much natural modularity MVG can explain, however, because it unclear how many biological environments change modularly, and whether they change at a high enough frequency to force this to play a significant role. A related theory that also assumes a constantly changing environment and selection for evolvability is that modularity arises to enable modifying one subcomponent without affecting others. There are other plausible hypotheses (reviewed in Wagner 2007), including that variation mechanisms, such as gene duplication, create a bias towards the generation of modular structures and that modularity evolves due to selection to make phenotypes robust to environmental perturbations.

We investigate an alternate hypothesis that has been suggested, but heretofore untested, which is that modularity evolves not because it conveys evolvability, but as a byproduct from selection to reduce connection costs in a network (Fig. 1). Such costs include manufacturing connections, maintaining them, the energy to transmit along them, and signal delays, all of which increase as a function of connection length and number. The concept of connection costs is straightforward in networks with physical connections (e.g. neural), but may also apply to other types of networks like metabolic and genetic pathways, as illustrated by the following examples; adding links in a pathway may incur delays; adding binding sites may slow replication and physically make regulation inefficient because polymerases recruited to upstream promoters would have to traverse longer stretches of sequence to reach protein-coding gene sequences; adding protein and metabolic interactions may increase constraints. The strongest evidence that biological networks face direct selection to minimize connection costs comes from the vascular system and from nervous systems, including the brain, where multiple studies suggest that the summed length of the wiring diagram has been minimized, either by reducing long connections or by optimizing the placement of neurons. Founding and modern neuroscientists have hypothesized that direct selection to minimize connection costs may, as a side-effect, cause modularity. This hypothesis has never been tested in the context of evolutionary biology. The most related study was on non-evolving, simulated neural networks with a specific within-life learning algorithm that produced more modularity when minimizing connection length in addition to performance, although the generality of the result was questioned when it was not replicated with other learning algorithms. Without during-life learning algorithms, carefully-constructed MVG environments, or mutation operators strongly biased toward creating modules, attempts to
Fig. 2. The addition of connection costs leads to higher-performing, functionally modular networks. (A) Networks evolve to recognize patterns (objects) in an eight-pixel retina. The problem is modularly decomposable because whether an object exists on the left and right sides can be separately determined before combining that information to answer whether objects exist on both sides (denoted by the AND logic function). (B) Networks from an example trial become more modular across evolutionary time (see SI for video) with a pressure to minimize connection costs in addition to performance (P&CC). (C) Median performance (± 95% bootstrapped confidence intervals) per generation of the highest-performing network of each trial, which is perfect only when minimizing connection costs in addition to performance. (D) Network modularity, which is significantly higher in P&CC trials than when selecting for performance alone (PA).

Given the impracticality of observing modularity evolve in biological systems, we follow most research on the subject by conducting experiments in computational systems with evolutionary dynamics. Specifically, we use a well-studied system from the MVG investigations, evolving networks to solve pattern-recognition tasks and Boolean logic tasks (Methods). These networks have inputs that sense the environment and produce outputs (e.g. activating genes, muscle commands, etc.), which determine performance on environmental problems. We compare a treatment where the fitness of networks is based on performance alone (PA) to one based on two objectives: maximizing performance and minimizing connection costs (P&CC). A multi-objective evolutionary algorithm is used with one (PA)
or two (P&CC) objectives: To reflect that selection is stronger on network performance than connection costs, the P&CC cost objective affects selection probabilistically only 25% of the time, although the results are robust to substantial changes to this (Methods). Two example connection cost functions are investigated. The default one is the summed squared length of all connections, assuming nodes are optimally located to minimize this sum (Methods), as has been found for animal nervous systems.\(^{27,33}\) A second measure of costs as solely the number of connections yields qualitatively similar results to the default cost function, and may better represent biological networks without connections of different lengths. More fit networks tend to have more offspring (copies that are randomly mutated), and the cycle repeats for a preset number of generations (Fig. 1) (Methods). Such computational evolving systems have substantially improved our understanding of natural evolutionary dynamics.\(^{27,33}\)

The main experimental problem involves a network that receives stimuli from eight inputs\(^{22}\). It can be thought of as an eight-pixel retina receiving visual stimuli, although other analogies are valid (Methods), such as a genetic regulatory network exposed to environmental stimuli. Patterns shown on the retina’s left and right halves may each contain an ‘object’, meaning a pattern of interest (Fig. 2a). Networks evolve to answer whether an object is present on both the left and right sides of the retina (the L-AND-R environment) or whether an object is displayed on either side (the L-OR-R environment). Which patterns count as an object on the left and right halves are slightly different (Fig. 2a).

Each network iteratively sees all possible 256 input patterns and answers true (\(\geq 0\)) or false (\(< 0\)). Its performance is the percentage of correct answers, which depends on which neurons are connected, how strongly, and whether those connections are inhibitory or excitatory (Methods). Networks are randomly generated to start each experiment. Their connections stochastically mutate during replication (Methods). Network modularity is evaluated with an efficient approximation\(^{27,33}\) of the widely used modularity metric \(Q\), which first optimally divides networks into modules then measures the difference between the number of edges within each module and the number expected for random networks with the same number of edges\(^{27,33}\).

**Fig. 3.** The highest-performing networks found for each combination of modularity and cost for the retina problem. Colors indicate the highest-performing network found at that point in the modularity vs. cost space, with yellow representing perfect performance. This map has been generated using the MOLE algorithm (Methods). The best-performing network at the end of each of the 50 PA and P&CC runs are overlaid on the map. Networks with perfect performance exist throughout the space, which helps explain why modularity does not evolve when there is selection based on performance alone. Below a cost threshold of around 125 there is an inverse correlation between cost and modularity for perfectly performing networks. The lowest cost networks—those with the shortest summed lengths—that are high-performing are modular.

**Fig. 4.** Evolving with connection costs produces networks that are more evolvable. (A) P&CC networks adapt faster to new environments than PA networks. Organisms were first evolved in one environment (e.g. L-AND-R) until they reached perfect performance and then transferred to a second environment (e.g. L-OR-R). Thick lines are medians, boxes extend from \(25\text{th}\) to \(75\text{th}\) data percentiles, thin lines mark \(1.5 \times IQR\) (interquartile range), and plus signs represent outliers. Fig. S7 is a zoomed-out version showing all of the data. (B) P&CC networks in an unchanging environment (dotted green line) have similar levels of modularity to the highest levels produced by MVG (solid blue line). Combining MVG with P&CC results in even higher modularity levels (solid green line), showing that the forces combined are stronger than either alone.

**Results**

After 25000 generations in an unchanging environment (L-AND-R), treatments selected to maximize performance and minimize connection costs (P&CC) produce significantly more modular networks than treatments maximizing performance alone (PA) (Fig. [4](#fig4)). A second measure of costs as solely the number of connections yields qualitatively similar results to the default cost function, and may better represent biological networks without connections of different lengths. More fit networks tend to have more offspring (copies that are randomly mutated), and the cycle repeats for a preset number of generations (Fig. 1) (Methods). Such computational evolving systems have substantially improved our understanding of natural evolutionary dynamics.\(^{27,33}\)

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creases performance and modularity, we searched for the highest-performing networks at all possible combinations of modularity and cost (Methods). For high-performing networks, there is an inverse correlation between cost and modularity, such that the lowest-cost networks are highly modular (Fig. 3). Many runs in the P&CC treatment evolved networks in this region whereas the PA treatments never did. There are also many non-modular, high-cost networks that are high-performing, helping to explain why modularity does not evolve due to performance alone (Fig. 3).

Comparing PA vs. P&CC populations across generations reveals that a connection cost pushes populations out of high-cost, low-modularity areas of the search space into low-cost, modular areas (Figs. 2h,i). Without the pressure to leave high-cost, low-modularity regions, many PA networks remain in areas that ultimately do not contain the highest-performing solutions (Fig. 3; dark green squares in the bottom right), further explaining why P&CC treatments have higher performance.

P&CC networks are also more evolvable than PA networks. We ran additional trials until 50 P&CC and 50 PA trials each had a perfectly performing network (Methods) and transferred these networks into the L-OR-R environment, which has the same subproblems in a different combination (Fig. S7). The presence (P&CC) or absence (PA) of a connection cost remained after the environmental change. We also repeated the experiment, except first evolving in L-OR-R and then transferring to L-AND-R. In both experiments, P&CC networks exhibit greater evolvability than PA by requiring fewer generations to adapt to the new environment (Fig. 4h; L-AND-R→L-OR-R: 3.0±2.0, 5.0 vs. 65/62, 69; p = 3 × 10−12; L-OR-R→L-AND-R: 12.0±7.0, 21.0 vs. 222.5±175.0, 290.0; p = 9 × 10−128). Modular networks thus evolve because their sparse connectivity has lower connection costs, but such modularity also aids performance and evolvability because the problem is modular. Minimizing connection costs can work in conjunction with other forces to increase modularity. Modularity levels are higher when combining P&CC with MVG environments (Fig. 4i; solid vs. dotted green line, p = 3 × 10−17). Overall, P&CC (with or without MVG) yields similar levels of modularity as MVG at its strongest, and significantly more when rates of environmental change are too slow for the MVG effect to be strong (Fig. 4j; green lines vs. blue solid line).

P&CC modularity is also higher than PA even on problems that are non-modular (Fig. 5a, p = 5.4 × 10−15). As to be expected, such modularity is lower than on modular problems (p = 0.0011, modular retina vs. non-modular retina). This non-modular problem involves answering whether any four pixels were on (black), which is non-modular because it requires information from all retina inputs. As mentioned previously, performance and modularity are also significantly higher with an alternate connection cost function based on the number of connections (P&CC-NC) instead of the length of connections (Figs. 5a, 5b). We also verified that modularity and performance are not higher simply because a second objective is used (Fig. 5c). We further tested whether modularity arises even when the inputs for different modules are not geometrically separated, which is relevant when cost is a function of connection length. Even in experiments with randomized input coordinates (Methods), a connection cost significantly increased performance (1.0±0.98, 1.0; p = 0.0012) and modularity (Q = 0.35±0.34, 0.38; p = 1 × 10−9), and performance and modularity scores were not significantly different than P&CC without randomized coordinates (Fig. S5).

All the results presented so far are qualitatively similar in a different model system: evolving networks to solve Boolean logic tasks. We tested two fully separable problems: one with five “exclusive or” (XOR) logic modules (Fig. 5d), and another with hierarchically nested XOR problems (Fig. 5e). P&CC created separate modules for the decomposed problems in nearly every trial, whereas PA almost never did (Figs. 5f, S5). P&CC Performance was also significantly higher (Fig. 5g) and there was an inverse correlation between cost and modularity (Figs. 5h, 11). Confirming the generality of the finding that connection costs improve adaptation rates and that high-performing, low-cost networks are modular is an interesting area for future research.

Discussion and Conclusion

Overall, this paper supports the hypothesis that selection to reduce connection costs causes modularity, even in unchanging environments. The results also open new areas of research into identifying connection costs in networks without physical connections (e.g. genetic regulatory networks) and investigating whether pressures to minimize connection costs may explain modularity in human-created networks (e.g. communication and social networks).

It is tempting to consider any component of modularity that arises due to minimizing connection costs as a ‘spandrel’, in that it emerges as a byproduct of selection for another trait. However, because the resultant modularity produces evolvability, minimizing connection costs may serve as a bootstrapping process that creates initial modularity that can then be further elevated by selection for evolvability. Such hypotheses for how modularity initially arises are needed, because selection for evolvability cannot act until enough modularity exists to increase the speed of adaptation. Knowing that selection to reduce connection costs produces modular networks will substantially advance fields that harness evolution for engineering, because a longstanding challenge therein has been evolving modular designs. It will additionally aid attempts to evolve accurate models of biological networks, which catalyze medical and biological research. The functional modularity generated also makes synthetically evolved networks easier to understand. These results will thus generate immediate benefits in many fields of applied engineering, in addition to furthering our quest to explain one of nature’s predominant organizing principles.

Methods

Experimental Parameters Each treatment is repeated 50 times with different stochastic events (i.e. different random number generator seeds). Analyses and visualizations are of the highest-performing network per trial with ties broken randomly. The main experiments (retina, non-modular retina, 5-XOR, and hierarchical XOR) last 25000 generations and have a population size of 1000.

Statistics For each statistic we report the median +/- 95% bootstrapped confidence intervals of the median (calculated by resampling the data 5,000 times). In plots, these confidence intervals are

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A Non-Modular Problem

![Network Diagram](network_diagram.png)

B Multiple, Separable Problems

![Network Diagram](network_diagram.png)

C Hierarchical, Separable Problems

![Network Diagram](network_diagram.png)

Fig. 5. Results from tests with different environmental problems. (A) Even on a non-modular problem, modularity is higher with P&CC, though it is lower than for modular problems. (B, C) P&CC performs better, is more modular, and has better functional decomposition than PA when evolving networks to solve five separate XOR functions and hierarchically nested XOR functions. The examples are the final, highest-performing networks per treatment. Figs. S3, S4, and S5 show networks from all trials.

Smoothed with a median filter (window size=200) to remove subsampling noise.

Length Cost For P&CC treatments, prior to calculating connection costs, we place nodes in positions optimal for minimizing connection costs given the topology of the network, which is biologically motivated and can be solved for mathematically. Inputs and outputs are at fixed locations (SI Text). Visualizations reflect these node placements.

Evolvability Experiment The evolvability experiments (Fig. 4A) are described in Fig. S7. To obtain 50 trials that each had a perfectly performing network in L-AND-R and L-OR-R, respectively, took 110 and 116 trials for P&CC and 320 and 364 trials for PA. 1000 clones of each of these networks then evolved in the alternate environment until performance was perfect or 5000 generations passed.

Overview of Network Models This section provides a brief overview of the network models in this paper. A more complete review of network models is provided in Alon 2007, Haykin 1999, Newman 2003, Barabási 2004, and cites therein.

Network models can represent many types of biological processes by representing interactions between component elements. Example biological systems that are commonly modeled as networks are neural, genetic, metabolic, and protein interaction networks. All such networks can be represented abstractly as nodes representing components, such as neurons or genes, and the interactions between such components, such as a gene inhibiting another or gene. The weight of connections indicates the type and strength of interactions, with positive values indicating activation, negative values indicating inhibition, and the magnitude of the value representing the strength of the interaction.

Multiple nodes can connect to form a network (e.g. Fig. 4B). Typically, information flows into the network via input nodes, passes through hidden nodes, and exits via output nodes. Examples include a gene regulatory network responding to changing levels of environmental chemicals or a neural network responding to visual inputs from the retina and outputting muscle commands.

Our model of a network is a standard, basic one used in machine learning, systems biology, and computational neuroscience. It also has been used in previous, landmark studies on the evolution of modularity. The networks are feedforward, meaning that nodes are arranged into layers, such that a node in layer n receives incoming connections only from nodes in layer n-1 and has outgoing connections only to nodes in layer n+1 (Fig. 4C). The maximum number of nodes per hidden layer is 8/4/2 for the three hidden layers in the retina problem, 8 for the single hidden layer in the 5-XOR problem, and 8/4/4 for the three hidden layers in the hierarchical XOR problem. The possible values for connection weights are the integers -2,-1,1, and 2. The possible values for thresholds (also called biases) are the integers -2,-1,0,1, and 2. Information flows through the network in discrete time steps one layer at a time. The output of each node in the network is the following function of its inputs: y_j = tanh(λ(Σ_i w_i y_i + b_j)) where y_j is the output of node j, i is the set of nodes connected to j, w_i is the strength of the connection between node i and node j, y_i is the output of node i, and b_j is a threshold (also called a bias) that determines at which input value the output transitions from negative to positive. The tanh(x) transfer function ensures an output range of [-1,1]. λ (here, 20) determines the slope of the transition between these inhibitory and excitatory extremes (Fig. 4C). This network model can approximate any function with an arbitrary precision provided that it contains enough hidden nodes.

Evolutionary Algorithm The evolutionary algorithm is based on research into algorithms inspired by evolution that simultaneously optimize several objectives, called multi-objective algorithms. These algorithms search for, but are not guaranteed to find, the set of optimal trade-offs: i.e., solutions that cannot be improved with respect to one objective without decreasing their score with respect to another one. Such solutions are said to be on the Pareto Front described formally below. These algorithms are more general than algorithms that combine multiple objectives into a single, weighted fitness function, because the latter necessarily select one set of weights for each objective, whereas multi-objective algorithms explore all possible tradeoffs between objective goals.

The specific multi-objective algorithm in this paper is the widely used Nondominated Sorting Genetic Algorithm, version II (NSGA-II) (Fig. 4D). As with most modern multi-objective
evolutionary algorithms, it relies on the concept of Pareto dominance, defined as follows:

An individual $x'$ is said to dominate another individual $x$, if both conditions 1 and 2 are true: (1) $x'$ is not worse than $x$ with respect to any objective; (2) $x'$ is strictly better than $x$ with respect to at least one objective.

However, this definition puts the same emphasis on all objectives. In the present study, we take into account that the first objective (performance) is more important than the second objective (optimizing connection cost). To reflect this, we use a stochastic objective (performance) is more important than the second objective

This stochastic application of the second objective is implemented as follows. Let $\lambda$ denote a random number in $[0,1]$ and $p$ the probability to take the second objective into account. A solution $x'$ is said to stochastically dominate another solution $x$, if one of the two following conditions is true: (1) $x'>p$ and $x'$ is better than $x$ with respect to the first objective; (2) $x'<p$ and $x'$ is not worse than $x$ with respect to either objective and $x'$ is better than $x$ with respect to at least one objective.

Stochastic Pareto dominance is used in the algorithm twice (Fig. 3H): (1) To select a parent for the next generation, two individuals $x_1$ and $x_2$ are randomly chosen from the current population; if $x_1$ stochastically dominates $x_2$, then $x_1$ is selected, if $x_2$ stochastically dominates $x_1$, then $x_2$ is selected. If neither dominates the other, the individual selected is the one which is in the less crowded part of the objective space (Fig. 3H). (2) To rank individuals, the set of stochastically non-dominated solutions is first identified and called the first Pareto layer (rank = 1, e.g., $t_1$ in Fig. 3I); these individuals are then removed and the same operation is performed to identify the subsequent layers (additional ranks corresponding to $t_2$, $t_3$, etc. in Fig. 3I).

Mutational Effects Mutations operate in essentially the same way as in the study by Kashan and Alon. In each generation, every new network is randomly mutated (Fig. 3H). Four kinds of mutation are possible, which are not mutually exclusive: (1) each network has a 20% chance of having a single connection added. Connections are added between two randomly chosen nodes that are not already connected and belong to two consecutive layers (to maintain the feed-forward property described previously); (2) each network has a 20% chance of a single, randomly chosen connection being removed; (3) each node in the network has a 1/244=4.16% chance of having its threshold (also called its bias) incremented or decremented, with both options equally likely; five values are available \((-2,-1,0,1,2\); mutations that produce values higher or lower than these five values are ignored; (4) each connection in the network has a separate probability of being incremented or decremented of $0.05/n$, where $n$ is the total number of connections of the network. Four values are available \((-2,-1,1,2\); mutations that produce values higher or lower than these four values are ignored.

The results in this manuscript are robust to varying these parameters. Because having more mutational events that remove connections than to add them might also produce sparsely connected, modular networks, we repeated the main experiment with mutation rates biased to varying degrees (Fig. 3H, b). These experiments show that even having remove-connection events be an order of magnitude more likely than add-connection events does not produce modular networks. In each of the experiments with biased mutation rates, the modularity and performance of the P&CC treatment with default mutation values was significantly greater than the PA treatment with biased mutation rate values (Fig. S9b).

Our main results are qualitatively the same when weights and biases are real numbers (instead of integers) and mutated via Gaussian perturbation. Nodes are never added nor removed. For clarity, following [37] nodes without any connections are not displayed or included in results.

Multi-Objective Landscape Exploration (MOLE) Algorithm It would be helpful to visualize the constraints, tradeoffs, and other correlations between different phenotypic dimensions that occur in evolving systems (e.g. in this study the performance, modularity, and length for each possible network). Because it is impossible for this study to determine such information via exhaustive or random search (SI Text), we designed an algorithm to find high-performing solutions with different combinations of modularity and length scores. We call this algorithm Multi-Objective Landscape Exploration (MOLE). It is a multi-objective optimization search (Fig. S1) with two objectives. The first objective prioritizes individuals that have high performance. The second objective prioritizes individuals that are far away from other individuals already discovered by the algorithm, where distance is measured in a Cartesian space with connection costs on the x axis and modularity on the y axis. Algorithms of this type have been shown to better explore the search space because they are less susceptible to getting stuck in local optima. Thus, unlike a traditional evolutionary algorithm that will only be drawn to a type of solution if there is a fitness gradient towards that type of solution, MOLE searches for high-performing solutions for every possible combination of modularity and cost scores. While this algorithm is not guaranteed to find the optimal solution at each point in the space, it provides a focused statistical sampling of how likely it is to discover a high-quality solution in each area of the search space. The MOLE maps in this paper show the highest performing network at each point in this Cartesian space found in 30 separate runs.

Exhaustive and random search fail to discover high-performing networks In this study it would help to know the performance, modularity, and length for each solution in the search space. If the search space is small enough, such values can be determined by exhaustively checking every possible solution. Such an approach is intractable for the problems in this msancript. For example, for the main problem in the paper, which is the retina problem, the number of possible weights is

$$\text{NumberOfWeights} = \begin{pmatrix} 8 \\ 8 \end{pmatrix} + \begin{pmatrix} 8 \\ 4 \end{pmatrix} + \begin{pmatrix} 4 \\ 2 \end{pmatrix} + \begin{pmatrix} 2 \\ 1 \end{pmatrix} + 23 = 129$$

(1)

due to the maximum possible number of nodes in the input, hidden, and output layers, as well as the bias for each of the 23 possible nodes. Each of these weights can be one of four values or a zero if no connection exists, and biases can be one of five values, leading to a search space of

$$\text{NumberOfSolutions} = 5^{129} \times 10^{90}.$$  

(2)

Given that it takes on average 0.0013 seconds to assess the fitness of a solution across all possible 256 inputs using a modern computer, it would take $4.1 \times 10^{79}$ years of computing time to exhaustively determine the performance, modularity, and cost for each solution in the search space. Because it is infeasible to exhaustively search the space, we randomly sampled it to see if we would find high-performing solutions with a variety of cost and modularity scores. Specifically, we randomly generated more than two billion solutions, but every solution had poor performance. The highest-performing solution gave the correct answer for only 62 out of 256 retina patterns (24.2%), which is far below the performance of 93% or greater for solutions routinely discovered by the evolutionary algorithm (Fig. 2). We thus concluded that randomly sampling the space would not lead to the discovery of high-performing solutions.
Geometric coordinates
Nodes exist at two-dimensional (i.e. \( x,y \)) Cartesian locations. The geometric coordinates of the inputs and outputs for all problems were fixed throughout evolution, including the treatment where the within-row location of inputs are randomized at the beginning of each separate trial, and are as follows. The inputs for all problems have \( y \) values of 0. For the retina problem, the \( x \) values for the inputs are \( \{-3.5, -2.5, -3.5\ldots\} \) and the output is at \( (4.0) \). For the problem with 5 XOR modules, the \( x \) values for the inputs are \( \{-4.5, -3.5, -4.5\ldots\} \) and the outputs all have \( y \) values of 2 with \( x \) values of \( \{-4.0, -2.0, 2.0\ldots\} \). For the problem with decomposable, hierarchically nested XOR functions, the \( x \) values for the inputs are \( \{-3.5, -2.5, ... , -3.5\} \) and the outputs all have \( y \) values of 4 with \( x \) values of \( \{-2.2\} \). The geometric location of nodes is consequential only when there is a cost for longer connections (i.e. the main P&CC treatment).

Video of networks from each treatment evolving across generations
A video is provided to illustrate the change in networks across evolutionary time for both the PA and P&CC treatments. It can be viewed at http://chronos.isir.upmc.fr/~mouret/tmp/modularity.avi. In it, the networks are visualized as described in the text.

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The evolutionary origins of modularity
– Supplementary Material

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Fig. S1. Overview of the model. (A) The multi-objective evolutionary algorithm (NSGA-II). Starting with a population of \( N \) randomly generated individuals, an offspring population of \( N \) new individuals is generated using the best individuals of the current population. The union of the offspring and the current population is then ranked according to the stochastic Pareto dominance (explained in Methods, here represented by having organisms in different ranks connected by lines labeled \( L_1, L_2, \ldots \)) and the best \( N \) individuals form the next generation. (B) An example network model. Networks can model many different biological processes, such as genetic regulatory networks, neural networks, metabolic networks, and protein interaction networks. Information enters the network when it is sensed as an input pattern. Nodes, which represent components of the network (e.g. neurons or genes), respond to such information and can activate or inhibit other components of the network to varying degrees. The strength of interactions between two nodes is represented by the weight of the connection between them, which is a scalar value, and whether the interaction is excitatory or inhibitory depends on whether the weight is positive or negative. In this figure all non-zero weights are represented by an arrow. The signal entering each node is passed through a transfer function to determine the output for that node. That output then travels through each of the node’s outgoing connections and, after being scaled by the weight of that outgoing connection, serves as a component of the incoming signal for the node at the end of that connection. Eventually an output pattern is produced, which for a neural network could be muscle commands or for a genetic regulatory network could be proteins. (C) The transfer function for each node. The sum of the incoming signal \( x \) for a node is multiplied by 20 before being passed through the transfer function \( \tanh(x) \). Multiplying by 20 makes the transition steep and similar to a step-like function. The \( \tanh(x) \) function ensures that the output is in the range \([-1, 1]\).
Fig. S2. Network visualizations and data from the main experiment. The highest-performing network at the end of each trial is visualized here, sorted first by fitness and second by modularity. For each network the performance (left-justified) and modularity score $Q$ (right-justified) are shown. An "L" or "R" indicates that the network has a single neuron that perfectly solves the left or the right subproblem, respectively. (A) Networks from the treatment where the only selection pressure is on the performance of the network. (B) Networks from the treatment where there are two selection pressures: one to maximize performance and one to minimize connection costs.
Fig. S3. Network visualizations and data for the experiment with five decomposable XOR Boolean logic functions. The highest-performing network at the end of each trial, sorted by fitness then modularity, and its performance (left-justified) and modularity score $Q$ (right-justified). (A) The environmental challenge in this experiment. (B and C) Networks from the PA and P-MCC treatments, respectively.
Fig. S4. Network visualizations and data for the experiment with decomposable, hierarchically nested XOR Boolean logic functions. The highest-performing network at the end of each trial is visualized here, sorted first by fitness and second by modularity. For each network the performance (left-justified) and modularity score $Q$ (right-justified) are shown. (A) A depiction of the environmental challenge in this experiment. (B) Networks from the treatment where the only selection pressure is on the performance of the network. (C) Networks from the treatment where there are two selection pressures: one to maximize performance and one to minimize connection costs.
Exactly 4 black pixels?

Fig. S5. Network visualizations and data from the experiment with a non-modular problem. (A) A non-modular version of the retina problem is created when networks have to answer whether any four pixels are on, which is non-modular because it involves information from anywhere in the retina. (B, C) The highest-performing network at the end of each trial is visualized here, sorted first by fitness and second by modularity. For each network the performance (left-justified) and modularity score $q$ (right-justified) are shown. (B) shows networks from the treatment where the only selection pressure is on the performance of the network. (C) shows networks from the treatment where there are two selection pressures: one to maximize performance and one to minimize connection costs.
Fig. S6. Modularity and performance results are robust to variation in the strength of selection to minimize connection costs. **(A)** Median performance per generation of the highest-performing network, which is improved by adding a selection pressure to minimize connection costs. The value of $p$ indicates the strength of the pressure (Methods), ranging from 0% (no pressure) through 10% (low pressure) to 100% (high pressure—equal to that for the main performance objective). **(B)** Performance of the highest-performing networks after 25000 generations for different values of $p$. The differences between PA ($p=0$%) and P&CC ($p>0$%) are highly significant (four asterisks indicate a p-value <0.001). **(C)** Median modularity per generation of the highest-performing network of each trial for different values of $p$. **(D)** Modularity of the highest-performing networks after 25000 generations, which is significantly higher when there is a selection pressure to reduce connection costs (i.e. when $p \neq 0$%). **(E)** A changing environment. The $x$-axis represents the number of generations between a switch from the L-AND-R environment to the L-OR-R environment or vice-versa. This figure is the same as Fig. 4 from the main text, but shows results from additional values of $p$. The results for P&CC ($p>0$) are consistent across different values of $p$ provided that the strength of selection on network connection costs is not equal to that of network performance (i.e. for all $p \neq 100$%). The $p=100$% line is anomalous because in that case cost is as important as performance, leading to mostly low-performing networks with pathological topologies: this effect is strongest when the environment changes quickly because such changes frequently eliminate the fitness benefits of high performance.
Environmental changes between two modular problems with shared subproblems. (A) In the first evolutionary phase, networks evolve to answer whether a left and right object are present (the L-AND-R environment). The problem can be modularly decomposed, since the presence of left and right objects can first be separately detected before answering the larger question of whether they are both present. A left object is considered present if one of the eight left object patterns (shown in Fig. 2 in the main text) is exposed to the left side of the retina, and vice-versa for right objects. Networks that could perfectly solve the L-AND-R problem after 5000 generations are then transferred to an environment in which the challenge is to determine if a left or right object is present (the L-OR-R environment), which is a different overall problem that shares the subproblems of identifying left and right objects. Evolution continues until networks can perfectly solve the L-OR-R problem or until 5000 generations elapse. (B) The same experiment is repeated, but first evolving in the L-OR-R environment and then transferring to the L-AND-R environment. (C) A fully zoomed-out plot of Fig. 4 from the main text. Trials last 5000 generations or until a network exhibits perfect performance in the new environment. For each treatment, for each of 50 networks that perform perfectly in the first environment, we conduct 50 trials in the second environment, meaning that each column in this figure (and Fig. 4 from the main text) represent 50 × 50 = 2500 data points.
Fig. S8. (A) Repeating the main experiment wherein selection is based on performance and connection costs (P&CC), but with connection costs solely measured as the number of connections (P&CC-NC), produces networks that look qualitatively similar to those produced with the default P&CC cost function (compare the networks visualized here to those in Fig. 3). The modularity and performance scores are also qualitatively similar and not significantly different (modularity $Q=0.36(0.22,0.4)$ vs. default cost function $Q=0.42(0.25,0.45)$, $p=0.15$; performance $=1.0(0.99,1.0)$ vs. default cost function performance of $1.0(1.0,1.0)$, $p=1.0$). Like the default cost function, the alternative cost function produced significantly more modularity ($p=1.0 \times 10^{-9}$) and higher performance ($p=1.0 \times 10^{-5}$) than PA. Also qualitatively similar between these cost functions is the percent of runs that have the inputs related to the left and right subproblems in separate modules after splitting the network once to maximize modularity (alternate: $52\%$, default: $56\%$, Fisher’s exact test: $p=0.84$). One minor qualitative difference is the percent of runs that have two neurons that each perfectly solve the left and right subproblems, respectively (alternate: $10\%$, default: $39\%$, Fisher’s exact test: $p=8 \times 10^{-9}$). (B) Randomizing the geometric location of input coordinates (P&CC-RL) eliminates the left-right geometric decomposition of the L-AND-R retina problem, yet such randomization does not change the result that a connection cost causes significantly higher performance and modularity. (C) Displayed are final, evolved P&CC-RL networks, which are shown both with randomized input coordinates (left) and with the left and right inputs in order to visualize problem decomposition (right). Despite the randomization of the input locations, many of the evolved modules still functionally decompose the left and right subproblems.
Fig. S9. (A,B) Biasing the mutation rate towards having more remove-connection mutations than add-connection mutations does not increase the modularity or performance of PA treatments. Setting the remove-connection mutation rate to be up to an order of magnitude higher than the add-connection mutation rate did not qualitatively change the results. The PA treatment with default values of 0.2 for the remove-connection and add-connection mutation rates did not have statistically different levels of modularity or performance from PA treatments with the same remove-connection mutation rate of 0.2, but a lower add-connection mutation rate of 0.15, 0.10, or 0.02 ($p > 0.05$). The P&CC treatment had statistically higher performance and modularity scores than every PA treatment, irrespective its mutation rate bias. (C,D,E) Networks evolved with a connection cost have shorter lengths, fewer nodes, and fewer connections. (C) The summed length of all connections is smaller for networks evolved in the P&CC regime than in the PA regime. The P&CC networks also have fewer nodes (D) and connections (E). Three asterisks indicate a value of $p < 0.0001$ and four indicate a value of $p < 0.0001$. 
A Multiple, Separable Problems

B Hierarchical, Separable Problems

Fig. S10. The highest-performing networks found for each combination of modularity and length for (A) the problem with five separable XOR functions and (B) the hierarchical XOR problem. To understand the performance potential of networks with different combinations of modularity levels and summed connection lengths we invented the Multi-Objective Landscape Exploration (MOLE) algorithm, which is described in Methods. Colors indicate the highest-performing network found at that point in the modularity vs. cost space, with yellow representing perfect performance. The best-performing network at the end of each of the 50 PA and P&CC runs are overlaid on the map. Networks with perfect performance exist throughout the space, which helps explain why modularity does not evolve when there is selection based on performance alone. There is also an inverse correlation between length and modularity for high-performing networks: The lowest cost networks—those with the shortest summed lengths—that are high-performing are modular.