Performance-optimized hierarchical models predict neural responses in higher visual cortex

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Edited by Terrence J. Sejnowski, Salk Institute for Biological Studies, La Jolla, CA, and approved April 8, 2014 (received for review March 3, 2014)

The ventral visual stream underlies key human visual object recognition abilities. However, neural encoding in the higher areas of the ventral stream remains poorly understood. Here, we describe a modeling approach that yields a quantitatively accurate model of inferior temporal (IT) cortex, the highest ventral cortical area. Using high-throughput computational techniques, we discovered that, within a class of biologically plausible hierarchical neural network models, there is a strong correlation between a model's categorization performance and its ability to predict individual IT neural unit response data. To pursue this idea, we then identified a high-performing neural network that matches human performance on a range of recognition tasks. Critically, even though we did not constrain this model to match neural data, its top output layer turns out to be highly predictive of IT spiking responses to complex naturalistic images at both the single site and population levels. Moreover, the model's intermediate layers are highly predictive of neural responses in the V4 cortex, a midlevel visual area that provides the dominant cortical input to IT. These results show that performance optimization—applied in a biologically appropriate model class—can be used to build quantitative predictive models of neural processing.

computational neuroscience | computer vision | array electrophysiology

Retinal images of real-world objects vary drastically due to changes in object pose, size, position, lighting, nonrigid deformation, occlusion, and many other sources of noise and variation. Humans effortlessly recognize objects rapidly and accurately despite this enormous variation, an impressive computational feat (1). This ability is supported by a set of interconnected brain areas collectively called the ventral visual stream (2, 3), with homologous areas in nonhuman primates (4). The ventral stream is thought to function as a series of hierarchical processing stages (5–7) that encode image content (e.g., object identity and category) increasingly explicitly in successive cortical areas (1, 8, 9). For example, neurons in the lowest area, V1, are well described by Gabor-like edge detectors that extract rough object outlines (10), although the V1 population does not show robust tolerance to complex image transformations (9). Conversely, rapidly evoked population activity in top-level inferior temporal (IT) cortex can directly support real-time, invariant object categorization over a wide range of tasks (11, 12). Midlevel ventral areas—such as V4, the dominant cortical input to IT—exhibit intermediate levels of object selectivity and variation tolerance (12–14).

Significant progress has been made in understanding lower ventral areas such as V1, where conceptually compelling models have been discovered (10). These models are also quantitatively accurate and can predict response magnitudes of individual neuronal units to novel image stimuli. Higher ventral cortical areas, especially V4 and IT, have been much more difficult to understand. Although first principles-based models of higher ventral cortex have been proposed (15–20), these models fail to match important features of the higher ventral visual neural representation in both humans and macaques (4, 21). Moreover, attempts to fit V4 and IT neural tuning curves on general image stimuli have shown only limited predictive success (22, 23). Explaining the neural encoding in these higher ventral areas thus remains a fundamental open question in systems neuroscience.

As with V1, models of higher ventral areas should be neurally predictive. However, because the higher ventral stream is also believed to underlie sophisticated behavioral object recognition capacities, models must also match IT on performance metrics, equalling (or exceeding) the decoding capacity of IT neurons on object recognition tasks. A model with perfect neural predictivity in IT will necessarily exhibit high performance, because IT itself does. Here we demonstrate that the converse is also true, within a biologically appropriate model class. Combining high-throughput computational and electrophysiology techniques, we explore a wide range of biologically plausible hierarchical neural network models and then assess them against measured IT and V4 neural response data. We show that there is a strong correlation between a model's performance on a challenging high-variation object recognition task and its ability to predict individual IT neural unit responses.

Extending this idea, we used optimization methods to identify a neural network model that matches human performance on a range of recognition tasks. We then show that even though this model was never explicitly constrained to match neural data, its output layer is highly predictive of neural responses in IT cortex—providing a first quantitatively accurate model of this highest ventral cortex area. Moreover, the middle layers of the model are highly predictive of V4 neural responses, suggesting top-down performance constraints directly shape intermediate visual representations.

Significance

Humans and monkeys easily recognize objects in scenes. This ability is known to be supported by a network of hierarchically interconnected brain areas. However, understanding neurons in higher levels of this hierarchy has long remained a major challenge in visual systems neuroscience. We use computational techniques to identify a neural network model that matches human performance on challenging object categorization tasks. Although not explicitly constrained to match neural data, this model turns out to be highly predictive of neural responses in both the V4 and inferior temporal cortex, the top two layers of the ventral visual hierarchy. In addition to yielding greatly improved models of visual cortex, these results suggest that a process of biological performance optimization directly shaped neural mechanisms.

Author contributions: D.L.K.Y., H.H., and J.J.D. designed research; D.L.K.Y., H.H., and E.A.S. performed research; D.L.K.Y. contributed new reagents/analytic tools; D.L.K.Y., H.H., C.F.C., and D.S. analyzed data; and D.L.K.Y., H.H., and J.J.D. wrote the paper.

The authors declare no conflict of interest.

This article is a PNAS Direct Submission.

Freely available online through the PNAS open access option.

See Commentary on page 8327.

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This article contains supporting information online at www.pnas.org/lookup/suppl/doi:10.1073/pnas.1403112111/-/DCSupplemental.

Results

Invariant Object Recognition Performance Strongly Correlates with IT Neural Predictivity. We first measured IT neural responses on a benchmark testing image set that exposes key performance characteristics of visual representations (24). This image set consists of 5,760 images of photorealistic 3D objects drawn from eight natural categories (animals, boats, cars, chairs, faces, fruits, planes, and tables) and contains high levels of the object position, scale, and pose variation that make recognition difficult for artificial vision systems, but to which humans are robustly tolerant (1, 25). The objects are placed on cluttered natural scenes that are randomly selected to ensure background content is uncorrelated with object identity (Fig. S1*A*).

Using multiple electrode arrays, we collected responses from 168 IT neurons to each image. We then used high-throughput computational methods to evaluate thousands of candidate neural network models on these same images, measuring object categorization performance as well as IT neural predictivity for each model (Fig. 1*A*; each point represents a distinct model). To measure categorization performance, we trained support vector machine (SVM) linear classifiers on model output layer units (11) and computed cross-validated testing accuracy for these trained classifiers. To assess models' neural predictivity, we used a standard linear regression methodology (10, 26, 27): for each target IT neural site, we identified a synthetic neuron composed of a linear weighting of model outputs that would best match that site on fixed sample images and then tested response predictions against actual neural site's output on novel images (*Materials and Methods* and *SI Text*).

Models were drawn from a large parameter space of convolutional neural networks (CNNs) expressing an inclusive version of the hierarchical processing concept (17, 18, 20, 28). CNNs approximate the general retinotopic organization of the ventral stream via spatial convolution, with computations in any one region of the visual field identical to those elsewhere. Each convolutional layer is composed of simple and neuronally plausible basic operations, including linear filtering, thresholding, pooling, and normalization (Fig. S2*A*). These layers are stacked hierarchically to construct deep neural networks.

Each model is specified by a set of 57 parameters controlling the number of layers and parameters at each layer, fan-in and fan-out, activation thresholds, pooling exponents, and local receptive field sizes at each layer. Network depth ranged from one to three layers, and filter weights for each layer were chosen randomly from bounded uniform distributions whose bounds were model parameters (*SI Text*). These models are consistent with the Hierarchical Linear-Nonlinear (HLN) hypothesis that higher level neurons (e.g., IT) output a linear weighting of inputs from intermediate-level (e.g., V4) neurons followed by simple additional nonlinearities (14, 16, 29).

Models were selected for evaluation by one of three procedures: (*i*) random sampling of the uniform distribution over parameter space (Fig. 1*A*; n = 2,016, green dots); (*ii*) optimization for performance on the high-variation eight-way categorization task (n = 2,043, blue dots); and (*iii*) optimization directly for IT neural predictivity (n = 1,876, orange dots; also see *SI Text* and Fig. S3). In each case, we observed significant variation in both performance and IT predictivity across the parameter range. Thus, although the HLN hypothesis is consistent with a broad spectrum of particular neural network architectures, specific parameter choices have a large effect on a given model's recognition performance and neural predictivity.

Performance was significantly correlated with neural predictivity in all three selection regimes. Models that performed better on the categorization task were also more likely to produce outputs more closely aligned to IT neural responses. Although the class of HLN-consistent architectures contains many neurally inconsistent architectures with low IT predictivity, performance provides a meaningful way to a priori rule out many of those inconsistent models. No individual model parameters correlated nearly as strongly with IT predictivity as performance (Fig. S4), indicating that the performance/IT predictivity correlation cannot be explained by simpler mechanistic considerations (e.g., receptive field size of the top layer).

Critically, directed optimization for performance significantly increased the correlation with IT predictivity compared with the random selection regime ($r = 0.78$ vs. $r = 0.55$), even though neural data were not used in the optimization. Moreover, when optimizing for performance, the best-performing models predicted neural output as well as those models directly selected for neural predictivity, although the reverse is not true. Together, these results imply that, although the IT predictivity metric is a complex function of the model parameter landscape, performance optimization is an efficient means to identify regions in parameter space containing IT-like models.

IT Cortex as a Neural Performance Target. Fig. 1*A* suggests a next step toward improved encoding models of higher ventral cortex: drive models further to the right along the x axis—if the correlation holds, the models will also climb on the y axis. Ideally, this would involve identifying hierarchical neural networks that perform at or near human object recognition performance levels and validating them using rigorous tests against neural data (Fig. 2*A*). However, the difficulty of meeting the performance challenge itself can be seen in Fig. 2*B*. To obtain neural reference points on categorization performance, we trained linear

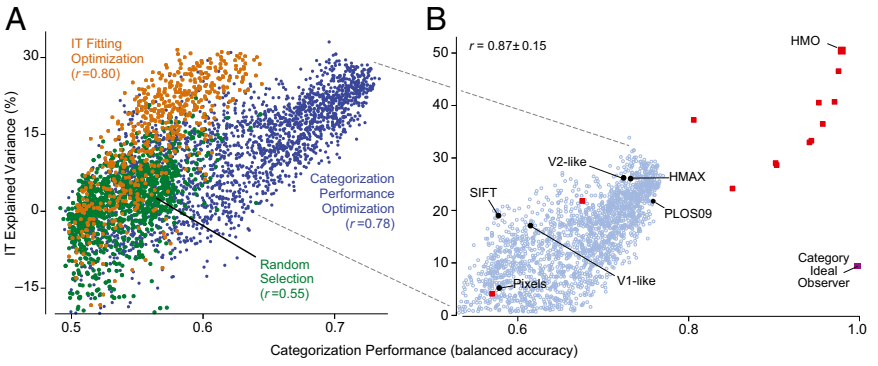

Fig. 1. Performance/IT-predictivity correlation. (*A*) Object categorization performance vs. IT neural explained variance percentage (IT-predictivity) for CNN models in three independent high-throughput computational experiments (each point is a distinct neural network architecture). The x axis shows performance (balanced accuracy, chance is 0.5) of the model output features on a high-variation categorization task; the y axis shows the median single site IT explained variance percentage ($n = 168$ sites) of that model. Each dot corresponds to a distinct model selected from a large family of convolutional neural network architectures. Models were selected by random draws from parameter space (green dots), object categorization performance-optimization (blue dots), or explicit IT predictivity optimization (orange dots). (*B*) Pursuing the correlation identified in *A*, a high-performing neural network was identified that matches human performance on a range of recognition tasks, the HMO model. The object categorization performance vs. IT neural predictivity correlation extends across a variety of models exhibiting a wide range of performance levels. Black circles include controls and published models; red squares are models produced during the HMO optimization procedure. The category ideal observer (purple square) lies significantly off the main trend, but is not an actual image-computable model. The r value is computed over red and black points. For reference, light blue circles indicate performance optimized models (blue dots) from *A*.

classifiers on the IT neural population (Fig. 2*B*, green bars) and the V4 neural population ($n = 128$, hatched green bars). To expose a key axis of recognition difficulty, we computed performance results at three levels of object view variation, from low (fixed orientation, size, and position) to high (180° rotations on all axes, 2.5× dilation, and full-frame translations; Fig. S1*A*). As a behavioral reference point, we also measured human performance on these tasks using web-based crowdsourcing methods (black bars). A crucial observation is that at all levels of variation, the IT population tracks human performance levels, consistent with known results about IT's high category decoding abilities (11, 12). The V4 population matches IT and human performance at low levels of variation, but performance drops quickly at higher variation levels. (This V4-to-IT performance gap remains nearly as large even for images with no object translation variation, showing that the performance gap is not due just to IT's larger receptive fields.)

As a computational reference, we used the same procedure to evaluate a variety of published ventral stream models targeting several levels of the ventral hierarchy. To control for low-level confounds, we tested the (trivial) pixel model, as well as SIFT, a simple baseline computer vision model (30). We also evaluated a V1-like Gabor-based model (25), a V2-like conjunction-of-Gabors model (31), and HMAX (17, 28), a model targeted at explaining higher ventral cortex and that has receptive field sizes similar to those observed in IT. The HMAX model can be trained in a domain-specific fashion, and to give it the best chance of success, we performed this training using the benchmark images themselves (see *SI Text* for more information on the comparison models). Like V4, the control models that we tested approach IT and human performance levels in the low-variation condition, but in the high-variation condition, all of them fail to match the performance of IT units by a large margin. It is not surprising that V1 and V2 models are not nearly as effective as IT, but it is instructive to note that the task is sufficiently difficult that the HMAX model performs less well than the V4 population sample, even when pretrained directly on the test dataset.

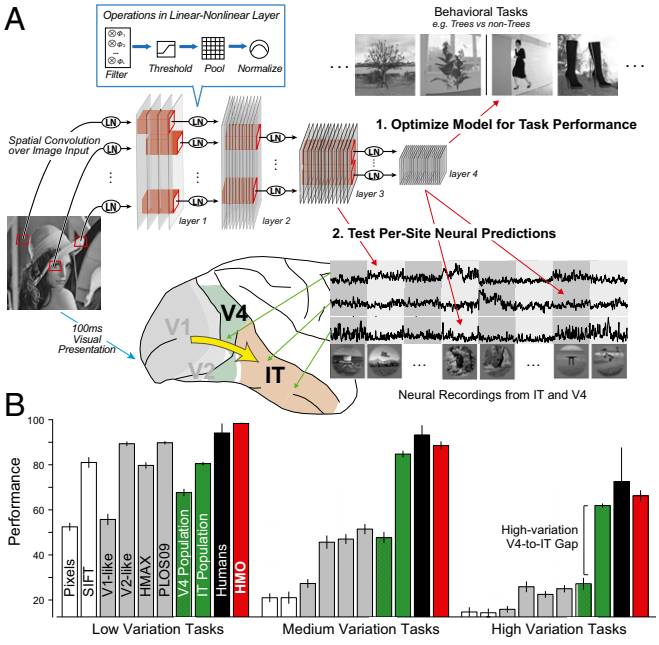

Fig. 2. Neural-like models via performance optimization. (*A*) We (*1*) used high-throughput computational methods to optimize the parameters of a hierarchical CNN with linear-nonlinear (LN) layers for performance on a challenging invariant object recognition task. Using new test images distinct from those used to optimize the model, we then (*2*) compared output of each of the model's layers to IT neural responses and the output of intermediate layers to V4 neural responses. To obtain neural data for comparison, we used chronically implanted multielectrode arrays to record the responses of multiunit sites in IT and V4, obtaining the mean visually evoked response of each of 296 neural sites to ∼6,000 complex images. (*B*) Object categorization performance results on the test images for eight-way object categorization at three increasing levels of object view variation (*y* axis units are 8-way categorization percent-correct, chance is 12.5%). IT (green bars) and V4 (hatched green bars) neural responses, and computational models (gray and red bars) were collected on the same image set and used to train support vector machine (SVM) linear classifiers from which population performance accuracy was evaluated. Error bars are computed over train/test image splits. Human subject responses on the same tasks were collected via psychophysics experiments (black bars); error bars are due to intersubject variation.

Constructing a High-Performing Model. Although simple three-layer hierarchical CNNs can be effective at low-variation object recognition tasks, recent work has shown that they may be limited in their performance capacity for higher-variation tasks (9). For this reason, we extended our model class to contain combinations (e.g., mixtures) of deeper CNN networks (Fig. S2*B*), which correspond intuitively to architecturally specialized subregions like those observed in the ventral visual stream (13, 32). To address the significant computational challenge of finding especially high-performing architectures within this large space of possible networks, we used hierarchical modular optimization (HMO). The HMO procedure embodies a conceptually simple hypothesis for how high-performing combinations of functionally specialized hierarchical architectures can be efficiently discovered and hierarchically combined, without needing to prespecify the subtasks ahead of time. Algorithmically, HMO is analogous to an adaptive boosting procedure (33) interleaved with hyperparameter optimization (see *SI Text* and Fig. S2*C*).

As a pretraining step, we applied the HMO selection procedure on a screening task (Fig. S1*B*). Like the testing set, the screening set contained images of objects placed on randomly selected backgrounds, but used entirely different objects in totally nonoverlapping semantic categories, with none of the same backgrounds and widely divergent lighting conditions and noise levels. Like any two samples of naturalistic images, the screening and testing images have high-level commonalities but quite different semantic content. For this reason, performance increases that transfer between them are likely to also transfer to other naturalistic image sets. Via this pretraining, the HMO procedure identified a four-layer CNN with 1,250 top-level outputs (Figs. S2*B* and S5), which we will refer to as the HMO model.

Using the same classifier training protocol as with the neural data and control models, we then tested the HMO model to determine whether its performance transferred from the screening to the testing image set. In fact, the HMO model matched the object recognition performance of the IT neural sample (Fig. 2*B*, red bars), even when faced with large amounts of variation—a hallmark of human object recognition ability (1). These performance results are robust to the number of training examples and number of sampled model neurons, across a variety of distinct recognition tasks (Figs. S6 and S7).

Predicting Neural Responses in Individual IT Neural Sites. Given that the HMO model had plausible performance characteristics, we then measured its IT predictivity, both for the top layer and each of the three intermediate layers (Fig. 3, red lines/bars). We found that each successive layer predicted IT units increasingly well, demonstrating that the trend identified in Fig. 1*A* continues to hold in higher performance regimes and across a wide range of model complexities (Fig. 1*B*). Qualitatively examining the specific predictions for individual images, the model layers show that category selectivity and tolerance to more drastic image transformations emerges gradually along the hierarchy (Fig. 3*A*, top four rows). At lower layers, model units predict IT responses only at a limited range of object poses and positions. At higher layers, variation tolerance grows while category selectivity develops, suggesting that as more explicit "untangled" object recognition

features are generated at each stage, the representations become increasingly IT-like (9).

Critically, we found that the top layer of the high-performing HMO model achieves high predictivity for individual IT neural sites, predicting $48.5 \pm 1.3\%$ of the explainable IT neuronal variance (Fig. 3 *B* and *C*). This represents a nearly 100% improvement over the best comparison models and is comparable to the prediction accuracy of state-of-the-art models of lower-level ventral areas such as V1 on complex stimuli (10). In comparison, although the HMAX model was better at predicting IT responses than baseline V1 or SIFT, it was not significantly different from the V2-like model.

To control for how much neural predictivity should be expected from any algorithm with high categorization performance, we assessed semantic ideal observers (34), including a hypothetical model that has perfect access to all category labels. The ideal observers do predict IT units above chance level (Fig. 3*C*, left two bars), consistent with the observation that IT neurons are partially categorical. However, the ideal observers are significantly less predictive than the HMO model, showing that high IT predictivity does not automatically follow from category selectivity and that there is significant noncategorical structure in IT responses attributable to intrinsic aspects of hierarchical network structure (Fig. 3*A*, last row). These results suggest that high categorization performance and the hierarchical model architecture class work in concert to produce IT-like populations, and neither of these constraints is sufficient on its own to do so.

Population Representation Similarity. Characterizing the IT neural representation at the population level may be equally important for understanding object visual representation as individual IT neural sites. The representation dissimilarity matrix (RDM) is a convenient tool comparing two representations on a common stimulus set in a task-independent manner (4, 35). Each entry in the RDM corresponds to one stimulus pair, with high/low values indicating that the population as a whole treats the pair stimuli as very different/similar. Taken over the whole stimulus set, the RDM characterizes the layout of the images in the high-dimensional neural population space. When images are ordered by category, the RDM for the measured IT neural population (Fig. 4*A*) exhibits clear block-diagonal structure—associated with IT's exceptionally high categorization performance—as well as off-diagonal structure that characterizes the IT neural representation more finely than any single performance metric (Fig. 4*A* and Fig. S8). We found that the neural population predicted by the output layer of the HMO model had very high similarity to the actual IT population structure, close to the split-half noise ceiling of the IT population (Fig. 4*B*). This implies that much of the residual variance unexplained at the single-site level may not be relevant for object recognition in the IT population level code.

We also performed two stronger tests of generalization: (*i*) object-level generalization, in which the regressor training set contained images of only 32 object exemplars (four in each of eight categories), with RDMs assessed only on the remaining 32 objects, and (*ii*) category-level generalization, in which the regressor sample set contained images of only half the categories but RDMs were assessed only on images of the other categories (see Figs. S8 and S9). We found that the prediction generalizes robustly, capturing the IT population's layout for images of completely novel objects and categories (Fig. 4 *B* and *C* and Fig. S8).

Predicting Responses in V4 from Intermediate Model Layers. Cortical area V4 is the dominant cortical input to IT, and the neural representation in V4 is known to be significantly less categorical

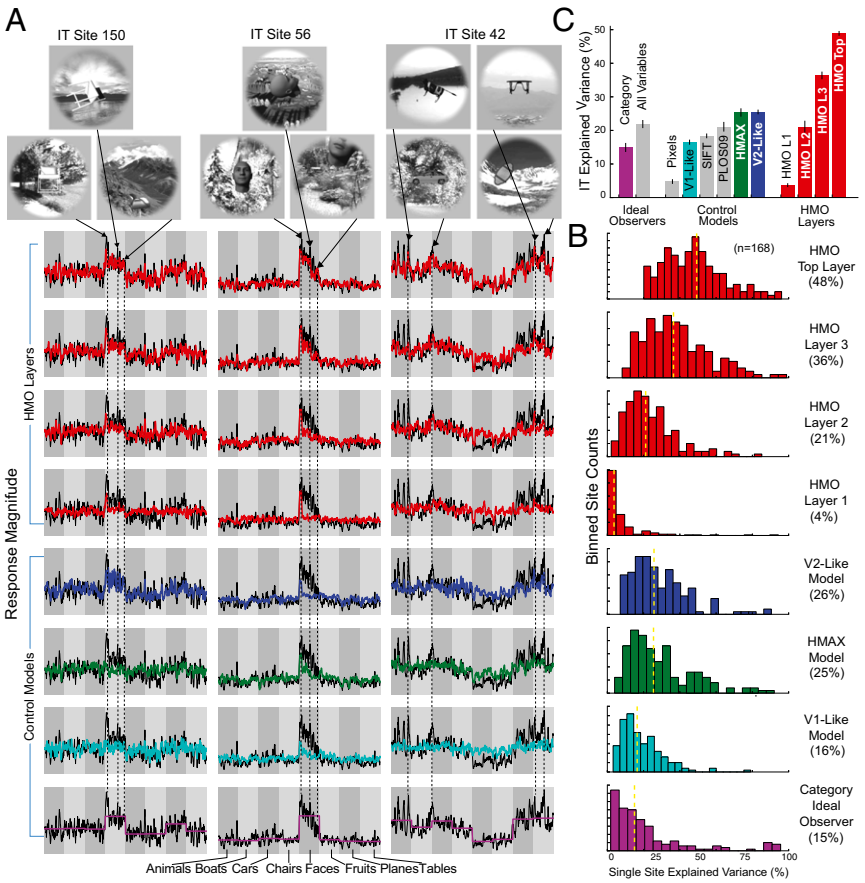

Fig. 3. IT neural predictions. (*A*) Actual neural response (black trace) vs. model predictions (colored trace) for three individual IT neural sites. The *x* axis in each plot shows 1,600 test images sorted first by category identity and then by variation amount, with more drastic image transformations toward the right within each category block. The *y* axis represents the prediction/response magnitude of the neural site for each test image (those not used to fit the model). Two of the units show selectivity for specific classes of objects, namely chairs (*Left*) and faces (*Center*), whereas the third (*Right*) exhibits a wider variety of image preferences. The four top rows show neural predictions using the visual feature set (i.e., units sampled) from each of the four layers of the HMO model, whereas the lower rows show the those of control models. (*B*) Distributions of model explained variance percentage, over the population of all measured IT sites ($n = 168$). Yellow dotted line indicates distribution median. (*C*) Comparison of IT neural explained variance percentage for various models. Bar height shows median explained variance, taken over all predicted IT units. Error bars are computed over image splits. Colored bars are those shown in *A* and *B*, whereas gray bars are additional comparisons.

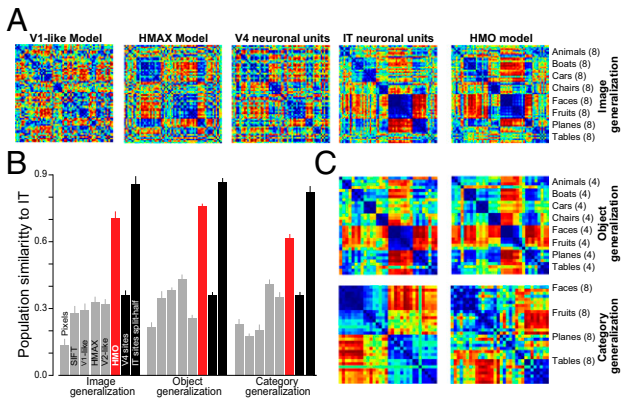

Fig. 4. Population-level similarity. (*A*) Object-level representation dissimilarity matrices (RDMs) visualized via rank-normalized color plots (blue = 0th distance percentile, red = 100th percentile). (*B*) IT population and the HMO-based IT model population, for image, object, and category generalizations (*SI Text*). (*C*) Quantification of model population representation similarity to IT. Bar height indicates the spearman correlation value of a given model's RDM to the RDM for the IT neural population. The IT bar represents the Spearman-Brown corrected consistency of the IT RDM for split-halves over the IT units, establishing a noise-limited upper bound. Error bars are taken over cross-validated regression splits in the case of models and over image and unit splits in the case of neural data.

than that of IT (12). Comparing a performance-optimized model to these data would provide a strong test both of its ability to predict the internal structure of the ventral stream, as well as to go beyond the direct consequences of category selectivity. We thus measured the HMO model's neural predictivity for the V4 neural population (Fig. 5). We found that the HMO model's penultimate layer is highly predictive of V4 neural responses ($51.7 \pm 2.3\%$ explained V4 variance), providing a significantly better match to V4 than either the model's top or bottom layers. These results are strong evidence for the hypothesis that V4 corresponds to an intermediate layer in a hierarchical model whose top layer is an effective model of IT. Of the control models that we tested, the V2-like model predicts the most V4 variation ($34.1 \pm 2.4\%$). Unlike the case of IT, semantic models explain effectively no variance in V4, consistent with V4's lack of category selectivity. Together these results suggest that performance optimization not only drives top-level output model layers to resemble IT, but also imposes biologically consistent constraints on the intermediate feature representations that can support downstream performance.

Discussion

Here, we demonstrate a principled method for achieving greatly improved predictive models of neural responses in higher ventral cortex. Our approach operationalizes a hypothesis for how two biological constraints together shaped visual cortex: (*i*) the functional constraint of recognition performance and (*ii*) the structural constraint imposed by the hierarchical network architecture.

Generative Basis for Higher Visual Cortical Areas. Our modeling approach has common ground with existing work on neural response prediction (27), e.g., the HLN hypothesis. However, in a departure from that line of work, we do not tune model parameters (the nonlinearities or the model filters) separately for each neural unit to be predicted. In fact, with the exception of the final linear weighting, we do not tune parameters using neural data at all. Instead, the parameters of our model were independently selected to optimize functional performance at the top level, and these choices create fixed bases from which any individual IT or V4 unit can be composed. This yields a generative model that allows the sampling of an arbitrary number of neurally consistent units. As a result, the size of the model does not scale with the number of neural sites to be predicted—and because the prediction results were assessed for a random sample of IT and V4 units, they are likely to generalize with similar levels of predictivity to any new sites that are measured.

What Features Do Good Models Share? Although the highest-performing models had certain commonalities (e.g., more hierarchical layers), many poor models also exhibited these features, and no one architectural parameter dominated performance variability (Fig. S3). To gain further insight, we performed an exploratory analysis of the parameters of the learned HMO model, evaluating each parameter both for how sensitively it was tuned and how diverse it was between model mixture components. Two classes of model parameters were especially sensitive and diverse (*SI Text* and Figs. S10 and S11): (*i*) filter statistics, including filter mean and spread, and (*ii*) the exponent trading off between max-pooling and average-pooling (16). This observation hints at a computationally rigorous explanation for experimentally

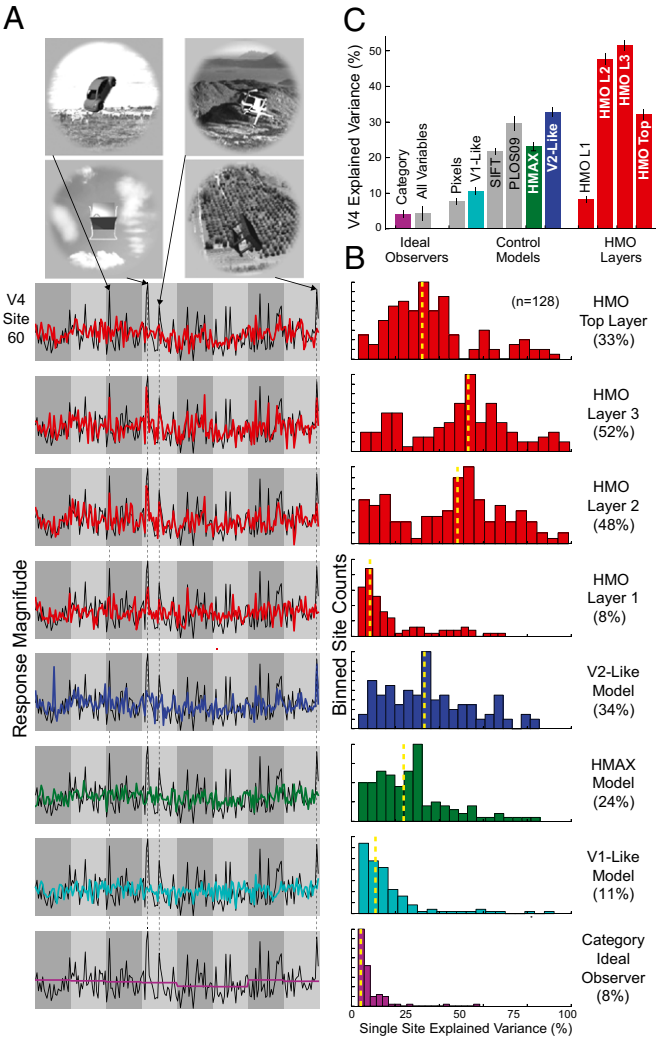

Fig. 5. V4 neural predictions. (*A*) Actual vs. predicted response magnitudes for a typical V4 site. V4 sites are highly visually driven, but unlike IT sites show very little categorical preference, manifesting in more abrupt changes in the image-by-image plots shown here. Red highlight indicates the best-matching model (*viz.*, HMO layer 3). (*B*) Distributions of explained variances percentage for each model, over the population of all measured V4 sites ($n = 128$). (*C*) Comparison of V4 neural explained variance percentage for various models. Conventions follow those used in Fig. 3.

observed heterogeneities in higher ventral cortex areas (13, 32), but much work remains to be done to confirm such a hypothesis.

Top-Down Approach to Understanding Cortical Circuits. A common assumption in visual neuroscience is that understanding the tuning curves of neurons in lower cortical areas will be a necessary precursor to explaining higher visual cortex. For example, significant work has gone into assessing the extent to which V4 neurons can be understood as a curvature-selective shape representation (27). Our results indicate that it is useful to complement this bottom-up approach with a top-down perspective characterizing IT as the product of an evolutionary/developmental process that selected for high performance on recognition on tasks like those used in our optimization. V4 may in turn be characterized as having been selected precisely to support the downstream computation in IT. This type of explanation is qualitatively different from more traditional approaches that seek explicit descriptions of neural responses in terms of particular geometrical primitives. However, our results show functionally relevant constraints can be used to obtain quantitatively predictive models even when such explicit bottom-up primitives have not been identified.

Going forward, we will bridge these bottom-up and top-down explanations by building links to lower and intermediate visual cortex, especially in V1 and V2. We will also explore recent high-performing computer vision systems with architectures inspired by the ventral stream (36). Our results show that behaviorally driven computational approaches have an important role in understanding the details of visual processing (37) and suggest that the overall approach may be applicable to other cortical areas and task domains.

Materials and Methods

Array Electrophysiology. Neural data were collected in two awake behaving rhesus macaques (*Macaca mulatta*, 7 and 9 kg) using parallel multielectrode array electrophysiology systems (Cerebus System; BlackRock Microsystems). All procedures were done in accordance with National Institutes of Health guidelines and approved by the Massachusetts Institute of Technology (MIT) Committee on Animal Care. 296 neural sites (168 in IT and 128 in V4) were selected as being visually driven. Fixating animals were presented with testing images for 100 ms, and scalar firing rates were obtained from spike trains by averaging spike counts in the period 70–170 ms after stimulus presentation. See *SI Text* for additional details.

Neural Predictivity Metric. For each IT neural site, we used linear regression to identify a linear weighting of model output units (from the top or intermediate layers) that is most predictive of that site's actual output on a fixed set of sample images (10, 26, 27). Using this "synthetic neuron," we then produced per-image response predictions on novel images not used in the regression training and compared them to the actual neural site's output for those images (Figs. 3*A* and 5*A*). We computed the goodness-of-fit r^2 value, normalized by the neural site's trial-by-trial variability, to obtain the explained variance percentage for that site. The overall area predictivity of a model is the median explained variance over all measured sites in that area (Figs. 3 *B* and *C* and 5 *B* and *C* and see *SI Text*).

ACKNOWLEDGMENTS. We thank Diego Ardila, Najib Majaj, and Nancy Kanwisher for useful conversations. This work was partially supported by National Science Foundation Grant IS 0964269 and National Eye Institute Grant R01-EY014970.

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Supporting Information

Yamins et al. 10.1073/pnas.1403112111

SI Text

Data Collection. We collected neural data, assessed human behavior, and tested models on a common image set. In this section, we discuss this image set and the data collection methods used.

Array electrophysiology. Neural data were collected in the visual cortex of two awake behaving rhesus macaques (*Macaca mulatta*, 7 and 9 kg) using parallel multielectrode array electrophysiology recording systems (Cerebus System; BlackRock Microsystems). All procedures were done in accordance with National Institute of Health guidelines and approved by the Massachusetts Institute of Technology (MIT) Committee on Animal Care guidelines. Six 96-electrode arrays (3 arrays each in two monkeys) were surgically implanted in anatomically determined V4, posterior inferior temporal (IT), central IT, and anterior IT regions (1). Of these, 296 neural sites (168 in IT and 128 in V4) were selected as being visually driven with a separate image set. Fixating animals were presented with testing images in pseudorandom order with image duration comparable to those in natural primate fixations (2). Images were presented one at a time on an LCD screen (SyncMaster 2233RZ at 120 Hz; Samsung) for 100 ms, occupying a central 8° visual angle radius on top of a gray background, followed by a 100-ms gray blank period with no image shown. Eye movements were monitored by a video tracking system (EyeLink II; SR Research), and animals were given a juice reward each time central fixation was maintained for six successive image presentations. Eye movement jitter within 2° from a 0.25° red dot at the center of screen was deemed acceptable, whereas presentations with large eye movements were discarded. In each experimental block, responses were recorded once for each image, resulting in 25–50 repeat recordings of the each testing image.

For each image repetition and electrode, scalar firing rates were obtained from spike trains by averaging spike counts in the period 70–170 ms after stimulus presentation, a measure of neural response that has recently been shown to match behavioral performance characteristics very closely (3). Background firing rate, defined as the mean within-block spike count for blank images, was subtracted from the raw response. Additionally, the signal was normalized such that its per-block variance is 1. Final neuron output responses were obtained for each image and site by averaging over image repetitions. Recordings took place daily over a period of several weeks, during which time neuronal selectivity patterns at each recording site were typically stable. Based on firing rates and spike-sorting analysis, we estimate that each individual electrode multiunit site in this study picks up potentials from one to three single neural units. To determine whether results would likely differ for direct single-unit recordings, we sorted single units from the multiunit IT data by using affinity propagation (4) together with the method described in ref. 5. Of these units, 21 had internal trial-to-trial consistency with an r value of 0.3. We assessed the hierarchical modular optimization (HMO) model's prediction ability for these single units, obtaining a median of $50.4 \pm 2.2\%$ explained variance, very close to that obtained directly from the multiunit data. Moreover, we supplemented with serially sampled, single-electrode recording (6,7) and found that neuronal populations from arrays have very similar patterns of image encoding as assembled single-electrode unit populations.

Test stimulus set. The test stimulus set (Fig. 1*A*) consisted of 5,760 images of 64 distinct objects chosen from one of eight categories (animals, boats, cars, chairs, faces, fruits, planes, tables), with eight specific exemplars of each category (e.g., BMW, Z3, Ford, etc., within the car category). The set was designed specifically to (*i*) include a range of everyday objects, (*ii*) support both coarse, basic-level category comparisons (e.g., animals vs. cars) and finer subordinate level distinctions (e.g., distinguish among specific cars) (8), and (*iii*) require strong tolerance to object viewpoint variation, e.g., pose, position, and size. Objects were placed on realistic background images, which were chosen randomly to prevent correlation between background content and object class identity.

Object view parameters were chosen randomly from uniform ranges at three levels of variation (low, medium, and high), and images were rendered using the photorealistic Povray package (9). The parameter ranges for the three variation levels were as follows:

i) Low variation: All objects placed at image center ($x = 0$, $y = 0$), with a constant scale factor ($s = 1$) translating to objects occluding 40% of image on longest axis, and held at a fixed reference pose ($rxy = rxz = ryz = 0$).

ii) Medium variation: Object position varies within one-half multiple of total object size ($|x|$, $|y| \leq 0.3$), varying in scale between $s = 1/1.3 \sim 0.77$ and $s = 1.3$, and between $-45°$ and $45°$ of in-plane and out-of-plane rotation ($\leq 45°$).

iii) High variation: Object position varies within one whole multiple of object size ($|x|$, $|y| \leq 0.6$), varying in scale between $s = 1/1.6 \sim 0.625$ and $s = 1.6$, and between $-90°$ and $90°$ of in-plane and out-of-plane rotation ($\leq 90°$).

Crowd-sourced human psychophysics. Data on human object recognition judgement abilities shown in Fig. 2*B* and Fig. S6 were obtained using Amazon's Mechanical Turk crowdsourcing platform, an online task marketplace where subjects can complete short work assignments for a small payment. A total of 104 observers participated in one of three visual task sets: an eight-way classification of images of eight different cars, an eight-way classification of images of eight different faces, or an eight-way categorization of images of objects from eight different basic-level categories. Observers completed these 30- to 45-min tasks through Amazons Mechanical Turk. All of the results were confirmed in the laboratory setting with controlled viewing conditions, and virtually identical results were obtained in the laboratory and web populations (Pearson correlation $= 0.94 \pm 0.01$). For the eight-way basic-level categorization task set, each human observer ($n = 29$) judged a subset of 400 randomly sampled images with blocks for each of the three variation levels (400 of 640 for low variation and 400 of 2,560 for medium and high variation levels). For the eight-way car ($n = 39$) and eight-way face ($n = 40$) identification task sets, each observer saw all 80 images at the low variation level and all 320 images at both medium and high variation levels. The presentation of images were randomized and counterbalanced so that the number of presentations of each class was the same in the given variation level. Each trial started with a central fixation point that lasted for 500 ms, after which an image appeared at the center of the screen for 100 ms; following a 300-ms delay, the observer was prompted to click one of eight response images that matched the identity or category of the stimulus image. Response images were shown from a fixed frontal viewpoint and remained constant throughout a trial block. All human studies were done in accordance with the MIT Committee on the Use of Humans as Experimental Subjects.

Performance was determined by computing accuracies for each task. For a given eight-way task set and variation level (e.g., high-variation basic-level categorization, medium-variation car subordinate identification, etc.), we constructed the raw 8×8 confusion matrix for each individual observer and computed the population confusion matrix summing raw confusion matrices across individuals.

From the population confusion matrix, we computed accuracy values for each task of recognizing one target class against seven distractor classes (a.k.a. binary task). We obtained 72 binary task accuracies by performing this procedure over all combinations of three task sets and three variation levels (3 task sets × 8 targets per task set × 3 levels of variation). We used standard signal detection theory to compute population accuracy from the population confusion matrix definition. The pooled performance scores were highly consistent, with a median (taken over the 72 tasks) Spearman-Brown corrected split-half Pearson-coefficient self-consistency of 0.99. To estimate the subject to subject variability, we selected one subject from each task set and combined the task performance of the three task sets to produce 72 individual human accuracies.

Data Analysis and Metrics. In this section, we discuss metrics that were used to characterize neural data and measure models' match to neurons. These metrics apply to any model and neural population and not just output from hierarchical feedforward neural networks. The only restriction on a model for our methods to be applicable is that the model be image computable, e.g., it is a rule for producing output on any arbitrary stimulus set and does not explicitly rely on stimuli being in a particular subclass of images (10, 11).

Individual neural site predictions. As described in the main text, we used a standard methodology for assessing a model's ability to predict individual sites (12, 13), in which each site is modeled as a linear combination of model outputs. In this procedure, linear regression was used to determine weightings of top-level model outputs which best fit a given neurons' output on a randomly chosen subset of the testing images. The remaining images were used to measure the accuracy of the prediction. Results from multiple random subsets were assessed independently and averaged to ensure statistical validity. Linear regressor results are reported for 10 splits of cross-validation, using 50%/50% train/test splits. Regression weights were obtained using a simple partial least squares (PLS) regression procedure, using 25 retained components (14, 15). For each measured site, separate neural response predictions and cross validated goodness-of-fit r^2 values were obtained. The percentage of explained variance was then computed on a per-site basis by normalizing the r^2 prediction value for that site by the site's Spearman-Brown corrected split-half self-consistency over image presentation repetitions.

To help interpret the meaning of this linear regression technique, consider a hypothetical case in which the responses for all IT neurons in one source animal are known on a set of image stimuli, and the goal is to use these data to predict the response of a random sample of IT neurons from a second target animal. This is a problem of neuron identification, e.g., for each target neuron in the target animal, determining which neuron(s) in the source animal correspond to that target neuron. Although it is known that at the population code level the IT responses of several different animals (and even different primate species) are similar (16), it is not known to what extent there is a 1-to-1 matching of responses between individual neural sites. There is likely to be significant individual variability between the specific tuning curves of units present in different animals, and it is not clear whether the IT units in all animals can be thought of as independent samples from a single master distribution of IT-like neurons. Hence, to explain a given IT unit in the target animal's IT might require linear combinations of multiple source animal IT units, even if a complete sample of neurons from the source animal was available. In more mathematical terms, it is plausible that the best linear fit from one animal's IT to another's would not be particularly sparse. Because it is currently not yet known how sparse the between-animal mapping actually is, in the present work each model's output units is treated a basis from which any observed IT must be constructed, with no prior on the expected sparsity of the weighted sums. Although in our experiments we did collect responses from units in two animals, we do not have enough units from either animal separately to draw a meaningful conclusion as to what the empircal sparsity distribution is, because accurate estimation would likely require on the order of $\sim 10^3$ units from a single animal. If recordings in multiple animals with enough units and images to assess cross-animal fitting sparsity becomes available, such data will be useful to falsify our—or any—model or IT, because the distributions of sparsenesses of the linear mappings from the model to any one population should match the typical animal-to-animal sparseness distribution.

This observation helps clarify the relationship between our work and some existing work on neural fitting (10, 11, 17). In that line of work, which has provided very useful insight into the units up to the V4 area, a different nonlinear model—roughly equivalent to a single convolutional neural network (CNN) network in our model, described below—is fitted separately for each observed visual neuron. Unlike that work, the present results yield a generative model of a neural population as a whole, one that can fit not just the tuning curves of observed neurons but also predicts what types of neurons a typical sample population should a priori contain.

We also implemented two stronger tests of generalization: (*i*) object-level generalization, in which the regressor sample set contained images of only 32 object exemplars (four in each of eight categories), with results assessed only on the remaining 32 objects, averaging results across many such object splits, and (*ii*) category-level generalization, in which the regressor sample set contained images of only half the categories (eight objects in each of, e.g., animal, boat, car, and chair categories), with results assessed only on images of the other categories (eight objects in face, fruit, plant, and table categories), averaged across many such category splits. Fig. S9 shows neural fitting results for object and category generalizations.

Prediction accuracy remains high for the object-level generalization, suggesting that the HMO model is effective at the generalizing neural predictions across a wide range of natural image variability. Neuron-level predictions of all models fall off somewhat in the category generalization case, although relative magnitude and ordering between models are preserved. To interpret this, it is again useful to consider the hypothetical animal-to-animal neural identification task described above. Even with completely comprehensive source animal response data (e.g., all the units in IT—the perfect model), the neuron identification task involves some uncertainty. If the training image stimulus set is not comprehensive enough to completely identify the target neuron, predictions from source to target will break down on images outside that image set. When the data used to identify the target neuron are narrowed to a very limited semantic slice of image space (e.g., a fraction of the object categories), it is expected that it will become difficult to identify that specific neuron from responses to just those images. For example, if all of the images in the training set were only of simple shapes of a uniform size and geometry, it would be impossible to effectively carry out the neuron identification procedure (via linear regression or any other technique). It is instructive to compare this to the results for the population level coding (see section on Representational Dissimilarity Matrices below), where even in the category generalization case, predictions remain accurate.

Linear classifier analysis. Object recognition performance was assessed by training linear classifiers on model and neural output. Linear classifiers are a standard tool for analyzing the performance capacity of a featural representation of stimulus data on discrete classification problems (6, 18). For any fixed population of output features (from either a model or neural population), a linear classifier determines a linear weighting of the units which best predicts classification labels on a sample set of training images. Category predictions are then made for stimuli held out from the weight

training set, and accuracy is assessed on these held-out images. To reduce the noise in estimating accuracy values, results are averaged over a number of independent splittings of the data into training and testing portions. In our case, the output features of a model on each stimulus are (by definition) the set of scalar values for each top-level model unit when evaluated on that stimulus, a typical procedure from computer vision studies (19, 20). For neuronal sites, the output features are defined as the vector of scalar firing rates for each unit, as is typical in neural decoding studies (6, 18).

To measure performance, we trained SVM (15) classifiers with $l2$ regularization for three types of tasks supported by the testing image set, including eight-way basic category classification (i.e., animals vs. boats vs. cars, etc.), eight-way car identification (astra vs. beetle vs. clio, etc.), and eight-way face identification, separately for each of the three levels of variation in the testing image set. Eight-way task choices were computed as a maximum over margins from eight binary one-vs.-all (OVA) classifiers (15). Fig. 2*B* shows cross-validated performance accuracies (defined as the fraction of correct predictions averaged over test splits) for the eight-way basic categorization task at the three variation levels. Fig. S6 shows accuracies for subordinate identification tasks as well.

The values shown in Fig. 2*B* and Fig. S6 are for classifiers trained with 75% train/25% test splits, averaged over 20 random category-balanced splits. However, the absolute values of performance for a linear classifier depend on the choice of the number of training examples used. To ensure that our conclusions were not dependent this choice, we computed performance curves for varying numbers of training examples. Although absolute performances did vary as a function of training examples, we found that the relative ordering of performances did not (Fig. S7*A*). Moreover, representations that were effective at high variation level (e.g., the IT neuronal population and the HMO model units) achieved most of their performance with comparatively small numbers of training examples.

Absolute performance also varies with the number of features used—the number of neuronal sites sampled in the case of neural data, or the number of top-end units in the case of models. As with the number of training examples, we would like to be sure that our results do not depend strongly on the number of sampled units. However, the analysis of dependence on number of units is somewhat less straightforward than analysis of training set size dependence, because it is not immediately clear how to fairly equate one neural unit with a fixed number of sample model units. Ideally, we would have extremely large numbers of both kinds of units and then simply make comparisons on complete population samples. Given the limitations of neural data collection, the limiting factor in this work is the number of neural sites sampled. We believe, however, that for the three key comparisons that we make, sample sizes issues do not strongly impact our results:

i) IT neural sample vs. V4 neural sample: At approximately the same number of neural samples (168–128), the performance values at high variation image set are extremely widely separated. Although it is unlikely that this difference is due to neural sample size, to ensure that this is true, we computed performance curves for subsamples of the population of different sizes (Fig. S7*B*), averaging over many subsamples of each fixed size. At all sizes, the IT population strongly outperformances the V4 population. Because these subsample curves appear to have a predictably logarithmic shape, we also fit the data to a logarithmic functional form to extrapolate approximately how many units would be required to achieve the performance measured from the human behavioral experiments. Our estimate suggests that $\sim 1{,}050 \pm 300$ IT units would be consistent with human performance, whereas $\sim 10^7$ V4 units would be required. Such estimates are necessarily very rough, but they illustrate the magnitude of the differences between these neural populations.

ii) IT neural sample vs. existing comparison models: In all cases the models sampled produced more output features than we had neural sites (4,096 in the case of HMAX, 24,316 for the V2-like model, and 86,400 for the V1-like model; see below for more information on the these models). The results in Fig. 2*B* show performances computed with the total number of model features in each case. The implication of this is that, even with thousands or tens of thousands of features, these models are not able to equal the performance level of even 168 randomly chosen IT units. Equating the number of features, either by increasing the number IT samples or decreasing the number of model features, would only make the magnitude of the gap larger.

iii) IT neural sample vs. the HMO model outputs. Our claim is that the HMO model is plausibly correct, i.e., it achieves roughly the right performance for a reasonable number of samples. The HMO model performs at approximately human levels with 1,250 top-end outputs, within the sampling error of the number of IT units suggested by extrapolation to achieve human performance. We also subsampled the HMO model to have as many features as our IT sample (168) and found that, although the performance degraded somewhat, it did not drop below measured IT performance levels. However, it is certainly possible that investigating the detailed dependence of model and IT performance on number of samples would allow us to falsify the HMO model. This falsification would be of interest for spurring future work, but for the reasons described above, it would be unlikely to invalidate the claims made in the present work.

Population code representational dissimilarity matrices. Given stimuli $S = s_1, \ldots, s_k$ and vectors of neural population responses $R = \vec{r}_1, \ldots, \vec{r}_k$ in which r_{ij} is the response of the jth neuron to the ith stimulus, we following ref. 16 by defining the representational dissimilarity matrix (RDM) as

$$\mathrm{RDM}(R)_{ij} = 1 - \frac{\mathrm{cov}(\vec{r}_i, \vec{r}_j)}{\sqrt{\mathrm{var}(\vec{r}_i) \cdot \mathrm{var}(\vec{r}_j)}}.$$

RDM structure is indicative of a range of behavior that a given neural population can support (21), and two populations can have similar RDMs on a given stimulus set (and similar population-level classification performance) even if the low-level details of the neural responses are somewhat different. Because they involve correlations over the feature dimension, RDMs alleviate some of the ambiguities just discussed in analyzing individual units. We produced RDMs for the IT and V4 neural populations, as well as for each of the model-based synthetic IT and V4 neural populations using weights obtained from the regressions for the individual site fits (Fig. 3 *D* and *E* and Fig. S8). Following Kriegeskorte (21), we measured similarity between population representations by assessing the Spearman rank correlations between the RDMs for the two populations. In addition to the standard image-level RDM, in which each pair of test images gives rise to an element of the RDM, we also computed object-level RDMs by averaging population responses for each object before computing correlations (so that each pair of objects gives rise to an element of the 64×64 object-level RDM). Similarity of the HMO model object-level RDMs with the IT object-level RDMs are what shown and quantified in Fig. 3 *D* and *E*.

The RDM for the IT neural population we measured has clear block-diagonal structure—associated with IT's exceptionally high categorization performance—as well as off-diagonal structure that characterizes the IT neural representation more finely than any single performance metric. In contrast, the RDM for the V4 population shows how high levels of variation blur out explicit categorical structure for intermediate visual areas, providing a clear visualization of the contrasting population responses underlying the high-variation V4-IT performance gap shown in Fig. 2*B*.

We also computed RDMs for object- and category-level generalizations, using the weightings from the regressions produced as described above in the section on individual neural site predictions. It is instructive to notice that the HMO model maintains high levels of IT similarity even at category-level generalizations (Fig. 3 *D* and *E*), suggesting that, although individual IT units may be hard to predict from a semantically narrow slice of image space (e.g., half the categories only), the overall population code structure remains well predicted.

Modeling. ***Comparison models.*** We compared results for performance, single site neural fitting, and population-level similarity for a variety of computational models, including the following:

i) The trivial Pixel control, in which 256 × 256 square images were flattened into a 65,536-dimensional feature representation. The pixel features provided a control against the most basic types of low-level image confounds.
ii) The baseline SIFT computer vision model (22). This model provided another control against low-level image confounds.
iii) An optimized V1-like model (23), built on grid of Gabor edges at a variety of frequencies, phases, and orientations. This model provided an approximation of a comparison point to lower levels in the ventral visual stream.
iv) A recent V2-like model (24), composed of conjunctions of Gabors. This model provides an approximation of the second level of the ventral stream.
v) HMAX (19, 25), a multilayer convolutional neural network model targeted at modeling higher ventral cortex. Because it is a deep network, HMAX has large IT-like receptive fields. HMAX is one of main existing first-principles-based models that attempts to build up invariance through hierarchical alternation of simple and complex cell-like layers.
vi) PLOS09, a recent three-layer convolutional neural network (26), which also has large IT-like receptive fields and which was discovered via a high-throughput screening procedure that was a predecessor to the HMO procedure.

Ideal observer semantic models. As shown in Figs. 3 and 5, we also computed the IT and V4 predictivity for ideal-observer semantic models (27). Although these ideal observers are not image computable models, given our perfect knowledge of image metadata, we were able to compute explained variance percentages using the same linear regression protocol applied to the image-computable models. We evaluated two ideal observers:

i) A category ideal observer. This model has eight features, one for each of the eight categories present in the test image set. For each image, the *i*th feature is 1 if the image contains an object of category *i*; otherwise, it is 0. For each IT unit, the eight linear regression weights for this feature set effectively describe how much each category contributes to that unit's response.
ii) An all-variable ideal observer. This model is given oracular access to all metadata parameter variables for the images, with one feature for each of 64 object identities (similar to the category ideal observer features above), in additional to features reporting object position, size, scale and image background.

If the IT or V4 explained variance for these (or any) ideal observers were close to 100%, then they would provide a conceptually interpretable explanation of neural variation, a very scientifically desirable result. In fact, the explained variance percentages are significantly less than 100% for the ideal observers we tested (although of course other better ones might be found, e.g., by taking into account 3D object curvature). These ideal observers therefore serve as useful controls to which other computational models can be compared. For example, the ideal category model serves to control for the minimum amount of IT explained variance that should be expected from any model that has high categorization performance. Insofar as a model with high categorization performance explains more explained variance than the ideal category model, that additional predictivity can be attributed to the constraints of the model class.

CNN model class. Here, we mathematically specify the basic class of CNN models used in this paper. These principles are consistent with a large parameter space of possible networks. The specific parameterized space of networks we use is close to that described in Pinto et al. (26), with one, two, or three convoluational layers. Each layer is characterized by a fixed set of parameters, but parameter values can differ between layers. This parameter space expresses an inclusive version of the hierarhical feedforward network concept and contains models similar to that used in many previous studies for different parameter values (19, 23, 24, 25).

More specifically, each individual layer is composed of operations including local pooling, normalization, thresholding, and filterbank convolution, which are combined as follows:

$$N_\Theta(X) = \text{Normalize}_{\theta_N}\left(\text{Pool}_{\theta_p}\{\text{Threshold}_{\theta_T}[\text{Filter}_{\theta_F}(X)]\}\right), \quad \textbf{[S1]}$$

where X is a 2D input image. The subscripts $\Theta = (\theta_p, \theta_N, \theta_T, \theta_F)$ denote the specific parameter choices for the constituent operations, setting radii, exponents, and thresholds, as described in Pinto et al. (26). Similar to previous studies, we also use randomly chosen filterbank templates in all models, but additionally allow the mean and variance of the filterbank to vary as parameters. Functions of the form N_Θ are the simplest computational units that we operate on and are thought to be plausible representations of what happens in a single cortical layer (28). To produce deep CNNs, layers of the form N_Θ are stacked hierarchically:

$$\ldots \mathbf{P}^{\ell-1}_{\theta_{P,\ell-1}} \xrightarrow{\text{Filter}} \mathbf{F}^{\ell}_{\theta_{F,\ell}} \xrightarrow{\text{Threshold}} \mathbf{T}^{\ell}_{\theta_{T,\ell}} \xrightarrow{\text{Pool}} \mathbf{N}^{\ell}_{\theta_{P,\ell}} \xrightarrow{\text{Normalize}} \mathbf{P}^{\ell}_{\theta_{N,\ell}} \ldots, \quad \textbf{[S2]}$$

where ℓ is layer number and the initial input at the 0th layer is the image pixel array X. We denote such a stacking operation as $\otimes$, so that the stacked hierarchical model can be written as

$$\mathbf{N} \equiv \otimes_{i=1}^{k} N_{\Theta_i}.$$

Let $\mathcal{N}_k$ denote the space of all stacked networks (N) of depth k or less. In this study, our CNNs are networks of depth $k = 3$ or less.

Mixture networks. We extend the class of CNNs by a fourth principle, namely that, at any stage, networks can consist of mixtures of CNNs where each component has a potentially distinct set of parameters (e.g., pooling size and number of filters), representing different types of units with different response properties (29). Such mixture networks may combine components of differing complexity, which correspond to anatomical bypass connections within the ventral stream (30) (Fig. S2*B*).

For a mathematical formulation of this idea, note that because the networks in $\mathcal{N}_3$ are convolutional, they can be combined in a standard fashion. Specifically, given a sequence of individual modules $\mathbf{N}(\Theta_{i1}, \Theta_{12}, \ldots, \Theta_{in_i})$ for $i \in [1, \ldots, J]$, possibly of different depths, the mixture network is defined by aligning the module output layers along the spatial convolutional dimension. Because the outputs of each of the modules is a 3D tensor, this alignment is well defined up to a rescaling factor in the spatial dimension. We denote this alignment operation by the symbol $\oplus$, so that a combined mixture network can be written as

$$\mathbb{N} \equiv \oplus_{i=1}^{J} \mathbf{N}(\Theta_{i1}, \Theta_{12}, \ldots, \Theta_{in_i}).$$

The total output of networks of this form is also a 3D tensor, so they too can be stacked with the $\otimes$ operation to form more

complicated, deeper hierarchies. By definition, the full class $\mathbb{N}$ consists of all of the networks formed by iteratively composed the stacking ($\otimes$) operation and the combination ($\oplus$) operation. Conceptually, members of $\mathbb{N}$ are nonlinear mixtures of modules chosen from a base class of simpler homogenous neural networks (e.g., the elements of $\mathcal{N}$). Schematically, $\otimes$ is a vertical composition relationship, increasing the depth complexity of the network. Biologically, it is plausible to think of $\otimes$ as corresponding to producing complex nonlinear representations by feedforward layering. Conversely, $\oplus$ is a horizontal composition relationship, increasing the breadth complexity of the network. Biologically, this may correspond to the idea of mixing heterogenous populations of different types of units in a given area.

HMO. The HMO procedure (31) is a computational optimization procedure designed to identify high-performing network architectures from the space $\mathbb{N}$. Intuitively, it is a version of adaptive boosting in which rounds of optimization are interleaved with boosting and hierarchical stacking (32). The process first analyses error patterns in the recognition predictions of candidate networks, picking complementary components, e.g., those with optimally nonoverlapping errors. Subsequent rounds of optimization attempt to optimize a criteria weighted toward those stimuli that are misclassified by the first-round results. As a result, complementary components emerge without having to prespecify the corresponding subtasks semantically (or in any other way), mapping the complex structure of high-variation recognition problems onto the parameter space of neurally plausible computations. These components are then aligned along their convolutional dimensions and used as inputs to repeat the same procedure hierarchically to build more complex nonlinearities. Although other possible optimization procedures could potentially be used to create high-performing neural networks (33), the HMO process may be particularly efficient because it explicitly takes advantage of the complementary strengths of different components within the large space of network architectures.

This section describes details of the HMO procedure. Suppose that $N \in \mathcal{N}$ and S is a screening stimulus set. Let E be the binary-valued classification correctness indicator, assigning to each stimulus image s 1 or 0 according to whether the screening task prediction was right or wrong, where the prediction for each s was made by using maximum correlation classifiers (MCCs) (34) on the output features of N with threefold cross-validation (see *Materials and Methods* describing screening set metric). Let

$$\text{performance}(N, S) = \sum_{s \in S} E[N(s)].$$

To efficiently find N that maximizes performance(N, S), the HMO procedure follows these steps:

i) Optimization: Optimize the performance function within the class of single-stack networks of some fixed depth d_1, obtaining an optimization trajectory of networks in $\mathcal{N}_{d_1}$ (Figs. S2*C* and S5*A*, *Left*). The optimization procedure that we use is hyperparameter tree parzen estimator, as described in ref. 35. This procedure is effective in large parameter spaces that include discrete and continuous parameters.

ii) Boosting: Consider the set of networks explored during step 1 as a set of weak learners and apply a standard boosting algorithm (Adaboost) to identify some number of networks $\mathrm{N}_{11}, \ldots, \mathrm{N}_{1l_1}$ whose error patterns are complementary (Fig. S2*C*, *Right*).

iii) Combination: Form the heterogenous network $\mathbb{N}_1 = \oplus_i \mathrm{N}_{1i}$ and evaluate $E[\mathbb{N}_1(s)]$ for all $s \in S$.

iv) Error-based reweighting: Repeat step 1, but reweight the scoring to give the jth stimulus s_j weight 0 if N_1 is correct in s_j and 1 otherwise. That is, the performance function to be optimized for N is now

$$\sum_{s \in S} E[N_1(s)] \times E[N(s)].$$

Repeat step 2 on the results of the optimization trajectory obtained to get models $N_{21}, \ldots N_{2k_2}$, and repeat step 3 (Figs. S2*C* and S5*A*, *Right*). Steps 1, 2, and 3 are repeated K times.

After K repetitions of this process, we will have obtained a mixture network $N = \oplus_{i \le K, j \le k_i} N_{ij}$. The process can then simply be terminated or repeated with the output of N as the input to another stacked network. In the latter case, the next layer is chosen using the model class $\mathcal{N}_{d_2}$ to draw from, for some fixed depth d_2, and using the same adaptive hyperparameter boosting procedure. The metaparameters of the HMO procedure include the numbers of components $l_1, l_2, \ldots$ to be selected at each boosting round, the number of times K that the interleaved boosting and optimization is repeated, and the number of times M that this procedure is stacked. For the purposes of this work, we fixed the metaparameters $K = 3$, $l_1 = l_2 = l_3 = 10$, and $M = 2$ (with $d_1 = 3$, $d_2 = 1$).

Model screening procedure. To construct a specific model network, we applied HMO to a screening task (Figs. S1*B* and S5). Like the testing set, the screening set was designed to be very challenging—having high levels of object pose, position, and scale variation (36). However, to ensure that a fair test could be made, in all other regards, the screening images were distinct from the testing image set, containing objects in totally nonoverlapping semantic categories, using none of the same background scenes, lighting, or noise conditions. The image set used for the HMO screening procedure consisted of 4,500 images of 36 distinct objects, chosen from one of nine categories, including bodies, building, flowers, guns, musical instruments, jewelry, shoes, tools, and trees. As in the testing set, in the high-variation subset, objects were shown in varying positions, sizes, and poses, placed in a variety of uncorrelated natural backgrounds scenes. Lighting was provided by ambient environment reflection, and speckle noise was added to simulate natural image distortions. Images were rendered with the Panda3d package (37).

The relationship between the screening set and testing set is intended to be similar to that between any two typical samples of natural images: having some high-level natural statistical commonalities, but otherwise quite different specific content. For this reason, any performance increases that could be demonstrated to transfer from the screening to the testing set are likely to also transfer, at least to some extent, to other high-variation image sets.

The screening objective sought to minimize classification performance error on the 36-way object classification task (no categorical semantic information was used), as assessed by training unregularized MCC classifiers with threefold cross-validated 50%/50% train/test splits. Using the HMO procedure on this screening set, we generated a network HMO_0, which produces 1,250-dimensional feature vectors for any input stimulus. HMO_0 is the model that we refer to throughout the paper as the HMO model and that we used for all testing evaluation.

In the optimization, candidate networks were first evaluated on overall performance metric, and performance gradients in parameter space were identified as seen in the trend toward decreasing screening loss (step 1; Fig. S5*A*, *Left*, blue dots). Ten components were identified by boosting (step 2) and combined. In subsequent rounds (Fig. S5*A*, *Right*, red dots), the optimization criterion was biased toward weighting more heavily errors of the architectures from earlier rounds (step 4). Decreasing loss in these later rounds indicates that models are improving at the subset of images that confused the components identified in round 1. The complementary model components identified in the two different optimization rounds were associated with different directions in the overall large parameter space of possible neural-like computations that effectively solve different subtasks

of the overall recognition task (Fig. S5*B*). As expected, training performance increases as components are combined (Fig. 4*C*).

Assessment. As described in the main text, we then assessed the HMO_0 model against the testing dataset (Fig. S1*A*). The HMO_0 model showed high performance on testing set, as described in the main text, Fig. 2*B*, and Fig. S6. Comparisons to neural data showed that the HMO_0 model also had significantly power to explain neural data, both at the individual site level (Figs. 3 *A–C* and 5) and the population level (Fig. 3 *D* and *E* and Fig. S8). The HMO model is a significantly closer match to IT population representations at all variation levels, but the difference is especially evident at the high variation level that most clearly exposes how the high-level IT representation differs from the lower-level V4 representation (Fig. S8, black bars).

Subsequently, we determined the stability of the HMO procedure by running it on a variety of alternative screening sets with different choices of objects and categories, varying the numbers of within-category exemplars and varying amounts of semantic similarity to the testing set. Performance and neural fitting ability were largely stable to these changes. Although some of these later models exhibited higher performance and neural explanatory power than the initial HMO_0 model, to prevent domain overfitting, we report only the results of the initial model HMO_0 constructed before any testing set results were obtained.

It is important to note how our screening process connects to the evaluation of other models. In the cases of the SIFT, V1-like, and V2-like models, we did not pretrain those models using the screening set: this is because those models do not accept pretraining data at all. In the case of HMAX, which does accept pretraining data, we used the testing data itself for pretraining, to give that model that highest chance of performance success. Separately, we also performed a pretraining of the HMAX model using the screening set and then reextracted it on the testing set, but found that this only further decreased final performance and neural fit results of the HMAX model (e.g., learned parameters did not effectively transfer from the screening to the testing set).

Another issue relevant to comparison of models is the question of numbers of total internal units. In the mixture models that we used to create the HMO model, the numbers of filters at each layer were kept very small ($\leq$24) to ensure that a total combined model composed of several such components would not be unmanageably large. In the HMO_0 model, the total number of units is approximately the same as that in the HMAX model, and the total number of output features is somewhat smaller (1,250 vs. 4,096).

Correlation experiments. Performance and neural predictivity results suggest that as performance on high-variation tasks increases, metrics of neural similarity also increase (Fig. 1b). To determine whether this correlation is a general feature of the deep feedforward architectures defined here, we ran several additional high-throughput experiments, evaluating a large number of candidate model architectures and measuring categorization performance and IT neural predictivity for each model (Fig. 1a and Fig. S3). Specifically, we performed three high-throughput searches of the parameter space $\mathcal{N}_3$ described in the above:

i) Random selection. We drew several thousand randomly sampled models from the parameter space $\mathcal{N}_3$. For each one, we computed linear classifiers for performance and linear regressors for IT predictivity, as described above. Each green point in Fig. S1*A* corresponds to one such model. In this condition, there is a significant correlation between performance and IT predictivity ($r = 0.55$, $n = 2{,}016$). Negative values on the y axis correspond to models having negative goodness of fit (the r^2 coefficient of determination statistic), due to overfitting on the training images. Fig. S3, *Left*, shows model performance for as a function of time during the procedure; the lack of any trend corresponds to random sampling of models.

ii) Performance optimization. Using the recently developed Hyperopt metaparameter optimization algorithm (35), we performed a directed search for network parameters that maximized performance on the high-variation eight-way categorization task (Fig. S1*A*, blue points). This optimization was carried out using the recently developed hyperparameter optimization algorithm Hyperopt (35). Via this optimization, absolute performance and fitting values were significantly improved compared with the random condition. Moreoever, although the optimization was done without reference to any neural data, the correlation between performance and IT predictivity actually increased significantly ($r = 0.78$, $n = 2{,}043$). Fig. S3, *Center*, shows the optimization criterion as a function of time step during the optimization procedure; the upward trend is due to the optimization process. Although the optimization gains toward the end of the optimization process are slow and appear to be plateau, small improvements are still observed.

iii) IT predicitivity optimization. In the third experiment, we directly optimized model architecture for IT predictivity, this time without reference to performance (Fig. S1*A*, orange dots). The correlation is comparable to the performance-optimized condition ($r = 0.80$, $n = 1{,}876$), but the optimization plateau occurs significantly earlier (Fig. S3, *Right*; we repeated the optimization multiple times, and obtained the same result each time; this suggests that continued optimization would not be effective). Moreover, the best-performing models from the performance-optimization experiment predict IT neural output as well as the models explicitly optimized for the predictivity objective, whereas the reverse does not hold.

The results of these experiments support three inferences. First, model performance is modestly correlated with neural predictivity in a random selection regime. Second, optimization pressure for either metric produces markedly better cross-validated accuracy on the optimized axis, and in doing so, significantly strengthens the correlations with the other nonoptimized metric. Third, when optimizing for performance, the best-performing models predict neural output approximately, as well as the most predictive models selected explicitly for neural predictivity, but not vice versa. The feedforward model architecture class itself imposes a relationship between high-level behavior (performance) and more detailed neural mechanisms, but directed optimization focuses on a region within network parameter space where this constraint is much stronger.

The inclusion of the category ideal observer (purple square in Fig. 3*D*) shows an effective negative control on the performance-predictivity relationship: it lies significantly off the main trend, making it visually clear how the correlation arises from a combination of architectural and performance constraints working in concert.* However, this ideal observer is not an image-computable model, It would be especially instructive to identify a image-computable algorithm that achieved invariant object recognition high performance but low neural IT neural consistency. If such an algorithm existed, its architecture might illustrate a very nonneural solution to object recognition tasks as a purely computer vision problem. With current understanding, we cannot rule out the possibility that such an algorithm does not exist—e.g., recent high-performing computer vision systems are deep convolutional neural networks (33).

Fig. 1*A* also implies that, even with intensive optimization, individual models in the $\mathcal{N}_3$ are limited in performance and

*Note that a converse control, in which a model has very high neural consistency for a population of IT units but low performance, cannot exist. IT units are already known to have high performance, so any model that matches IT units sufficiently well must also have high performance.

neural prediction ability, underscoring the need for an enlarged model class. However, further analysis of the results of these optimization experiments provides insight into how to construct a more effective model class. In Fig. S10, we show scatter plots of model performance on pairs of binary subtasks, e.g., performance on the two-way cars-vs.-planes task compared with performance on the two-way boats-vs.-chairs task. These plots show that, as the optimization algorithm explores parameter space, it identifies mutually exclusive subspaces that are effective for some of the natural subtasks defined in the overall task space. The highest performing architectures for one subtask are often significantly suboptimal for other subtasks, leading to V-shaped subtask-vs.-subtask scatter plots. In choosing a single architecture that is best for overall performance, the optimization is forced to tradeoff performance on some of these subtasks.

The effectiveness of optimized mixture models (such as HMO) may be understood in the context of Fig. S10, which suggests that models composed of mixtures from the $\mathcal{N}_3$ class might be significantly more effective than any single model alone. Such mixtures are also suggested by the observation from neurophysiology studies that patches within IT are selectively responsive for distinct object classes (38–40). Intuitively, such subregions might correspond to architecturally specialized structures within the larger feedforward class. Mixture models avoid the tradeoffs inherent in individual feedforward structures by combining several pareto-optimal network architectures. By identifying particularly effective mixture combinations, the HMO procedure overcomes these limitations efficiently. In addition, however, a key ingredient for the HMO model's success is that the components constituting the model, which were (by construction) complementary on the original screening set, were still complementary on the testing set. This holds even though the testing set had entirely distinct object categories, so the basis on which the complementarity of the components was originally discovered—nonoverlapping error patterns in screening set object identity judgements—is no longer even applicable. This strongly rules out image domain-specific overfitting and suggests that mixture components discovered by performance optimization may form a generically useful visual representational basis that can be recombined to solve new object recognition problems. In fact, achieving high performance and neural fitting capability appears to require diversity in many of the parameters of the constituent components (Fig. S11).

Model parameter diversity analysis. We characterized model parameters in terms of per-component tuning specificity vs. intercomponent diversity. Tuning specificity is a measure of how specifically each parameter needed to be tuned to produce optimal performance. To compute this, we analyzed the distribution of each parameter's values along the optimization trajectory near the optimal point using the concept of entropy. By definition, the entropy of (N samples from) a distribution P is

$$E(P) = \log(N) - \frac{1}{N}\sum_i n_i \log(n_i),$$

where N is the number of samples from the distribution, the sum is taken over possible values i of the distribution, and n_i is the number of samples with value i.

Suppose an optimal module component Θ^* occurs at timepoint t^* in the trajectory of one optimization run in the HMO process. Then, let $P_{p,k}(\Theta^*)$ be the distribution of values of parameter p in the k-neighborhood around t^* in the optimization trajectory

$$P_{p,k}(\Theta^*) = (\text{value of parameter } p \text{ at time points } t \in [t^* - k, \ldots, t, \ldots, t^* + k]).$$

The specificity of parameter p around optimal point Θ^* is, by definition,

$$-E\left[P_{p,k}(\Theta^*)\right].$$

Intuitively, this is because, if the distribution $P_{p,k}(\Theta^*)$ had high entropy, this indicated that the value of the parameter near the optimal point did not matter very much and therefore was not tuned very specifically. If, on the other hand, the distribution had low entropy, it was tightly clustered around one or a few optimal values that the optimization had identified as being important, suggesting it was highly tuned. For the purposes, we took $k = 25$ time steps, but values were not strongly sensitive to k with the range of 10–100. For each parameter p, we report the median tuning specificity of that parameter, taken over all component modules.

Intercomponent diversity is a measure of how variable a parameter is between the component modules. This was measured by computing, for each pair of components, how well separated the distributions of the parameter's values around each component were from each other. More formally, the d-prime discriminability index, d', for two distributions P_1 and P_2 is defined by

$$d'(P_1, P_2) = \frac{|\langle P_1 \rangle - \langle P_2 \rangle|}{\sqrt{0.5[\text{var}(P1) + \text{var}(P2)]}}.$$

(The sample d' uses the sample versions of the mean and variances.) Suppose Θ_1^* and Θ_2^* are two optimal components chosen by the HMO procedure. Then we measure separability for these two components as

$$d'\left[P_{p,k}(\Theta_1^*), P_{p,k}(\Theta_2^*)\right].$$

For each parameter p, we define intercomponent diversity as the median of this separation value taken over all pairs of components Θ_1 and Θ_2. The higher the diversity, the more different the components were from each other, and vice versa.

Parameters that have both high tuning specificity and high intercomponent diversity are both critical for performance and required to be heterogenous. Our results highlight certain types of parameters as being simultaneously highly tuned and diverse. This is particularly true for two broad classes of parameters, as can be seen Fig. S11, upper right: (*i*) local filter statistics, including filter mean and spread and (*ii*) the pooling exponents trading off between max-pooling and average-pooling (41). Other types of parameters are highly tuned but less diverse (nonlinear activation thresholds; lower right), whereas some appear less important overall (higher-level pooling and normalization kernel sizes; lower left). Interestingly, we observe that the parameter controlling the number of network layers (depth) is both comparatively highly tuned and diverse suggests that allowing network modules of different levels of complexity in the heterogeneous models is important for achieving high model performance. As a result, the final model has a significant proportion of lower-complexity units projecting directly to the final layer, suggesting that bypass connections (e.g., projects from V1 to V4 or V2 to IT) may be a key functional feature of the ventral stream (30).

Taken together, these results point to a computationally rigorous explanation for why heterogeneity is observed in the receptive fields of ventral stream neurons both at the unit and subarea levels (29, 38, 30, 42).

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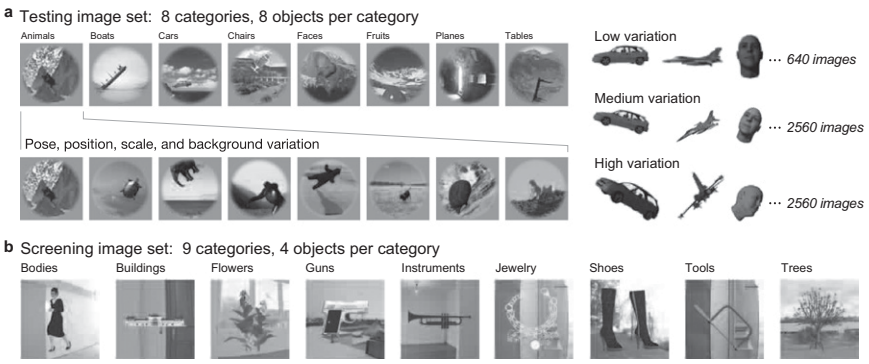

Fig. S1. (*A*) The neural representation benchmark (1) testing image set on which we collected neural data and evaluated models contained 5,760 images of 64 objects in eight categories. The image set contained three subsets, with low, medium, and high levels of object view variation. Images were placed on realistic background scenes, which were chosen randomly to be uncorrelated with object category identity. (*B*) The screening image set used to discover the HMO model contained 4,500 images of 36 objects in nine categories. As with any two uncorrelated samples of images from the world—such as those images seen during development vs. those seen in adult life—the overall natural statistics of the screening set images were intended to be roughly similar to those of the testing set, but the specific content was quite different. Thus, the objects, semantic categories, and background scenes used in screening were totally nonoverlapping with those used in the testing set. Moreoever, different camera, lighting and noise conditions, and a different rendering software package, were used.

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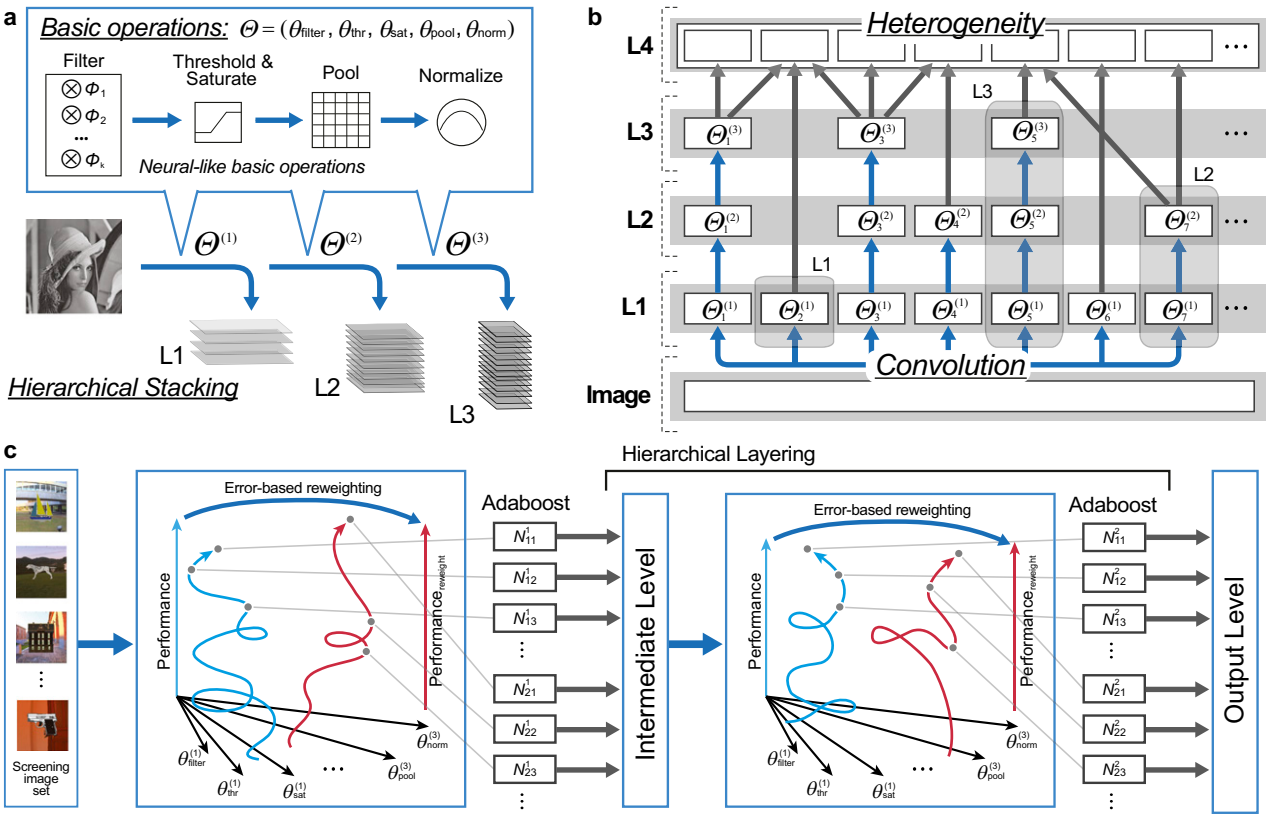

Fig. S2. In this work, we use CNN models. CNNs consist of a series of hierarchical layers, with bottom layers accepting inputs directly from image pixels, with units form the top and intermediate layers used to support training linear classifiers for performance evaluation and linear regressors for predicting neural tuning curves. (*A*) Following a line of existing work, we limited the constituent operations in each layer of the hierarchy to linear-nonlinear (LN) compositions including (*i*) a filtering operation, implementing AND-like template matching; (*ii*) a simple nonlinearity, e.g., a threshold; (*iii*) a local pooling/aggregation operation, such as softmax; and (*iv*) a local competitive normalization. These layers are combined to produce low complexity (L1), intermediate complexity (L2), and high complexity (L3) networks. All operations are repeated convolutionally at each spatial position, corresponding to the general retinotopic organization in the ventral stream. (*B*) In creating the HMO model, we allow mixture of several of these elements to model heterogenous neural populations, each acting convolutionally on the input image. The networks are structured in a manner consistent with known features of the ventral stream, as a series of areas of roughly equal complexity, but which permit bypass projections. (*C*) HMO is a procedure for searching the space of CNN mixtures to maximize object recognition performance. With several rounds of optimization, HMO creates mixtures of component modules that specialize in subtasks, without needing to prespecify what these subtasks should be. Errors from earlier rounds of optimization are analyzed and used to reweight subsequent optimization toward unsolved portions of the problem. The complementary component modules that emerge via this process are then combined and used as input to repeat the procedure hierarchically (*Materials and Methods* and *SI Text*).

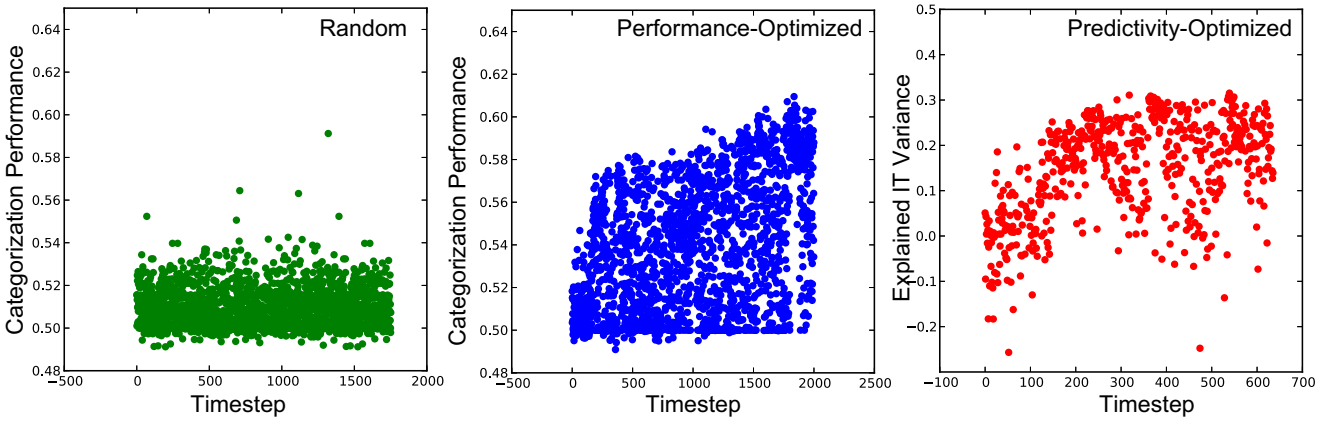

Fig. S3. Optimization time traces for the high-throughput experiments shown in Fig. 1. In the performance and fitting-optimized the *y* axis shows the optimization criterion—in the random selection case (*Left*), no optimization was done, and the performance data were ignored.

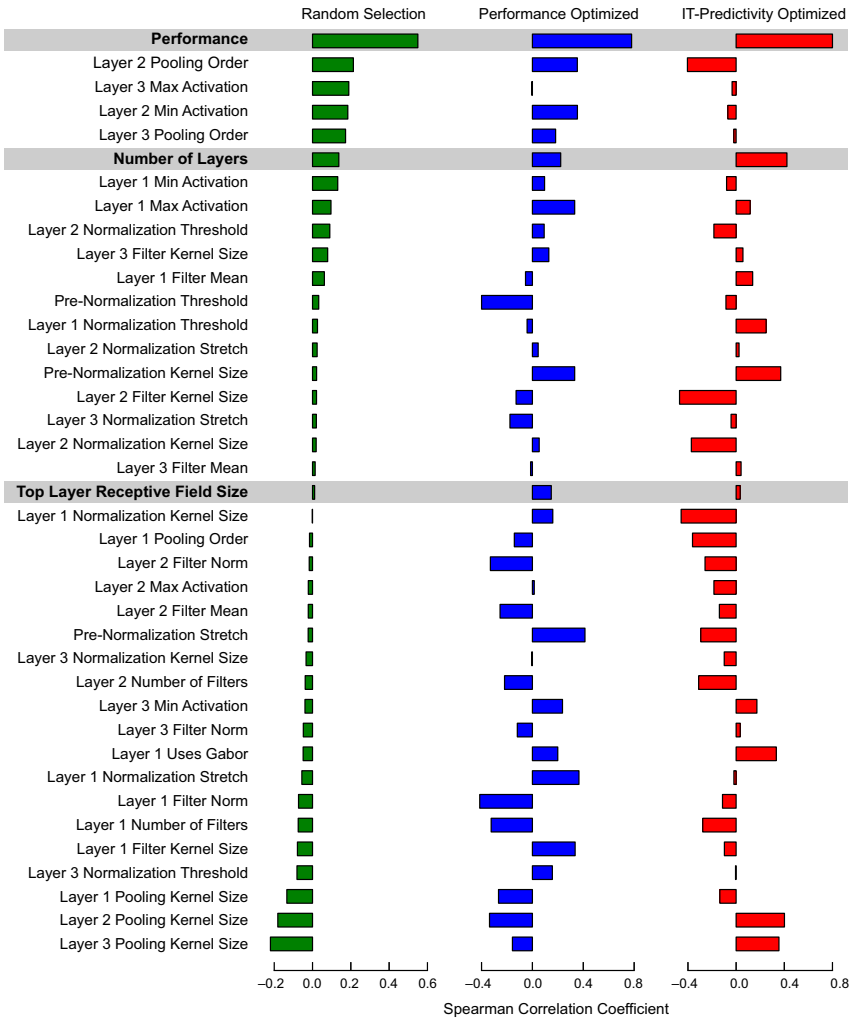

Fig. S4. Correlation of model parameters with IT predictivity for the three high-throughput experiments shown in Fig. 1. Parameters for which the correlation is significantly different from 0 are shown. Also included are several additional metrics that are not direct model parameters but that represent measurable quantities of interest for each model, e.g., model object recognition performance. The *x* axis is Spearman *r* correlation of the given parameter with IT predictivity for the indicated model selection procedure, including random (*Left*, green bars), performance-optimized (*Center*, blue bars), and IT predictivity optimized (*Right*, red bars). Parameters are ordered by correlation value for the random condition. Performance strongly correlates with IT predictivity in all selection regimes. Number of layers (model depth) consistently correlates as well, but much more weakly. Interestingly, one obvious metric—receptive field size at the top model layer—is only very weakly associated with predictivity, because, although the best models tended to have larger receptive field sizes, a large number of poor models also shared this characteristic.

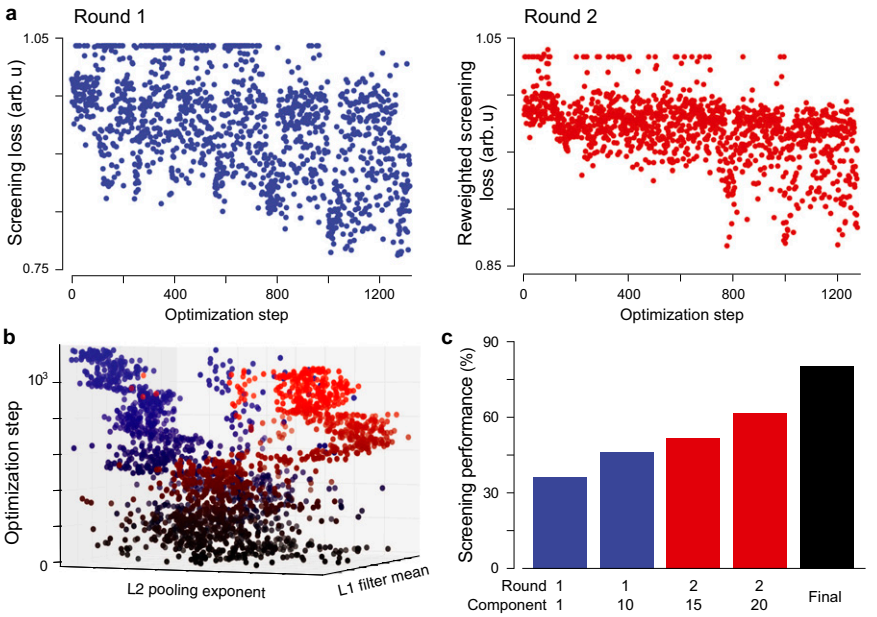

Fig. S5. (*A*) Optimization loss traces during the HMO procedure showing decreased loss as optimization proceeded. (*B*) Parameter-space trajectories during two optimization rounds shown in *A* (round 1 are blue dots; round 2 are red dots). This 3D plot shows parameter values for two chosen parameters (L1 filter mean and L2 pooling exponent) out of many, but it is evident that subsequent rounds of optimization (e.g., red) gravitate toward different paremeter combinations (i.e., different network architetures) than earlier rounds of optimization (e.g., blue). (*C*) Training performance as a function of model complexity, showing dramatic increases as components from round 1 (blue bars) and round 2 (red bars) were added. The final model (black bar) consists of 30 components identified with three complementary rounds of optimization, plus one L1 layer that, anatomically, stacks on top of those 30 components and, functionally, produces nonlinear combinations of their outputs.

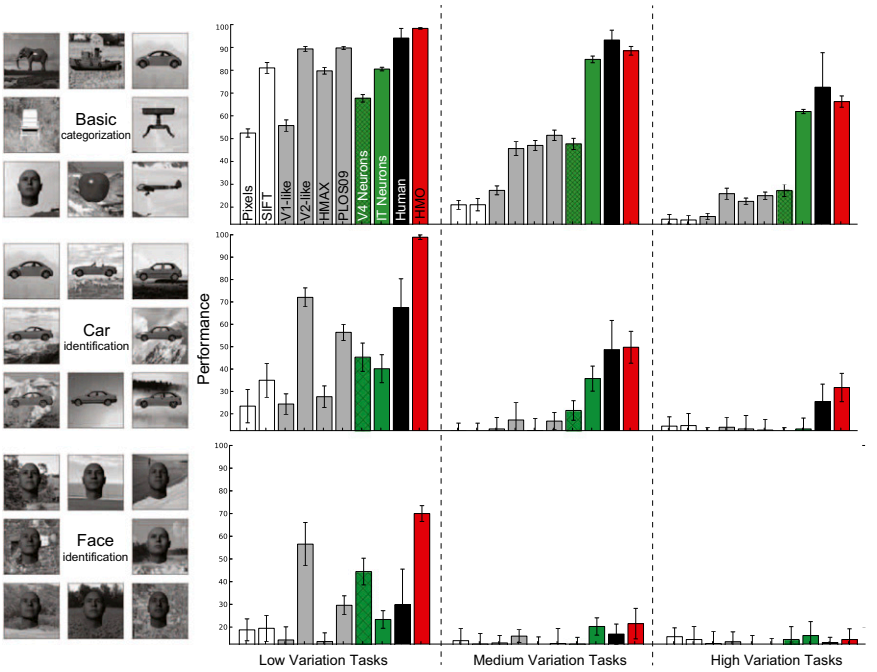

Fig. S6. Classification results for tasks including basic eight-way basic categorization (*Top*), eight-way subordinate car identification (*Middle*), and eight-way subordinate face identification (*Bottom*). Each task was assessed at low, medium, and high levels of image variation (*SI Text*). Comparison was made between neural data, human data, existing models from the literature, and the HMO model outputs. The tasks span a wide range of difficulty, from low-variation basic eight-way categorization where humans perform at greater than 95% accuracy to high-variation subordinate face identification, where human performance is indistinguishable from chance.

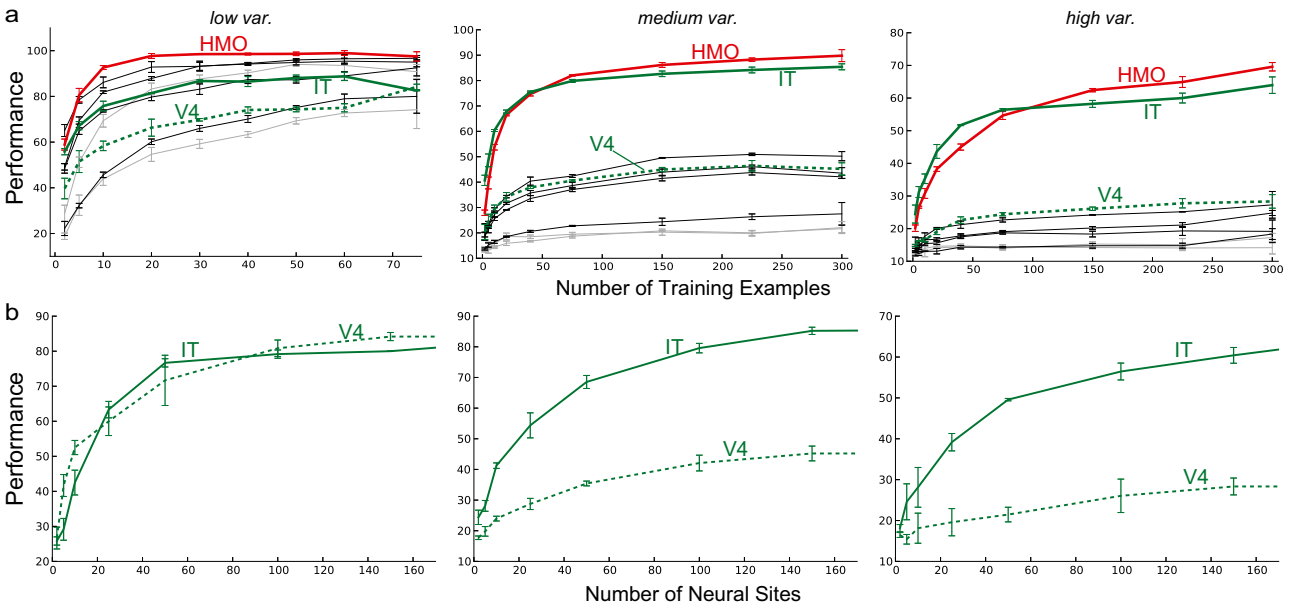

Fig. S7. (*A*) Dependence of performance on number of training examples for models and neural populations. HMO model is shown in red; IT population in solid green; V4 in dotted green; all other control models are shown in black. (*B*) Direct comparison of dependence of performance on number of neural sites, for the IT (solid green) and V4 (dotted green) neural populations.

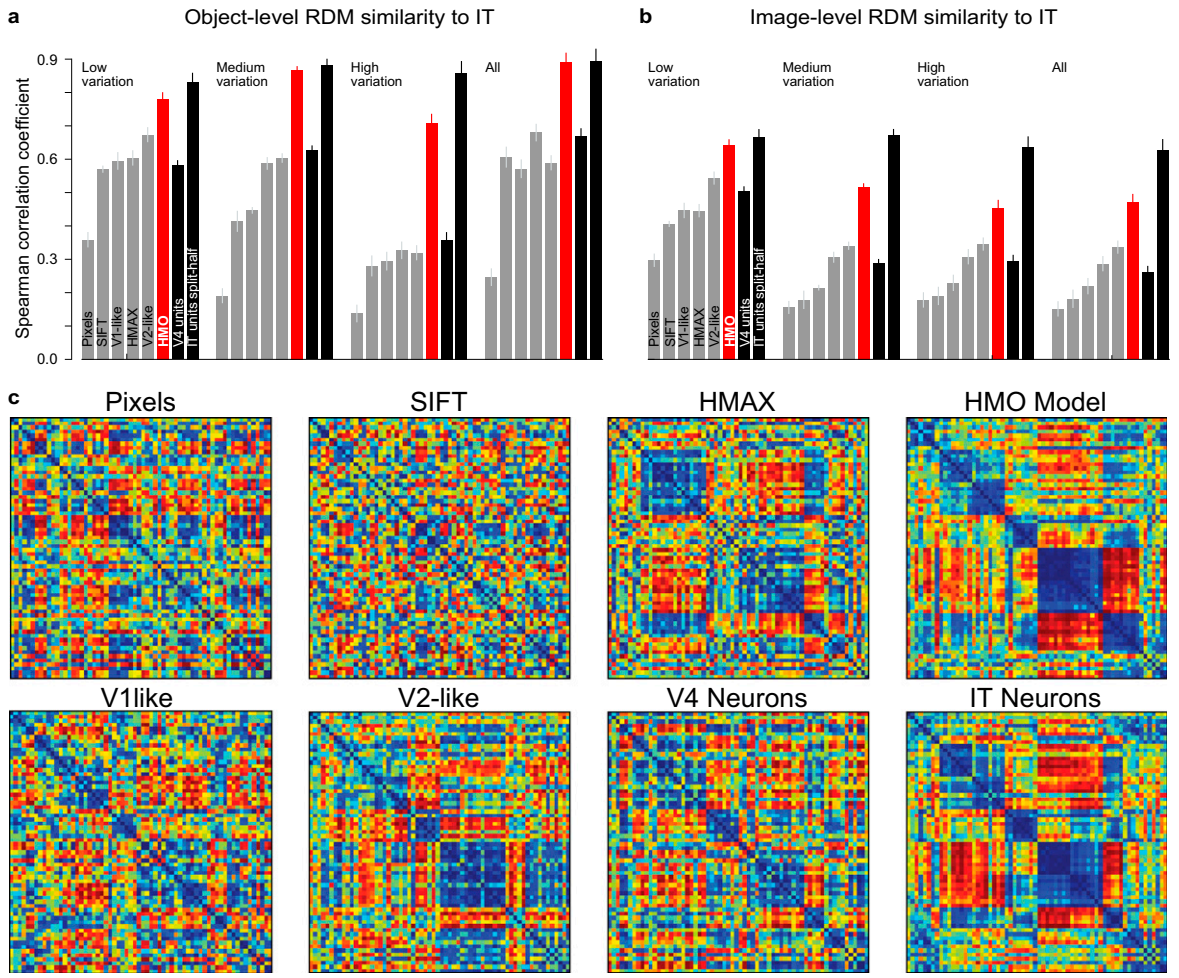

Fig. S8. Additional RDM comparisons to IT population structure. As in Fig. 3 *D* and *E*, each bar shows the Spearman correlation of an RDM for a model (or V4 population) with the RDM for the IT neural population on the same stimulus set. We show comparisons for three subsets of the test image set separated by variation level (Low, Medium, and High), as well as for the whole stimulus set (All). (*A*) Comparisons of RDMs at the object level, in which population representation vectors are averaged on a per-object basis before taking the pairwise correlations to make the RDM matrices. (*B*) More detailed image-level RDMs comparisons, with each stimulus represented separately. (*C*) Object-level RDMs for a variety of models and the V4 and IT neural populations.

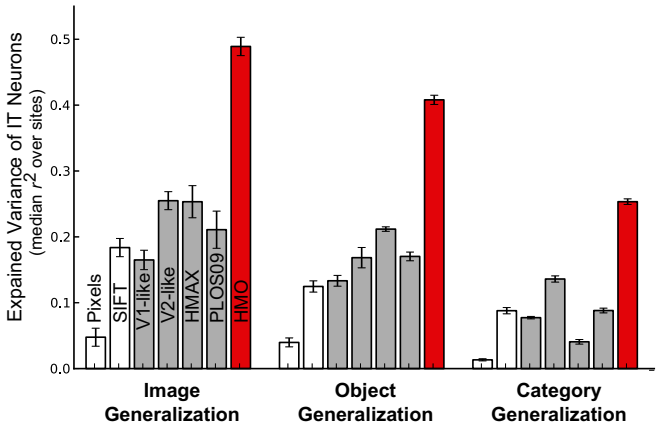

Fig. S9. IT explained variance for each model, fit with training/test image splits generated by (*1*) image generalization, a random selection process in which train and test splits contain images of the same 64 objects, but on different backgrounds and at widely different poses, positions, and sizes; (*2*) object generalization, in which train and test images are split so that they contain no overlapping objects, so that predictions are tested for generalization across object identity as well as position, pose, size and background variation; and (*3*) category generalization, in which train an test images are split so that they contain no overlapping categories, so that predictions are tested across category boundaries as well. Fig. 3*E* shows the corresponding results at the population RDM level.

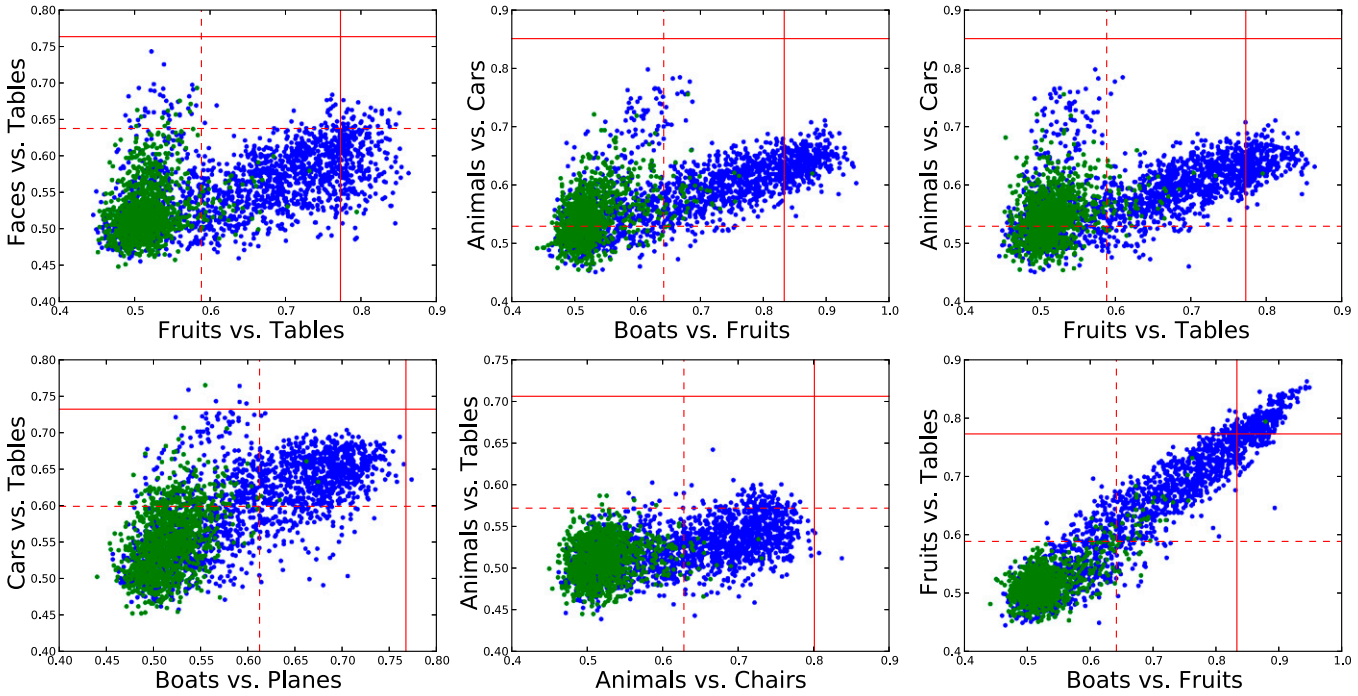

Fig. S10. Tradeoffs between subtask-optimal architectures. Each panel shows pairwise relative performance of the models from the high-throughput experiments in Fig. 1*A* and Fig. S3 on a variety of binary subtasks. As in that figure, random selections are shown in green and performance-optimized selections are shown in blue. Sometimes performance on one binary subtask—e.g., Boats-vs.-Fruits and Fruits-vs.-Tables (lower right corner panel)—directly correlates with performance on another. More commonly, there is a tradeoff between subtask performance in the models explored during optimization, leading to the V pattern observed in subtask pairs. Because the procedure was maximizing overall performance (as opposed to performance on any one subtask), one arm of the V is heavier than the other, corresponding to the optimization process being forced to make a single choice in each of these tradeoffs.

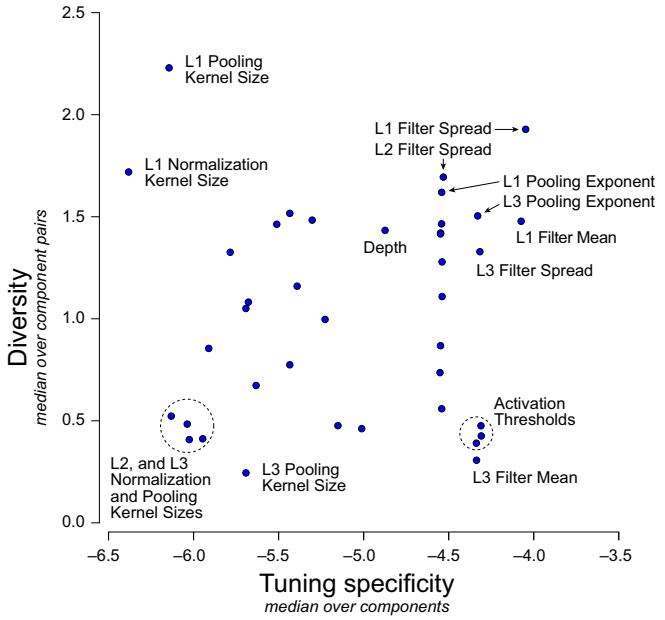

Fig. S11. Characterization of selected model parameters in terms of per-component tuning specificity vs. intercomponent diversity. Each point in this plot represents an architectural parameter in the HMO model. Parameters in the upper right corner are highly tuned but also highly diverse in their tunings between model components. See *SI Text* for the definition of diversity and tuning specificity.