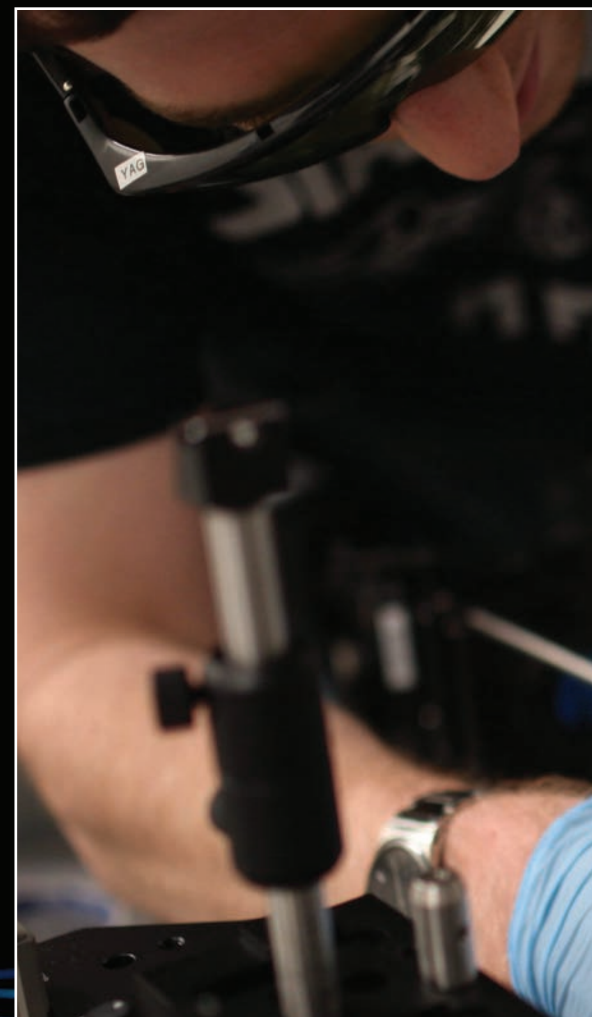
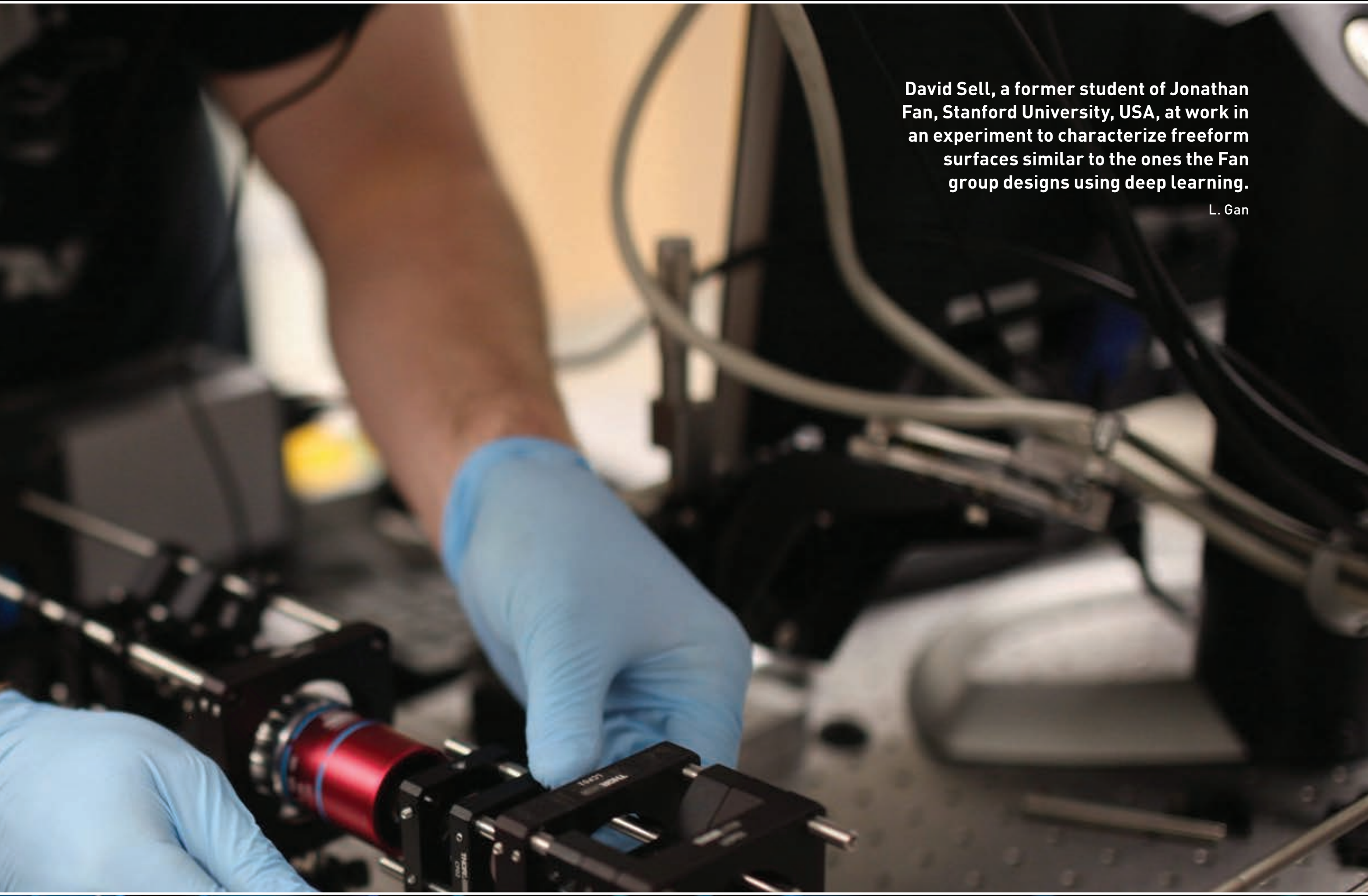
Edwin Cartlidge

Deep Design for Optical Devices



Neural networks can create blueprints for complex device designs that would be difficult if not impossible to generate with traditional techniques.



David Sell, a former student of Jonathan Fan, Stanford University, USA, at work in an experiment to characterize freeform surfaces similar to the ones the Fan group designs using deep learning.

L. Gan

W. Lin / Getty Images

Generative networks can create realistic-looking faces from scratch.
T. Karras et al. arXiv:1710.10196v3 [cs.NE] (2018)

In today's interconnected and data-rich world, there seem to be few areas of life where artificial intelligence (AI) is not making inroads. Enabled by ever more powerful computer hardware and ubiquitous digital information, deep learning—a technology modeled on the workings of the brain—is being exploited in everything from machine vision to natural-language processing and image recognition to game playing. All of these applications, and more, rest on spotting and generalizing patterns within vast data sets.

Scientists have enthusiastically embraced the technology. High-energy physicists use it to sift through the debris of particle collisions, looking for signs of exotic matter, while medical scientists exploit its classification ability to diagnose diseases. Microscopy also stands to benefit, as deep neural networks can, in effect, boost the resolution of optical microscopes after being trained to associate lower- and higher-resolution versions of specific images with one another.

But deep learning is not limited to the analysis or manipulation of data from pre-existing devices. Increasingly, researchers are also showing its use in designing new devices in the first place. This is the case in optics and photonics, where advanced fabrication techniques have diversified the possible shapes, sizes and structural compositions that devices can possess—particularly in the boom area of nanophotonics, where subwavelength features allow light to be manipulated in ways not possible at larger scales.

As Jonathan Fan of Stanford University, USA, puts it, rather than designing new optical systems based on simple, intuitive shapes, researchers can now fashion devices with unusual structures to generate unique electromagnetic responses. "Deep networks are a very good fit for this objective," he says. "They are well suited to identifying non-obvious connections between structure and function within the framework of physical constraints—in our case, Maxwell's equations."

Lightening the legwork

Physicists typically design new optical devices by starting from a random or intuitive layout and using a computer simulation based on Maxwell's equations to calculate the structure's optical response. They then use one of a number of techniques, such as so-called genetic algorithms or adjoint methods, to work backward and adjust the design to close the gap between the simulated and desired response. But each iteration requires a fresh simulation, making this process—known as inverse design—very resource hungry and time consuming as the number of design parameters increases.

Rather than simulating Maxwell's equations directly, neural networks instead approximate the equations by learning the relationship between the input and output—the design structure and its optical response. This involves feeding a network numerous examples of the former and iteratively adjusting the network's parameters so that, eventually, it accurately predicts the response from a given structure. This process usually relies on a conventional technique to provide the training data, which again involves generating large numbers of processor-intensive simulations. However, the simulations here represent a one-time cost. The network, once trained, can typically calculate optical responses in a fraction of a second.

"One run of a neural network takes about 200 ms," says Ravi Hegde of the Indian Institute of Technology

1047-6938/22/09/38/8-$15.00 ©Optica

Deep learning is not limited to the analysis or manipulation of data from pre-existing devices. Increasingly, researchers are also showing its use in designing new devices in the first place.

in Gujarat, "whereas a Maxwell solver typically takes hours."

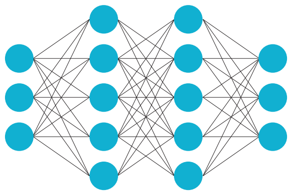
Deep neural networks of various shapes and sizes all consist of interconnected layers of processing units called neurons (see "The network effect," below). When learning, networks adjust neurons' weights and biases through "backpropagation." This involves feeding the difference between the calculated and desired optical response into a user-defined "loss function," and using that function to work out the size of the adjustments layer by layer, moving backward from the output.

A trained network can carry out inverse design by again using backpropagation. In this case, however, the neural weights are kept fixed while the inputs are varied to alter the proposed structure. Starting from a random or intuitive structure, the inputs are progressively tuned by backpropagating the difference between the desired output and the latest calculated output—and then stopping when the design generates outputs close enough to the target response.

Scientists as far back as the 1990s used this approach to design fairly simple centimeter-scale devices at microwave frequencies, including transmission lines, amplifiers and antennas. But with advances in computer power and network architecture, the new wave of AI has since allowed scientists to investigate designs all

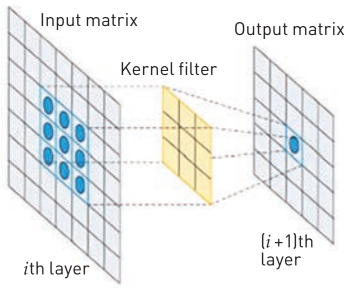
The network effect

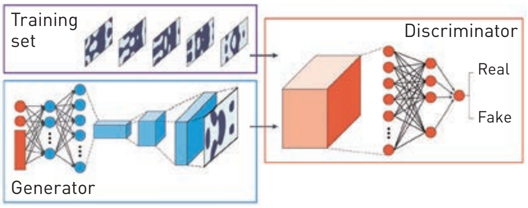
Scientists use a range of neural networks to design and optimize optical devices, employing backpropagation during training to adjust the weights of their neurons. Below are some of the most prominent networks.



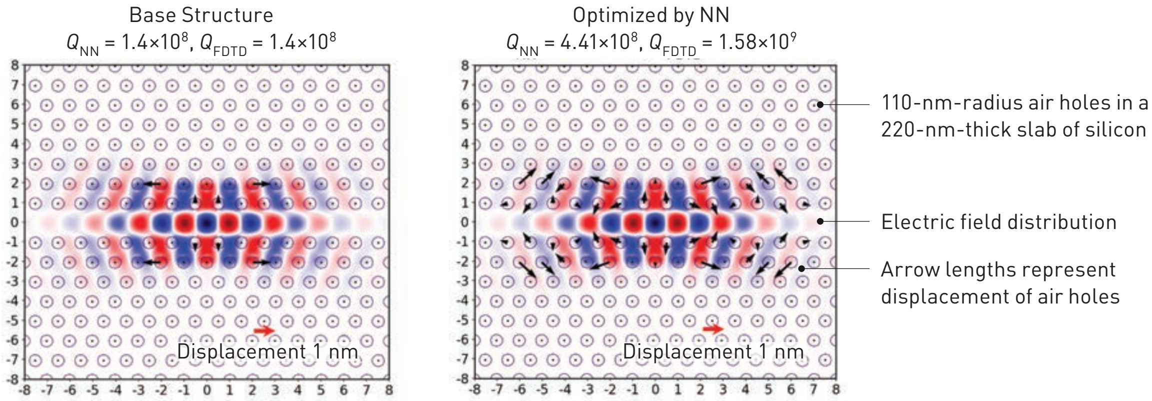
Fully connected network
The most traditional form, this tends to be used when optimizing relatively few parameters. Each neuron in one layer is connected to every neuron in the previous (and successive) layer. Neurons calculate the weighted sum of all the incoming links and then apply a nonlinear function, sending the result to neurons in the next layer.

Convolutional network
This is generally used to process high-dimensional inputs in the form of images. It scans a small matrix known as a kernel across the grid of input data, calculates the weighted sum from each region of the grid and then applies a nonlinear function. Storing the result as a single value in the next layer, it repeats the process across regions and then from layer to layer, using a different kernel. The result is a more manageable number of data points that provide information about large features in the image.





Generative adversarial network
Used to design complex freeform devices, this involves a tug-of-war between a generator that tries to mimic a set of training data and a discriminator that attempts to tell the difference between the two data sets. The generator creates its "fake" structures by applying certain parameters to a random input distribution and is guided to the "real" structures by dueling with the discriminator.



Susumu Noda and Takashi Asano, Kyoto University, Japan, used a neural network to optimize the position of air holes, and thus the Q factor, in the design of a photonic-crystal nanocavity.

S. Noda and T. Asano

the way down to the nanoscale and across increasingly large swaths of design space.

The next dimension

In 2018, Marin Soljačić and colleagues at the Massachusetts Institute of Technology, USA, reported using a fully connected network with four hidden layers to simulate light scattering from a multilayer nanoparticle. They trained the network via tens of thousands of Monte Carlo simulations to learn the relationship between the thicknesses of eight silica/titanium dioxide layers—the input—and the scattering cross-section at seven different wavelengths—the output. Having done so, they found they needed just a few design iterations to work out the nanoparticle geometry that could generate a given output spectrum.

This work relied on just a handful of geometric parameters while extending research down to very small spatial scales. Many inverse-design problems, in contrast, involve freeform devices defined as images built up from hundreds or thousands of pixels or voxels. Because the quantity of training data needed to properly sample a design space scales exponentially with the number of parameters, fully connected networks require many layers to design such devices.

To deal with this "curse of dimensionality," computer scientists use so-called convolutional neural networks to process image data by cutting the number of dimensions that have to be processed. They do so using small matrices to progressively reduce the number of data points from layer to layer while retaining information about ever-larger features from the image.

Susumu Noda and Takashi Asano of Kyoto University, Japan, employed a convolutional neural network to improve the design and the Q factors of nanocavities made by removing a certain number of air holes from 2D silicon photonic crystals. To optimize displacements of 50 other air holes from their baseline positions around the central gap, they trained the network with 1,000 random arrangements of the holes and their associated Q-values. They then used backpropagation to progressively improve device performance—showing that after 1,000 iterations, the Q factor increased by more than an order of magnitude compared to manual optimization.

Noda and colleague Menaka De Zoysa also built a convolutional network to control the beam pattern of photonic-crystal surface-emitting lasers, whose high-power, high-quality beams might benefit smart manufacturing in the future. The researchers say that, by learning the relationship between beam patterns and injection-current profiles, the network was able to control beams on demand in the face of fabrication errors and environmental noise.

Inverted inversion

One serious issue of inverse design is the "one-to-many problem"—while any specific design will yield a unique response under a given input, a specific output can be generated by multiple devices. Another problem is that the design-searching algorithm can get stuck in a local maximum—a good design but not the best—rather than finding the global maximum. Circumventing these problems calls for a thorough exploration of the design space during both training and design.

In their nanocavity work, Noda and Asano took a number of steps to boost the variety of their candidate designs. One was to set up several neural networks and train each one in a different order. They also tweaked their loss function to navigate larger portions of the design space and retrained their networks multiple

The design-searching algorithm can get stuck in a local maximum—a good design but not the best—rather than finding the global maximum.

times using the candidate designs from the previous rounds' results.

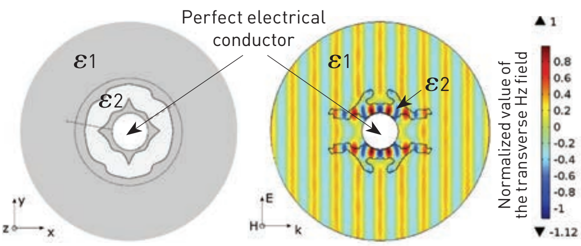
An alternative approach to inverse design is simply to invert the network's inputs and outputs—training the network with multiple examples of optical responses and correcting its weights and thresholds based on the associated device structure. In principle, the desired structure should then pop out once the target response is fed in at the front. However, the one-to-many problem again comes into play, with the network's surrogate model failing to converge.

In 2017, Zongfu Yu and colleagues at the University of Wisconsin–Madison, USA, proposed a "tandem" network as a solution to this problem. Their idea was to pre-train a standard forward-modeling network with device designs and their associated responses, and then use the forward network to guide an inverted network attached to its inputs. The inverted network is trained by adjusting its weights based on the difference between its input—a certain electromagnetic response—and the forward network's output—the calculated response. Because the forward network is not a perfect physical simulator, it produces a simplified design space that makes converging on certain designs easier for the inverse network.

That scheme has since been used by several groups to demonstrate innovative inverse designs. Researchers in the Republic of Korea, for example, showed that it enabled the simultaneous specification of nanoparticles' structural and material properties, and a group in Italy used it to establish the parameters of a complex topological insulator. Scientists in Israel, meanwhile, demonstrated the technique's ability to design nanostructures sensitive to certain substances, potentially leading to new devices for sensing, imaging and spectroscopy.

Starting from scratch

Not content to rest on their laurels, computer scientists have, over the last few years, developed an entirely new class of neural network that essentially generates new data sets rather than discerning patterns within existing ones. The inputs of such a "generative network" are not design (or response) parameters but a random variable sampled from a standard probability distribution and



Deep neural networks were used to work out the optimum configuration of two materials with different dielectric constants, yielding an optical cloak that reduces scattering of electromagnetic waves almost to zero.

(In)visible progress

Optical cloaks made from carefully chosen metamaterials hide objects by diverting electromagnetic waves around those objects so that to downstream observers, it appears that the radiation has propagated forward unimpeded. Proposed in 2006 and subsequently demonstrated at microwave frequencies, cloaks can now be made simply by varying the geometry of isotropic dielectric materials.

Olivier Martin and Andre-Pierre Blanchard-Dionne at the École Polytechnique Fédérale de Lausanne, Switzerland, showed how the design of such a cloak can be optimized by combining a generative adversarial network with a forward network. The former generates a series of candidate layouts consisting of 64×64-pixel images, in which each pixel represents a material with one of two dielectric constants. The forward network, previously trained using data generated by finite-element simulations, then calculates the scattering coefficient of each layout, compares this against the desired coefficient and backpropagates the difference to the generative network to optimize the cloaking design.

To ensure that the scheme yields the lowest possible scattering coefficients, Martin and Blanchard-Dionne added an extra step—using finite-element simulation to refine the calculation of scattering coefficients and using the results to iteratively retrain the forward network. Doing so for a 6-μm-diameter cloak exposed to infrared radiation, they found they could reduce the scattered field compared with the case of no cloak by more than a factor of 100—comparable, they say, to what can be done with conventional topology optimization but without any initial assumptions about the cloak's layout.

Adapted from A.-P. Blanchard-Dionne and O.J. F. Martin. OSA Continuum **4**, 87 (2021)

Aydogan Ozcan's group used deep learning to design a new kind of assay-based sensor to diagnose Lyme disease.
Reprinted with permission from H.-A. Joung et al. ACS Nano **14**, 229 (2020); © 2020 ACS

conditional labels. Processed by the network's hidden layers—typically several fully connected layers followed by a number of inverse convolutional ones—these inputs are transformed into a set of high-dimensional images.

One way of training a generative network is to hook it up to a conventional "discriminative network" so that the two act as adversaries. The loss function of the former attempts to minimize the difference between its output and a set of training images of device designs, while the latter is geared up to spot this difference. When the discriminative network can no longer tell the two sets of images apart, the generative network is trained and ready to produce new and improved device designs—as researchers in Switzerland have done to design an optical cloak (see "(In)visible progress," p. 43).

While this and other implementations of generative networks rely on training data, Jonathan Fan and Jiaqi Jiang at Stanford have instead shown how to train a generative network using a Maxwell simulator, as they did with their "global topology-optimization network" (GLOnet) to find the global maximum. GLOnet relies on an exponential weighting within the loss function, meaning the distribution of possible device designs is very narrow and ideally centered on the globally optimum design.

Fan and Jiang found they could outperform conventional simulations when optimizing the design of silicon metagratings. Setting up several dozen networks with different combinations of operating wavelength and deflection angle, they saw that in the vast majority of cases, the GLOnets yielded devices that were able to channel light in a particular direction at least as efficiently as those formulated conventionally.

Traditional optics, too

Exploring beyond the nanoscale, researchers are also exploiting deep-learning technology to optimize the arrangement of micrometer-scale components on photonic chips and at the centimeter scale of traditional optics, according to Hegde. The latter category contains compound lenses of interest for smartphone cameras and semiconductor lithography, whose design parameters include the curvature of each lens and the distance between lenses, Hegde notes.

Another emerging application of deep learning to more conventional optical systems is in the design of intelligent sensors. Aydogan Ozcan at the University of California, Los Angeles, USA, envisages using neural networks to "lock in" the benefits of AI within the sensing hardware itself—rather than to simply improve analysis of data from a pre-existing device.

Ozcan and colleagues have demonstrated the potential of this approach for medicine by developing a new kind of assay-based sensor to diagnose Lyme disease—a tick-borne illness that can lead to conditions such as arthritis and palsy. The researchers used a fully connected neural network to identify which combination of antibodies should be tested for in potentially infected people to maximize the chances of a correct diagnosis. Using 50 human serum samples to train the network and another 50 for blind testing, they found they could reduce both false positives and false negatives to less than 10%—a significant improvement, they say, compared with existing point-of-care assays.

Back at the nanoscale, simulating the electromagnetic response of an extremely broad range of structures is crucial for inverse design. Several groups have shown how deep networks themselves can execute this function and thereby speed up device development. For example, Peter Wiecha and Otto Muskens at the University of Southampton, UK, have used a convolutional network to predict the electric field produced by arbitrary 3D nanostructures when illuminated by plane waves. After training the network using commercial-level simulation software, they found it could accurately and quickly predict both the near and far fields as well as a variety of secondary quantities, such as higher-order antenna resonances and non-radiating anapole states.

Fan's group at Stanford has also developed a convolutional network for simulation, but one that draws

Another emerging application of deep learning to more conventional optical systems is in the design of intelligent sensors.

on physics as well as training data. The network learns to predict the magnetic near field of a nanoscale structure and then uses Maxwell's equations to calculate the electric field, having been trained in part by using the equations as a physical constraint within its loss function. By incorporating this simulator into their GLOnet algorithm, Fan and colleagues found they could optimize the design of a certain type of dielectric metagrating nearly as effectively as they could using a conventional simulator, but some 7,000 times faster.

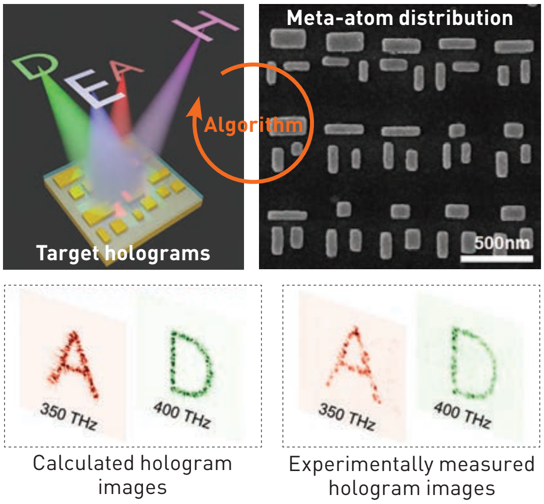
Despite the outliers

For all the deep-learning-fueled optics research, Yongmin Liu of Northeastern University, USA, says that, so far, very little of it has led to commercial devices. But he is confident that will change, arguing that neural networks enable designs with counter-intuitive functionalities that would be impossible to realize with traditional techniques—and that will ultimately lead to new applications in imaging, communications and computing.

Indeed, Liu and co-workers reported earlier this year that a combination of different neural networks can optimize the design of metasurfaces. With the right arrangement of "meta-atoms," a single metasurface can yield as many as eight independent responses when exposed to near-infrared light with the right frequencies and polarizations, as the researchers demonstrated experimentally via multiplexed holograms and lenses. "That is only possible with machine learning," says Liu.

Others are more cautious, however. Wiecha says that in around 5% of cases, his team's work modeling electric fields generated outliers—results with significant errors—just as other neural networks do. Outliers can be minimized by throwing more training data at a network, he says, but it doesn't always make sense to devote the necessary time and resources. Unless there is a need to produce many similar devices from a single training set, he argues that conventional optimization can often get the job done quicker and more accurately. "People often think that deep learning can do miracles for inverse design," he says. "But it is not like this."

Sharing data for network training is one of the aims of MetaNet, an online database set up by Fan



Yongmin Liu and colleagues used neural networks to arrange tiny metal–insulator–metal pillars on a metasurface to generate frequency-dependent holograms.
Adapted with permission from W. Ma et al. Adv. Mat. **34**, 2110022 (2022)

and colleagues in 2020 to try to introduce common benchmarks for assessing neural networks and device designs. But more than two years on, only two other researchers have uploaded data to the site, says Fan. He reckons this is partly because photonics researchers value new physics more than new techniques. "For some subfields of optics, specialized researchers can and will work together," he says, "but it will be case by case."

Despite the difficulties, Fan shares Liu's sense of optimism about machine learning's potential, particularly for designing metamaterials. Hegde, too, is excited, arguing that physics-based learning will help create more accurate neural networks and thereby "enable us to attack complex design problems that are intractable today." Even Martin is enthusiastic, having obtained very promising results in a new project to develop nanomotors—after being initially skeptical that deep learning could go significantly beyond the training data. "I am amazed that it works so well," he says. OPN

Edwin Cartlidge (edwin.cartlidge@yahoo.com) is a freelance science writer based in Rome, Italy.

For references and resources, go online: **optica-opn.org/link/deep-design**.

References and Resources

- T. Asano and S. Noda. "Optimization of photonic crystal nanocavities based on deep learning," Opt. Express **26**, 32704 (2018).
- J. Peurifoy et al. "Nanophotonic particle simulation and inverse design using artificial neural networks," Sci. Adv. **4**, eaar420 (2018).
- M. Chen et al. "WaveY-Net: Physics-augmented deep learning for high-speed electromagnetic simulation and optimization," arXiv:1710.10196v3 [cs.NE] (2018).
- H.-A. Joung et al. "Point-of-Care Serodiagnostic Test for Early-Stage Lyme Disease Using a Multiplexed Paper-Based Immunoassay and Machine Learning," ACS Nano **14**, 229 (2020).
- P.R. Wiecha and O.L. Muskens. "Deep Learning Meets Nanophotonics: A Generalized Accurate Predictor for Near Fields and Far Fields of Arbitrary 3D Nanostructures," Nano Lett. **20**, 329 (2020).
- A.-P. Blanchard-Dionne and O.J.F. Martin "Successive training of a generative adversarial network for the design of an optical cloak," OSA Continuum **4**, 87 (2021).
- J. Jiang et al. "Deep neural networks for the evaluation and design of photonic devices," Nat. Rev. Mater. **6**, 679 (2021).
- W. Ma et al. "Pushing the Limits of Functionality-Multiplexing Capability in Metasurface Design Based on Statistical Machine Learning," Adv. Mater. **34**, 2110022 (2022).