excel at generalizing those patterns to new data. For instance, search engines use this technology to automatically label the contents of billions of internet photos.

The authors use a convolutional neural network to learn the relationship between millions of daytime satellite images (which are rich in detail) and nighttime images (where light areas are assumed to be wealthy). In this way, the network learns which features in the daytime imagery are indicative of economic activity (see the figure). Knowledge of those features enabled the authors to accurately reconstruct survey-based indicators of regional poverty, improving on results from simpler models that relied solely on nightlights or mobile phone data.

How might these results change the way that we measure and target poverty? Perhaps the most immediate application is as a source of inexpensive, interim national statistics. Jean *et al.*'s results indicate that a model trained in one country can be used in another, creating options for countries where no recent survey data exist. For social welfare programs, some of which already use satellite imagery to identify eligible recipients (*14*), higher-fidelity estimates of poverty can help to ensure that resources get to those with the greatest need.

Other applications are on the horizon. Remotely sourced satellite and mobile phone data are updated frequently and can be used to generate nearly real-time estimates of regional vulnerability. Once it is possible to estimate short-term changes in wealth and poverty, new approaches to program monitoring and impact evaluation will follow.

Considerable validation and calibration are required before proof-of-concept studies such as that of Jean *et al.* can be used in practice. However, as their study illustrates, there is exciting potential for adapting machine learning to fight poverty. As the economist Sendhil Mullainathan has asked, "Why should the financial services industry, where mere dollars are at stake, be using more advanced technologies than the aid industry, where human life is at stake" (*15*)? ■

REFERENCES

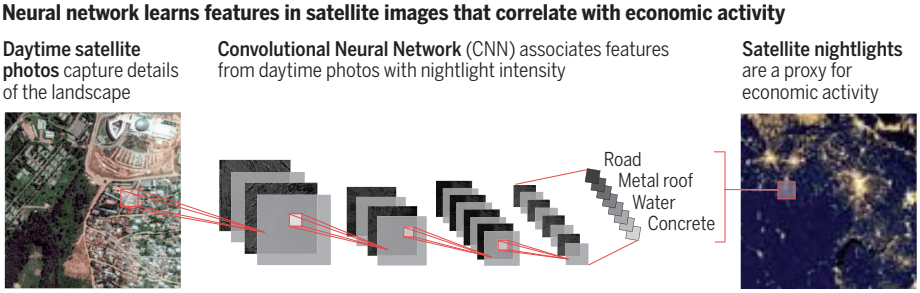
1. N. Jean *et al.*, *Science* **353**, 790 (2016).
2. A. Deaton, *The Analysis of Household Surveys: A Microeconometric Approach to Development Policy* (World Bank Publications, 1997).
3. A. Banerjee *et al.*, *Science* **348**, 1260799 (2015).
4. D. Donaldson, A. Storeygard, "Big Grids: Applications of Remote Sensing in Economics," working paper, 2016; https://dl.dropboxusercontent.com/u/2734209/Donaldson_Storeygard_JEP.pdf.
5. J. V. Henderson *et al.*, *Am. Econ. Rev.* **102**, 994 (2012).
6. X. Chen, W. D. Nordhaus, *Proc. Natl. Acad. Sci. U.S.A.* **108**, 8589 (2011).
7. Y. S. Lee, "International Isolation and Regional Inequality: Evidence from Sanctions on North Korea," working paper, 2016; https://web.stanford.edu/~yongslee/NKsanctions_030216.pdf.
8. H. Choi, H. Varian, *Econ. Rec.* **88**, 2 (2012).
9. A. Llorente *et al.*, *PLOS ONE* **10**, e0128692 (2015).
10. N. Eagle *et al.*, *Science* **328**, 1029 (2010).
11. J. E. Blumenstock *et al.*, *Science* **350**, 1073 (2015).
12. J. E. Blumenstock *et al.*, *J. Dev. Econ.* **120**, 157 (2016).
13. D. Björkegren, D. Grissen, "Behavior Revealed in Mobile Phone Usage Predicts Loan Repayment," working paper, 2015; http://dan.bjorkegren.com/files/danbjork_credit-scoring.pdf.
14. J. Haushofer, J. Shapiro, *Q. J. Econ.* 10.1093/qje/qjw025 (2016).
15. S. Mullainathan, "Satellite images can pinpoint poverty where surveys can't," *New York Times*, 1 April 2016; www.nytimes.com/2016/04/03/upshot/satellite-images-can-pinpoint-poverty-where-surveys-cant.html?_r=0.

10.1126/science.aah5217

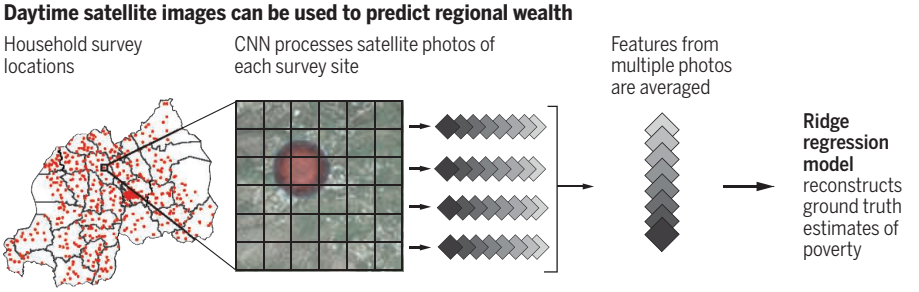
Predicting poverty

Satellite images can be used to estimate wealth in remote regions.

Neural network learns features in satellite images that correlate with economic activity



Daytime satellite images can be used to predict regional wealth



CRYSTALLOGRAPHY

Now you see me too

Attaching chiral molecules to a chiral framework allows their molecular structures to be determined

By **Lars Öhrström**

Knowledge of three-dimensional (3D) molecular structures is crucial for scientific advances in fields ranging from materials chemistry to medicine. For solar cell materials, human proteins, or new drugs, the revelation of the exact arrangement of atoms and bonds vastly advances understanding of their properties. On page 808 of this issue, Lee *et al.* (*1*) report an approach that allows better structural data to be obtained for large, complex organic molecules that are difficult to crystallize on their own.

The method of choice to obtain structure information is single-crystal x-ray diffraction, a method so important that UNESCO declared 2014 the International Year of Crystallography. However, this method requires not only a pure substance, but also the ability to grow crystals of it—no crystals, no crystal structure data. The main complementary method, nuclear magnetic resonance, mainly provides structures of compounds in solution, often at great detail, but sometimes with inherent uncertainty, especially for chiral (handed) molecules with complicated stereochemistry.

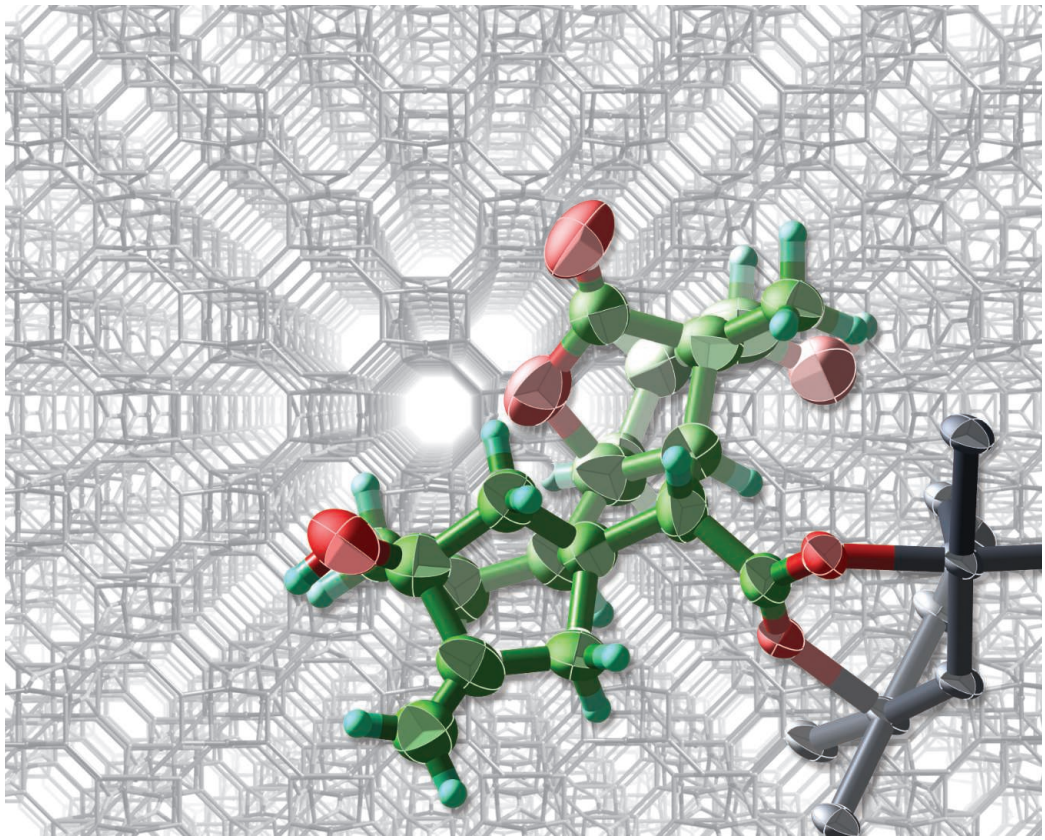
Although long hours in the lab may produce crystals, some substances are notoriously difficult to crystallize or yield crystals with defects and disorder that prevent a complete structure determination. On the other hand, the molecular structures of small solvent molecules, trapped between the larger molecules that are the principal constituents of a specific crystal, are determined over and over again; for example, 1989 molecular structures of pyridine, C_5H_5N, are reported in the Cambridge Crystallographic Database (*2*). This occurs because the form and intermolecular interactions of the larger molecules sometimes generate voids in the crystal. Scientists

Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden. Email: ohrstrom@chalmers.se

have therefore been exploring the idea that difficult-to-crystallize molecules could benefit from a similar approach if large enough voids could be deliberately engineered to trap the target molecules in.

An early example of such void engineering is the use of resorcinarenes and related substances (bowl-shaped molecules that assemble into hollow dimers) to encapsulate compounds and determine their structures (*3*). However, it was not until the discovery of coordination polymers and metal-organic frameworks (MOFs) (*4*) that a general protocol could be developed for the inclusion and structure determination of difficult-to-crystallize molecules.

MOFs consist of metal ions or clusters bridged by organic molecules (ligands) to form crystalline 3D networks with large potential voids and channels. First-generation MOF-based structure determination matrices were based solely on the void properties and are known as crystalline sponges (*5*). They work by soaking up the desired molecules from a solution. Information on molecular chirality has been obtained from molecules trapped in crystalline sponges (*6*), but the crystalline sponges themselves are nonchiral. They therefore do not provide a frame of reference (like a system of left hands could easily distinguish between right- and left-handed gloves) for absolute chirality assignment. Also, the probed molecules are only weakly attached to the framework. This can result in large thermal motions in the crystal and thus less precise data.



Lee *et al*. determined the structure of the plant hormone gibberellin A1 [carbon (green), hydrogen (light green), oxygen (red)] by trapping it inside MOF-520 (gray). The hormone is attached to aluminum ions (slate blue) in the MOF. The shapes of the atoms reflect data quality, with smaller and more spherical atoms indicating better precision (closer to attachment points to the MOF).

Lee *et al*. present a substantial improvement in data quality by using MOF-520. The bridging ligand in this MOF, 1,3,5-benzenetribenzoate, has a propeller-like handedness. The MOF forms separate crystals of either chirality, even though the 3D network in itself, assigned the topology symbol "sum," is not intrinsically chiral (*7*, *8*) (a well-known achiral topology is that of diamond; a chiral topology is that of quartz). The chiral framework makes it much easier to determine the stereochemistry of the trapped molecule; this information is crucial for understanding its potential biological activity.

To create the crystals, the authors first impregnated MOF-520 with fresh solvent and then soaked it in a saturated solution of the target molecule. The latter substitutes the small formate ions ($HCOO^-$) that are part of the original framework. The target molecule is thus firmly attached to the framework, reducing thermal motion and improving the precision of the data. However, it requires the probed substances to have a functional group that can be coordinated to a metal site. Fortunately, such functional groups are common in the molecules of interest.

"The approach...is an important advance, especially for difficult-to-crystallize natural products."

The approach reported by Lee *et al*. is an important advance, especially for difficult-to-crystallize natural products. However, having the molecular structure does not solve all crystallographic problems associated with a potential drug molecule. For legislation and patent reasons, a crystal structure of the pure compound or any of its pharmaceutically acceptable salts or co-crystals are also needed.

Beyond structure determination, Lee *et al*. show that MOFs could be used to exactly position molecular components. Such crystal engineering is, for example, of interest for solar energy applications (*9*), where it may reduce the need for costly covalent organic synthesis (*10*). Indeed, an early idea was that MOFs could be used to hang molecules on. Lee *et al*. show that MOF-520 provides both good hangers and a chiral wardrobe for complex molecular structures. ■

GRAPHIC: LARS ÖHRSTRÖM/CHALMERS UNIVERSITY OF TECHNOLOGY

REFERENCES

1. S. Lee, E. A. Kapustin, O. M. Yaghi, *Science* **353**, 808 (2016).
2. C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, *Acta Crystallogr. B* **72**, 171 (2016).
3. A. Scarso, A. Shivanyuk, J. Rebek Jr., *J. Am. Chem. Soc.* **125**, 13981 (2003).
4. S. R. Batten *et al.*, *Pure Appl. Chem.* **85**, 1715 (2013).
5. Y. Inokuma *et al.*, *Nature* **495**, 461 (2013).
6. S. Yoshioka, Y. Inokuma, M. Hoshino, T. Sato, M. Fujita, *Chem. Sci.* **6**, 3765 (2015).
7. M. O'Keeffe, M. A. Peskov, S. Ramsden, O. M. Yaghi, *Acc. Chem. Res.* **41**, 1782 (2008).
8. F. Gándara, H. Furukawa, S. Lee, O. M. Yaghi, *J. Am. Chem. Soc.* **136**, 5271 (2014).
9. P. Mahato *et al.*, *J. Am. Chem. Soc.* **138**, 6541 (2016).
10. M. Ghazzali, V. Langer, K. Larsson, L. Öhrström, *CrystEngComm* **13**, 5813 (2011).

10.1126/science.aah5367

Now you see me too

Lars Öhrström

Science **353** (6301), 754-755.
DOI: 10.1126/science.aah5367