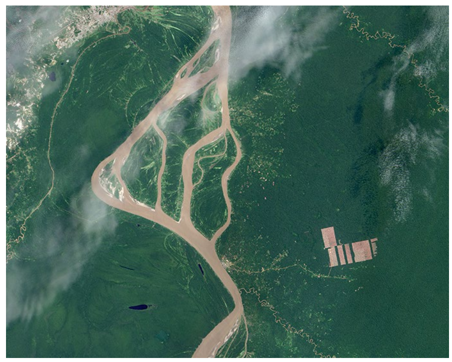
Achieving net zero emissions with machine learning: the challenge ahead

There is growing interest in using machine learning to mitigate climate change. But as avoiding catastrophic temperature rises becomes more urgent, action is also needed to understand the environmental impact of machine learning research.

Bangladesh and India were hit in June this year by one of the worst floods ever seen in a century as a result of climate change, leaving millions in need of aid. Rising temperatures are also causing heatwaves, droughts, wildfires, floods and other catastrophic events worldwide, while underprivileged regions are paying the biggest price for the world's failure so far to reduce carbon emissions. Governments should not need further wake-up calls to act swiftly and cap global warming to 1.5 °C above pre-industrial level. The Intergovernmental Panel on Climate Change report *Climate Change 2022: Mitigation of climate change*, which was released in April, concludes that "without immediate and deep emissions reductions across all sectors, limiting global warming to 1.5 °C is beyond reach"[1]. According to the report, in order to reach the goal, global greenhouse gas emissions should peak before 2025 and decrease by 43% by 2030. Eventually, net zero carbon dioxide emissions need to be reached by 2050. In Europe, an added incentive for swift movement to sustainable energy solutions is Europe's need for independence from Russian gas supplies. With these objectives in mind, transformative technologies are needed to create, store and distribute renewable energy, monitor carbon emissions and deforestation, reduce waste and make sustainable production chains more economical. Machine learning is envisioned to play an important role in the realization of such technologies.

A recently published report by Climate Change AI, a volunteer-driven non-profit organization founded in 2019 that brings together representatives from industry and academia, provides a long list of areas and applications in which machine learning could help to tackle climate change in the short or long term[2]. An example is using computer vision to track greenhouse gas emissions based on remote sensing and satellite data, as tackled by Climate Trace, a coalition of universities, tech companies and nonprofit organizations. Another area in which machine learning is expected to have a positive impact is in supporting societies' transition to run on electricity from sustainable sources. Machine learning can be used in forecasting energy supply and demand for efficient energy distribution, thereby minimizing waste and avoiding outages. Recently, Google announced that it will sell its wind power forecast service, developed by DeepMind in 2019, via Google Cloud.



Deforestation in Peru in 2013 captured by NASA's Landsat satellite. Machine learning and data-driven methods can be used to monitor deforestation and carbon emissions based on satellite image data. Credit: B.A.E. Inc. / Alamy Stock Photo

A related opportunity is the development of improved battery-storage and energy-conversion systems. As the availability of renewable energy from sources such as wind and solar is variable and intermittent, batteries are needed to store surplus energy and supply it to power grids when availability is low (or demand is high). Beyond energy supply and demand prediction, machine learning could be a game-changer in molecular design and material discovery in batteries and energy conversion. The Open Catalyst Project, a joint initiative of Carnegie Mellon University and Meta AI, has released two databases[3,4]. These datasets can be used to train machine learning models to identify suitable low-cost electrocatalysts for the conversion of renewable energy to storable forms and other environmental applications[5]. The first dataset consists of over 1.2 million density functional theory (DFT) relaxation calculations that describe the adsorption of molecules onto catalysts' surfaces[3], whereas the second dataset supplements the former with over 62,000 DFT relaxations specifically focusing on oxide electrocatalysis[4], for which available data were previously scarce. Last June, the Open Catalyst Project announced the second edition of their challenge, which consists of training machine learning models to predict relaxed state energies of catalyst-adsorbate structures starting from a given initial structure. Submissions are currently open, and winners will be announced in December at the NeurIPS 2022 Competition Track.

Another promising direction in this area is the design of molecules for aqueous redox flow batteries. In this issue of *Nature Machine Intelligence*, Shree Soundarya S. V. and collaborators present a molecular optimization framework based on AlphaZero and on an objective function made of two graph neural networks trained on DFT simulations to enforce chemically informed constraints. The resulting reinforcement learning algorithm searches the combinatorially large space of feasible organic radicals to identify unknown stable electrolytes that simultaneously fulfill predetermined reduction and oxidation requirements. The article is highlighted by a News & Views piece written by Yang Cao and colleagues in this same issue.

As the report[2] by Climate Change AI emphasizes, machine learning is not a 'silver bullet' solution. Moreover, some of its applications, such as in fossil fuel exploration and extraction, can worsen the climate crisis. Another concern, for all machine learning applications, is the carbon footprint of training and running machine learning models. It is therefore essential to consider the impact of machine learning holistically, as discussed in a recent *Nature Climate Change* Perspective article by Lyn H. Kaack and colleagues. According to the authors, researchers need to stop focusing on performance advances in terms of just accuracy and instead aim for optimizing the tradeoff between accuracy and carbon emissions/energy consumption. The authors recommend that researchers report the carbon emissions impact of their models in scientific publications, "even if only at the level of order-of-magnitude or qualitative assessments." A dedicated workshop, 'Tackling Climate Change with Machine Learning', taking place at NeurIPS 2022 and continuing a series of conference workshops on the topic, will focus on "climate change-informed metrics" to evaluate the impact of machine learning methods on climate change.

The machine learning community has already started grappling with the substantial impact that machine learning has on society in a broad sense. NeurIPS and other venues are prompting authors to add a 'broader impact' statement in their papers to discuss potential downstream positive and negative implications of their research. With a growing urgency of focusing on climate change mitigation, it is time to consider the need to include an assessment of environmental impact as part of that discussion. ❐

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