ML4CC: Lecture 11

Sit with your discussion groups (same as last time)

Assignments reminder

Keep doing your PMIRO+Q

Apr 17 - Project check-ins **during class**

Apr 24 - Exam II

May 1 - Project Presentations

Project reports due May 8th.

Summary of last paper

P - Want to advance methods for real-world reinforcement learning problems like EV charging

M - Create a benchmark dataset and try standard RL methods

I - Uses real world data related to sustainability problems

R - Standard methods don't do particularly well, leaving room for improvement

O - how high can performance be on this problem?

Climate Change in the News

CLIMATEWIRE

Trump declares war on state climate laws

By Adam Aton, Lesley Clark | 04/09/2025 06:52 AM EDT

The president signed an executive order late Tuesday that aims to "stop the enforcement" of a broad swath of state climate regulations.

President Donald Trump speaks at the National Republican Congressional Committee dinner at the National Building M in Washington on Tuesday. Pool photo

In a sweeping executive order signed late Tuesday, Trump ordered Attorney General Pam Bondi to "stop the enforcement of State laws" on climate change that the administration says are unconstitutional, unenforceable or preempted by federal laws.

The order names California, New York and Vermont as specific targets, while also listing a broad range of state policies that the administration would seek to nullify — from cap-and-trade systems to permitting rules.

The executive order also targets the array of lawsuits that mostly Democratic-led states, cities and counties have brought against oil majors, seeking compensation for the ravages of climate change, such as rising tides and more frequent wildfires.

"These State laws and policies are fundamentally irreconcilable with my Administration's American energy," Trump said in the order. "They should not stand."

The move came as Trump presided over a White House event Tuesday aimed at reviving which has withered against competition from less expensive natural gas and renewables

Some legal experts said the White House's executive order would be "toothless," though climate advocates worry about gambling with a judiciary dominated by conservative appointees. And in a statement, Democratic governors said Trump would not intimidate them from climate action.

"The federal government cannot unilaterally strip states' independent constitutional authority," New York Gov. Kathy Hochul and New Mexico Gov. Michelle Lujan Grisham said in a statement. The two Democrats co-chair the U.S. Climate Alliance, representing 22 states committed to reaching net-zero emissions.

"We are a nation of states — and laws — and we will not be deterred," they said. "We will keep advancing solutions to the climate crisis that safeguard Americans' fundamental right to clean air and water, create good-paying jobs, grow the clean energy economy, and make our future healthier and safer."

Climate Change in the News

Science

Renewables provided record share of global electricity in 2024

Nuclear and renewables together provided more than 40% of electricity generation

Thomson Reuters · Posted: Apr 08, 2025 9:26 AM EDT | Last Updated: April 8

For the first time, renewable energy plus nuclear — sources that don't directly emit greenhouse gases — generate more than 40 per cent of global demand for electricity, says a new report from an international research group.

Renewable power generation provided a record 32 per cent of global electricity last year, while nuclear power contributed nine per cent, down slightly from 9.1 per cent in 2023, a report by energy think-tank Ember said on Tuesday. Overall electricity demand grew four per cent, driven by heat waves and data centres.

Solar energy is doubling every three years globally, says Richard Black, policy head at Ember Energy, a European research group. Nearly half the growth is in China, but the curve is up in many regions, including California and Texas in the U.S., Hungary, Spain, Chile and Pakistan, he said.

Energy security fears, exacerbated by a trade war prompted by U.S. President Donald Trump's sweeping tariffs, could further boost demand for renewable power this year, Ember electricity and data analyst Euan Graham told Reuters.

Paper 9 Discussion

Reduced Optimal Power Flow Using Graph Neural Network

Thuan Pham
Student Member, IEEE
Department of Electrical and Computer Engineering
University of Houston
Houston, TX, USA
tdpham7@cougarnet.uh.edu

Xingpeng Li
Senior Member, IEEE
Department of Electrical and Computer Engineering
University of Houston
Houston, TX, USA
xli82@uh.edu

Attendance

Select one person from the group to go to fill out the attendance form (link in Brightspace)

Discussion Question 1

What is a ROPF and why is it desirable here?

Reduced Optimal Power Flow problem

formulation of the OPF problem [13]. For this paper, we designed a GNN model that can predict overloaded and congested lines in the power network with different given load profiles. Predictions from the GNN model are used to identify a subset of critical lines for supervision. We want to lower the number of monitoring lines or number of line flow limit constraints in the OPF problem, in essence, producing a reduced OPF (ROPF) problem. With an ROPF model, it is expected that the amount of computing time for finding the optimal solution will decrease, especially for large and complex power systems.

OPF problems grow with complexity as more components and constraints are added to the grid.

By identifying a subset of the grid to focus our constraints on, we can make the OPF problem easier.

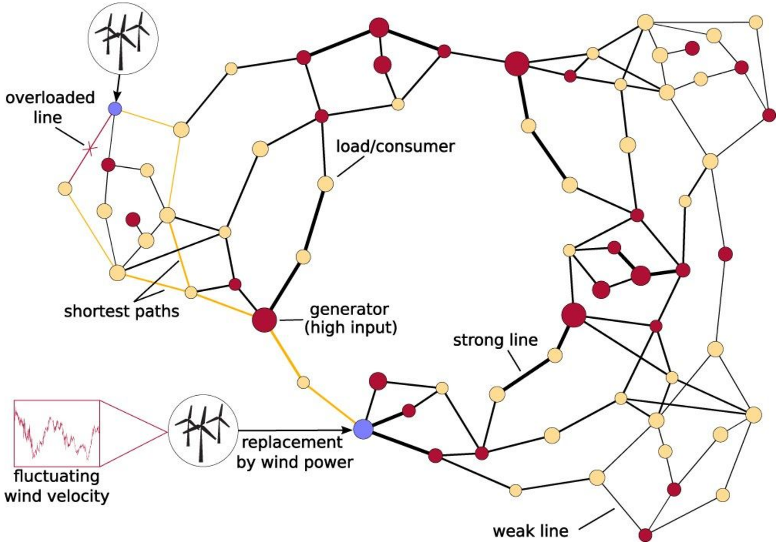
Formulation	Variables	Number of variables	Number of equations
BIM	$V_i = (v_i e^{j\delta_i})$ $S^G_g = (p^G_g + jq^G_g)$ $S^L_l = (p^L_l + jq^L_l)$	$N + G + L$ $(2N + 2G + 2L)$	N $(2N)$
BFM	$V_i = (v_i e^{j\delta_i})$ $S^G_g = (p^G_g + jq^G_g)$ $S^L_l = (p^L_l + jq^L_l)$ $I^s_{ij} = (i^s_{ij} e^{j\gamma^s_{ij}})$ $S_{ij} = (p_{ij} + jq_{ij})$ $S_{ji} = (p_{ji} + jq_{ji})$	$N + G + L + 3E$ $(2N + 2G + 2L + 6E)$	$N + 3E$ $(2N + 6E)$

Discussion Question 2

How is the data generated here?

By solving the OPF problem for a bunch of fake examples

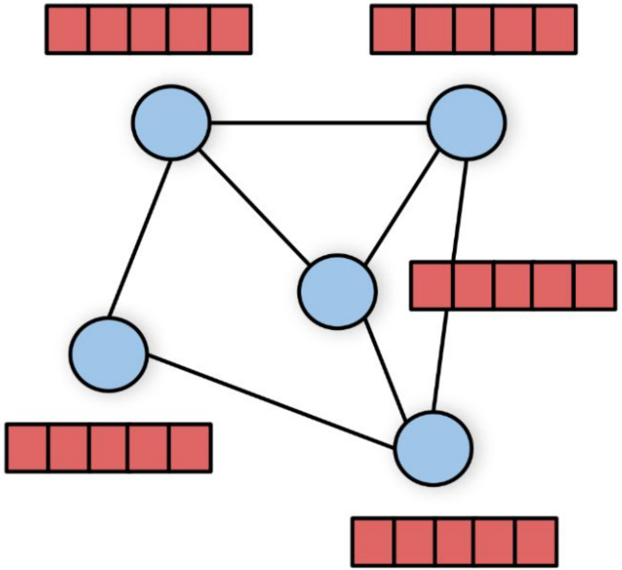
To generate a large number of samples to sufficiently train and test a GNN model, we run normal OPF simulations on the IEEE 73-bus system with different load profiles to collect 20,000 samples. The load profile of each sample is varied within ±10% of the base load profile. From the 20,000 generated samples, the data set is divided into three groups: 80% for training, 10% for validation, and 10% for testing. Then, we used Pyomo library in python to solve for the optimal solution of each sample [15] [16]. Based on the solution, we created labels for each branch based on a pre-specified loading threshold that is defined as a percentage of the line rating limit. For example, if the line rating limit is 100MW and the loading threshold is 80%, a branch will be classified/labeled as heavily loaded/congested when its flow is over 80MW. The labels are represented as one-hot encoding and used as output during the training process.



Lines that, according to the OPF solution, would need to be working at a large percentage of their capacity are labeled as congested.

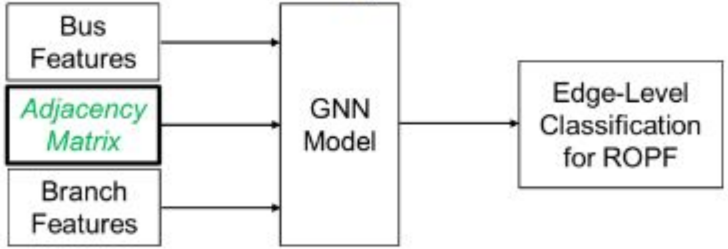
Discussion Question 3

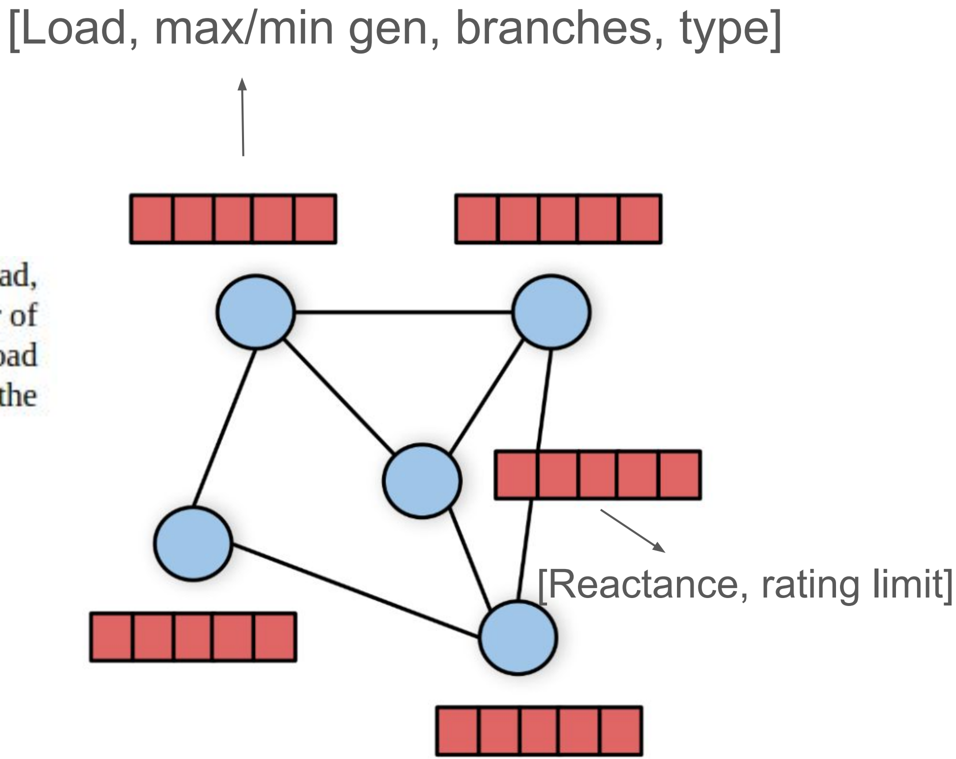
What is the input to the GNN model? What does the model output?



Input: Node and Edge Info

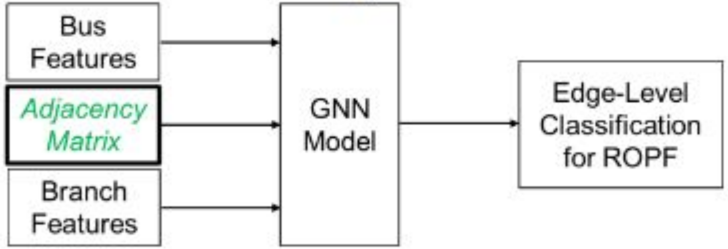
For each sample, the node features are the nodal load, maximum and minimum generation at each bus, the number of branches (edges) connected to each bus, and bus types (load bus, generator bus and slack bus). The edge features include the line reactance and the line rating limit.

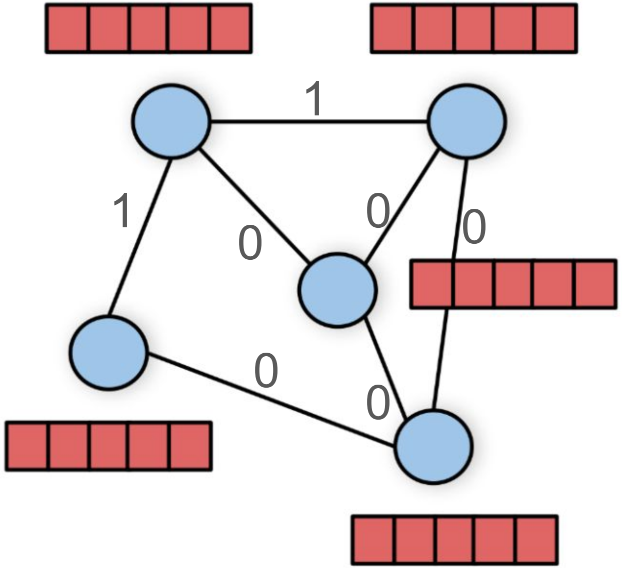




Output: Edge Classification

For each sample, the node features are the nodal load, maximum and minimum generation at each bus, the number of branches (edges) connected to each bus, and bus types (load bus, generator bus and slack bus). The edge features include the line reactance and the line rating limit.





Discussion Question 4

What other model architectures are trained? How do they differ in structure from the GNN?

Regular ANN and Convolutional NN

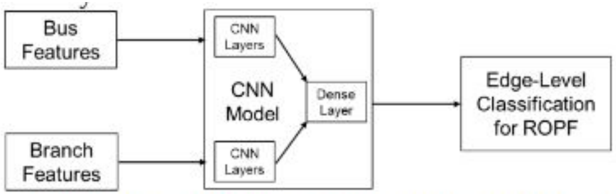


Fig. 5. Illustration of the CNN model. (4 CNN layers for bus features, 4 CNN layers for branch features, and 1 Dense layer to combine both features)

To evaluate how the GNN model perform against typical NN and CNN models, we built separate NN and CNN models that mimic the GNN model. For these models, node features and branch features are each passed and trained separately through four layers. Then, the outputs are combined in a dense layer with softmax activation. As we can see from Fig. 5 and Fig. 6, there is no adjacency matrix to keep track of network topology or global context during the training process.

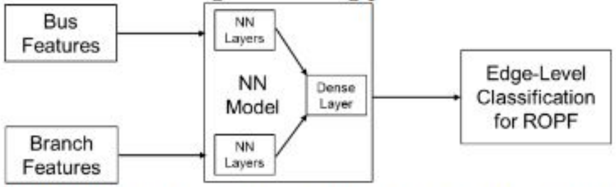
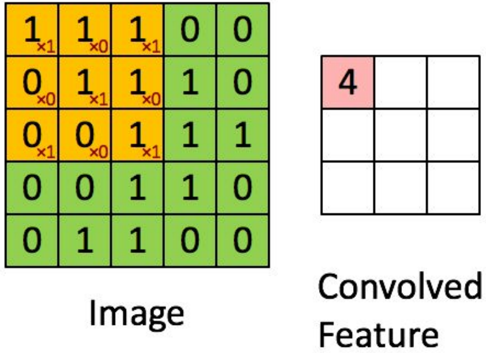


Fig. 6. Illustration of the NN model. (4 NN layers for bus features, 4 NN layers for branch features, and 1 Dense layer to combine both features)

Convolution:



These other models do not take in the adjacency matrix. They also process branch and bus features separately until the end of the network

Discussion Question 5

Describe Figure 10 in your own words

Error distribution

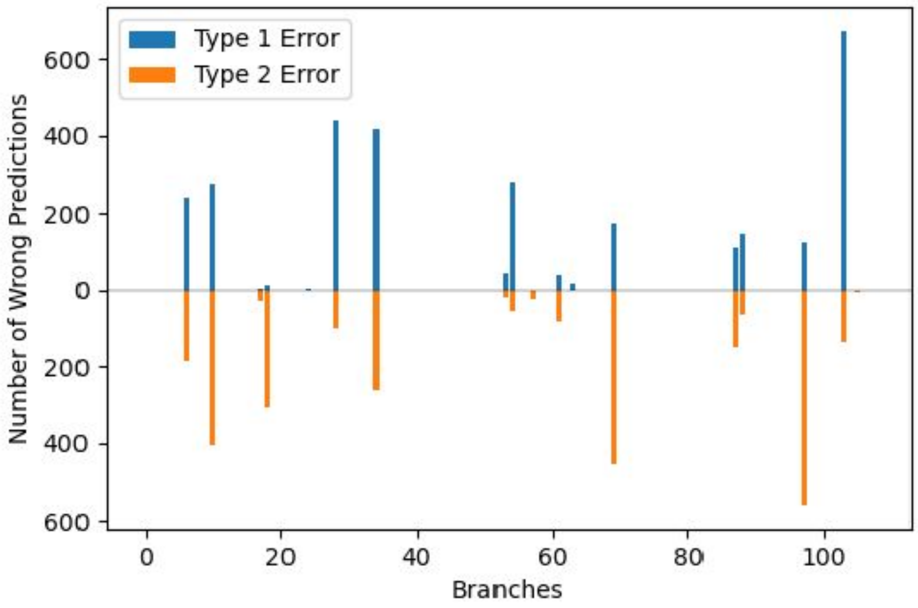


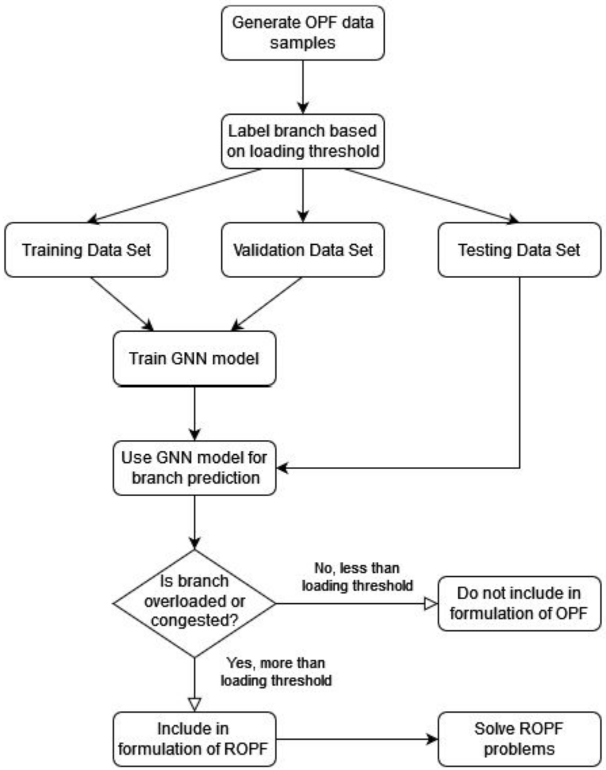
Fig. 10. Number of wrong predictions for Type 1 vs. Type 2 error per branch.

The plot shows that false positive errors (saying a line is congested when it isn't) and false negative errors (saying it is not congested when it is) tend to occur on the same lines, suggesting a small set of lines are generally hard to predict.

Discussion Question 6

Explain figure 13 in your own words. Why does this result make sense?

False negatives lead to physical violations



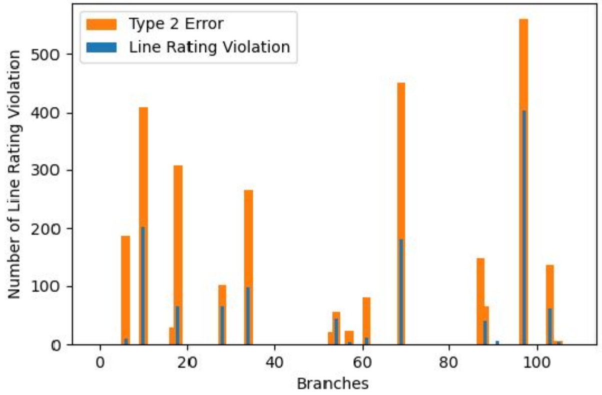


Fig. 13. Line rating violation is superimposed on top of type 2 error per branch.

When branches are incorrectly labeled as non-congested, their limits are not included in the ROPF problem. This means the ROPF solution is not required to obey these line limits. Therefore, the solution sometimes does indeed violate them.

Discussion Question 7

Describe the trends shown in Figures 14 and 15. Why do the changes as a function of threshold make sense?

Increasing threshold increases error and reduces compute time

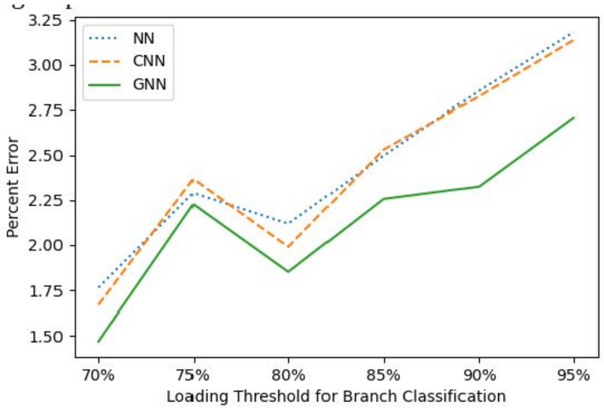
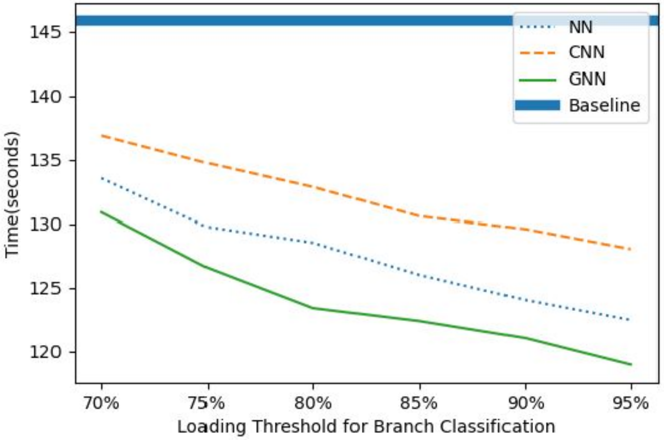


Fig. 14. Percent error of prediction at multiple loading thresholds from different ML models.



The GNN performs best and runs in the least time.

Increasing the threshold for what counts as congested reduces the number of line constraints included in the ROPF (and therefore the run time) but may involve ignoring lines that are congested.

Discussion Question 8

Share what questions you wrote in your PMIRO+Q and decide as a group what you’d like to ask.

Update your PMIRO+Q

Submit a second file to the Brightspace assignment (don’t overwrite the original):

It should:

Update your PMIRO as needed

Answer your own Q

You can be talking with your group during this!

15 min break

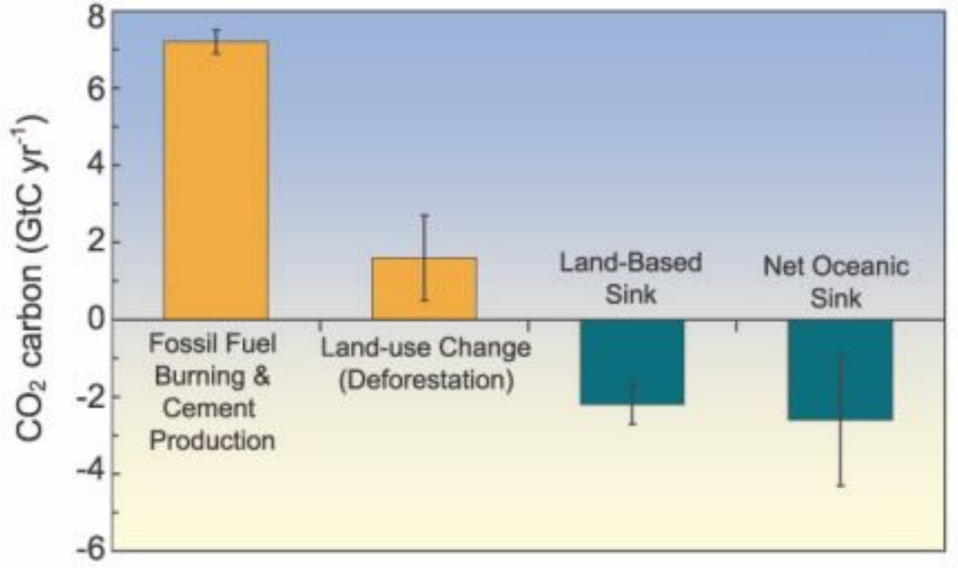
Lecture

Climate Content: Carbon dioxide removal

Machine learning: Review of many topics, Multi-task learning

“Net zero”

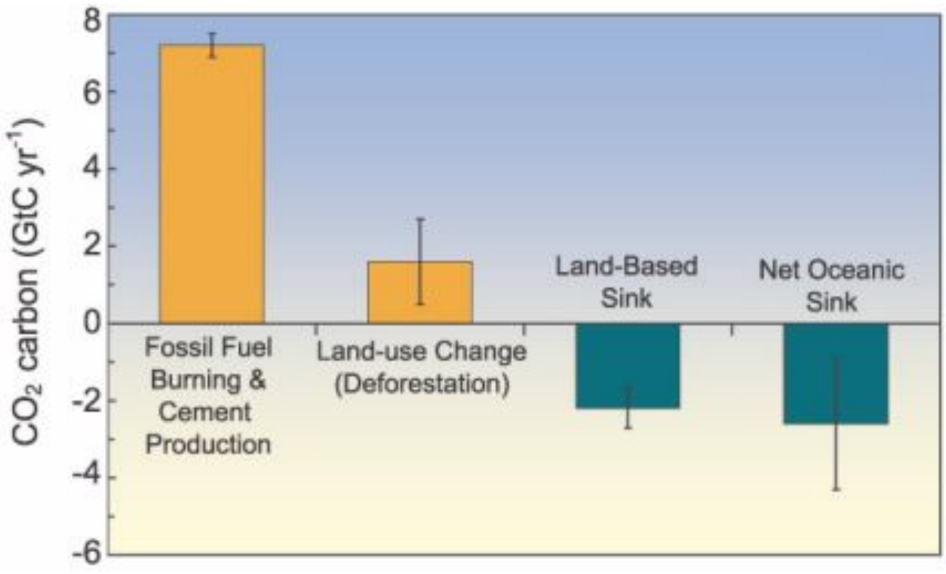
‘Net-zero emissions’ means that all sources of emissions are balanced out by the removal of GHGs.



“Net zero”

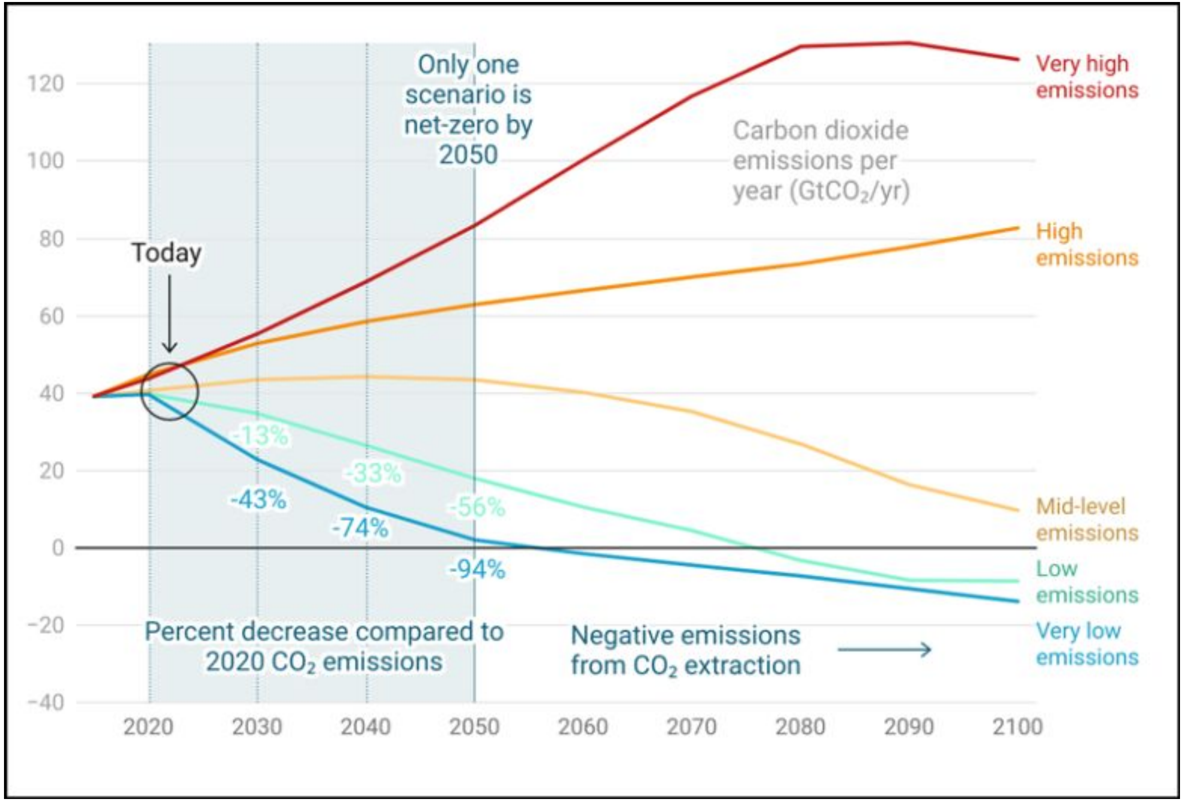
‘Net-zero emissions’ means that all sources of emissions are balanced out by the removal of GHGs.

Net *negative* emissions means that more GHGs are removed from the atmosphere than emitted



Negative emissions

Most models of how we can now stay below 2 degrees C require net negative emissions at some point.



The IPCC on carbon dioxide removal

Methods for removing CO2 from the atmosphere are “unavoidable” if the world is to reach net-zero – both globally and nationally, the report says.

It states with *high confidence* that net-zero can only be achieved if CO2 removal is used to balance “difficult-to-abate” emissions from sectors that will find it harder to slash their climate impact, such as aviation, agriculture and some industrial processes.

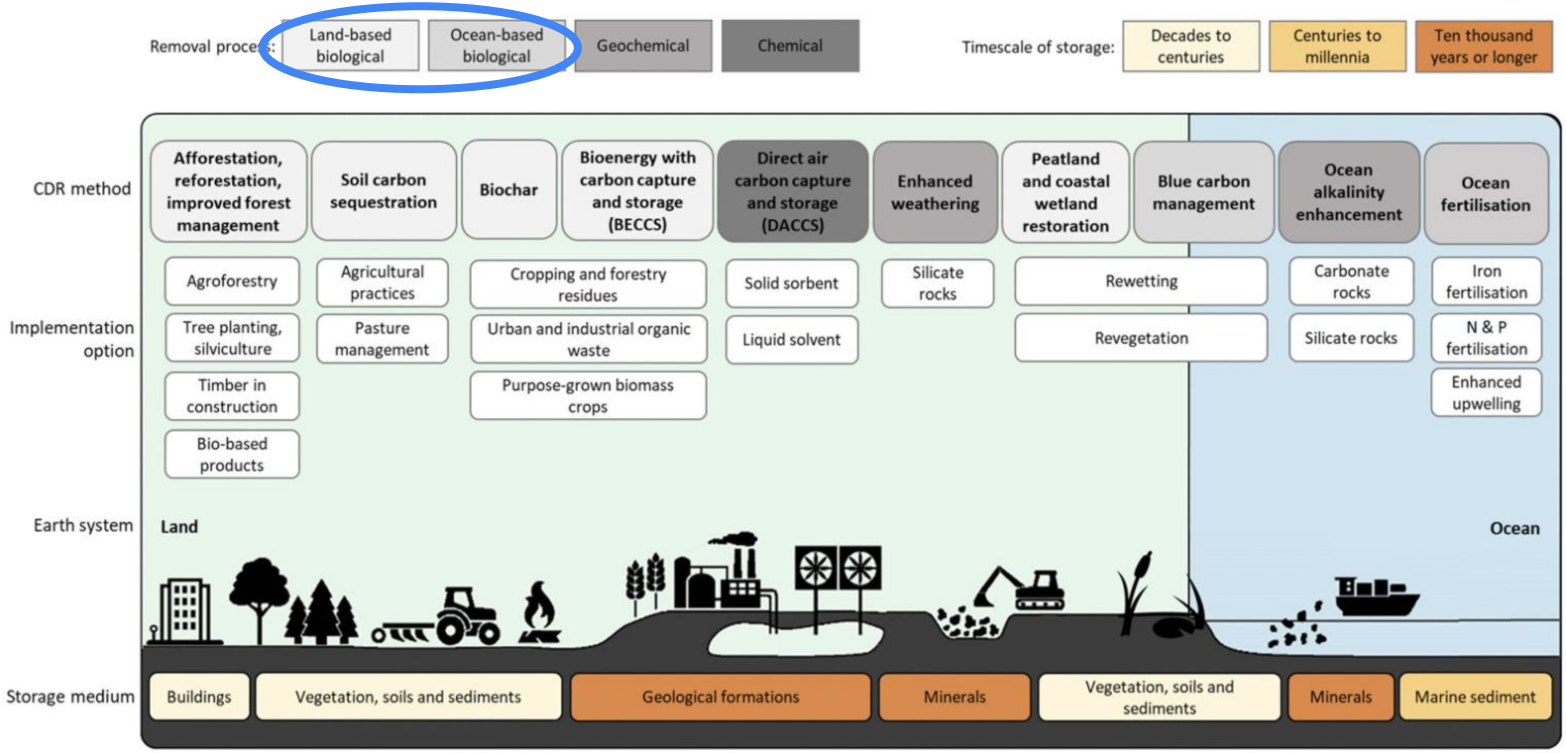
In the longer term, upscaling CO2 removal could provide “net-negative CO2 emissions at the global level”, allowing a “reversal of global warming”, the report says with *medium confidence*.

https://www.carbonbrief.org/in-depth-qa-the-ipccs-sixth-assessment-on-how-to-tackle-climate-change/#co2removal

How can GHGs be removed from the atmosphere?

How can GHGs be removed from the atmosphere?

IPCC



When evaluating removal methods, need to consider process (including energy) and permanence.

ML for ecological restoration

collaborative earth

Global Forests

Aron Boettcher
University of Hawaii
Kyle Fisher Andre Otte

We are building an accurate and global model for predicting potential rates of reforestation and resulting carbon sequestration. Such a model could have a transformational impact on global reforestation efforts by opening new streams of financing in the form of carbon credit futures.

Bison

Jason Baldes NWF & ITBC
Gisel Booman RegenNetwork
Emily Austin Colin Hill
Valérie Lechêne Justin Lewis
Jens Owen Jason Prasad

Across the continent, a number of first nations are reintroducing bison to grasslands where they were once an ecologically vital species. Initial experiences and evolutionary considerations suggest that this may be ecologically beneficial in terms of biodiversity, carbon cycle, and resilience to climate change. However, these questions have not yet been studied at scale. In this lab, we will leverage remote sensing to scale up from ground measurements, establishing the large-scale patterns of bison impact.

Coastal Forested Wetlands

Elliott White Jr.
Stanford University
Nikhil Raj Deep Aaron Hirsh
Stephanie Kao Layla Tadjpour

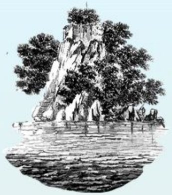
The goal of our lab is to create a high-spatial resolution map of coastal forested wetlands at global scale. If we know precisely where these ecologically critical but fragile forests are located, we can manage freshwater flows to counteract saltwater introgression due to rising sea levels, and we can assist in their migration inland, preserving their critical function in protecting coastlines and sequestering carbon.

Beaver

Grace Lindsay
New York University
Avinash Mahech Cary Murray
Chris Norcross Wendy Owens
Rios Quintin Tyree

Beaver dams are known to result in greener, more drought-resilient waterways in semi-arid environments. We are using computer vision to spot dams in satellite imagery, generating a large dataset that we can use to train models that will tell us what the ecological effects of a dam will be at any point on a waterway. The goal is to create a tool to guide efficient restoration through the introduction of small dams.

Ganges



Anthony Acciavatti
Yale University
Sarthak Arora Markley Boyer
Nikhil Raj Deep Jiby Matthew
James Smoot Michael
Warner

In our pursuit of a successful and thriving relationship between humanity and natural systems, the Ganges river basin represents an extreme challenge. It is densely populated, remains agriculturally productive, and subject to an extremely powerful monsoon. We are mapping and analyzing a key feature of the Ganges basin—naalas—to understand how new forms of green infrastructure, such as parks, bioswales, and bioremediation, can rejuvenate this vital and sacred river.

Assisted Forest Regeneration

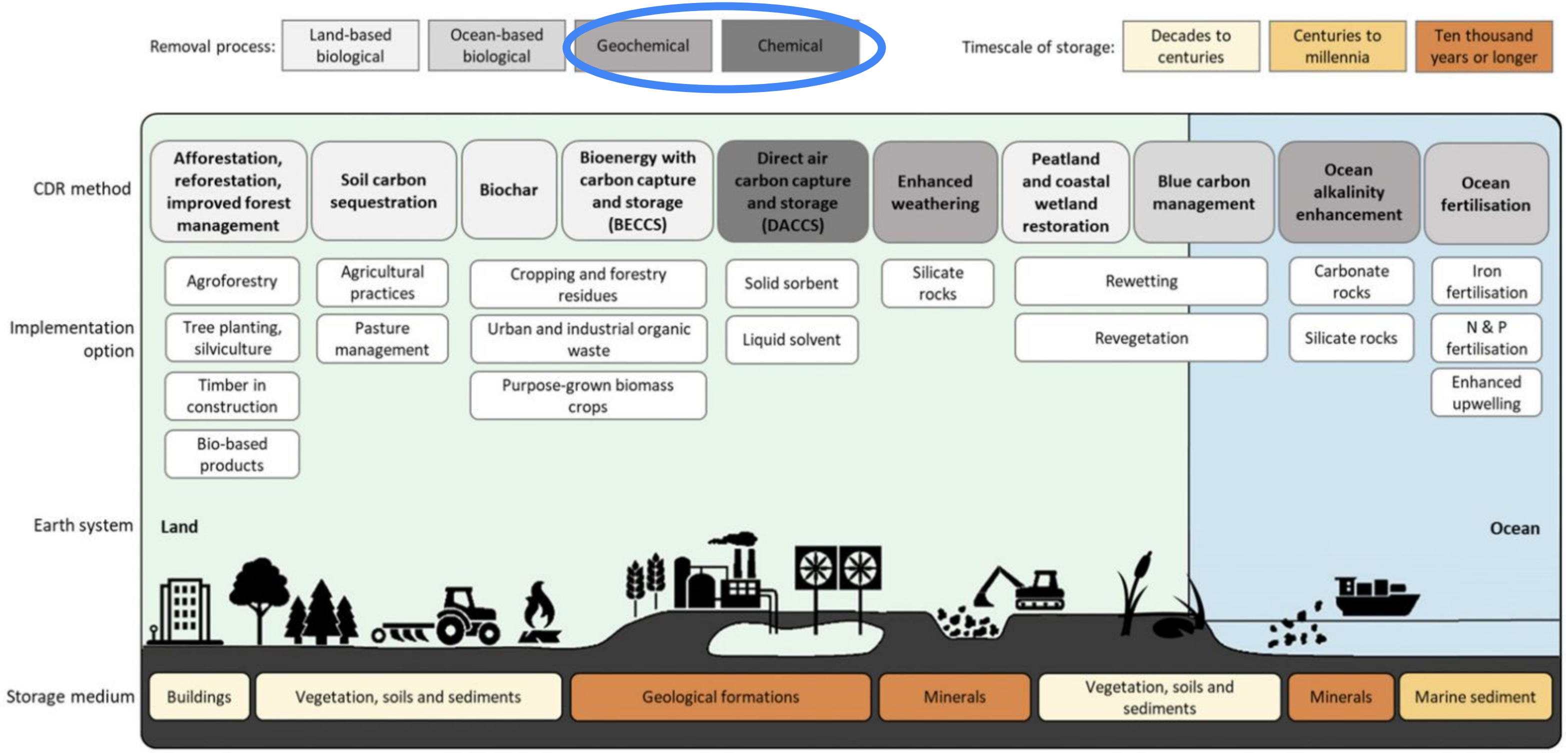
Leland Werden
ETH Zürich
Collaborative Earth AFR Data Team

This project is pioneering the idea of a massively open literature review. We aim to quantify potential carbon capture and plant biodiversity recovery of forest, savannah, and mangrove assisted restoration projects. To do so, we are gathering and synthesizing unpublished data from field partners, integrating as much information from non-English sources as possible. There is a wealth of wisdom that has not been published in academic journals, and we aspire to integrate these insights into our review.

According to the IPCC, tree-planting and ecosystem restoration are the only “widely deployed” forms of CO2 removal.

How can GHGs be removed from the atmosphere?

IPCC



When evaluating removal methods, need to consider process (including energy) and permanence.

(Geo)chemical carbon dioxide removal

Enhanced Weathering: A speedup of a natural process...

(Geo)chemical carbon dioxide removal

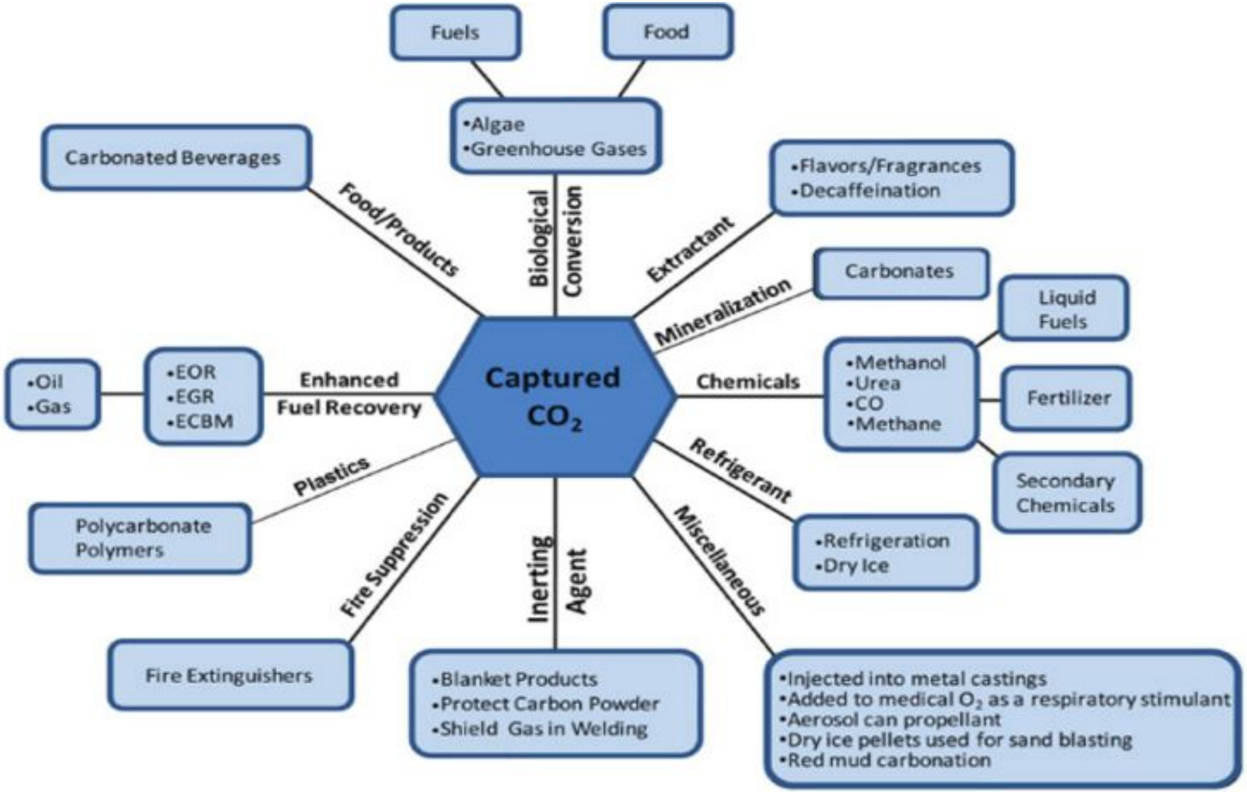
Direct air capture (DAC) aims to pull carbon dioxide out of the air.

(A separate technology, “carbon capture”, tries to recapture carbon dioxide released during fuel burning. This cannot create net-negative emissions)

According to the IPCC: Despite limited use at present, technologies such as direct air capture, are projected to make a “moderate to large” contribution to future CO2 removal

(Geo)chemical carbon dioxide removal

Uses of captured carbon



Aspen Institute

Deals

Occidental buys carbon air capture tech firm for $1.1 billion

By **Sabrina Valle** and **Sourasis Bose**

August 15, 2023 6:38 PM EDT · Updated 8 months ago

Aa

The logo for Occidental Petroleum is displayed on a screen on the floor at the New York Stock Exchange (NYSE) in New York, U.S., April 30, 2019. REUTERS/Brendan McDermid/File Photo *Purchase Licensing Rights*

Aug 15 (Reuters) - U.S. oil and gas producer Occidental Petroleum (OXY.N) on Tuesday agreed to pay $1.1 billion for technology supplier Carbon Engineering Ltd to help it develop a string of carbon-capture sites it hopes will profit from tackling climate change.

The U.S. oil producer aims to build about 100 plants using direct air capture (DAC) technology that strips

Equivalent to the annual emissions of about 33,000 Americans

- Occidental Petroleum is a pioneer in direct air capture (DAC) technology thanks to its $1.1B acquisition of Carbon Engineering in 2023.
- Occidental Petroleum will launch its STRATOS plant in 2025 to capture 500K metric tonnes of carbon dioxide (C02) annually.
- Occidental subsidiary 1PointFive has struck deals with Amazon, Airbus and Microsoft to sell millions of tons of carbon dioxide removal (CDR) carbon credits, which will be generated through its Stratos and future DAC plants.

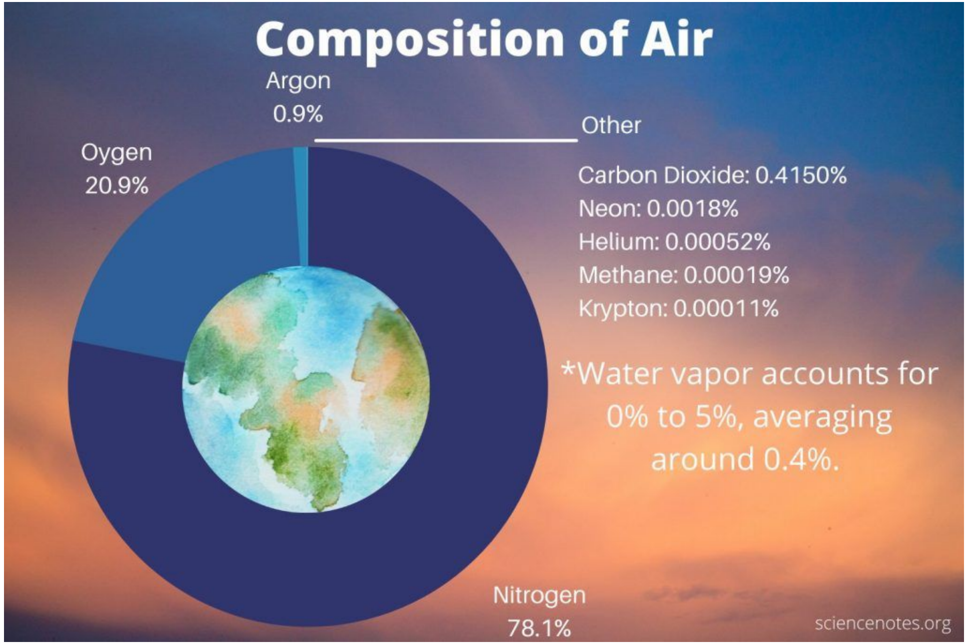
According to the IPCC...

The upscaling of many CO2 removal methods faces “various feasibility and sustainability constraints”

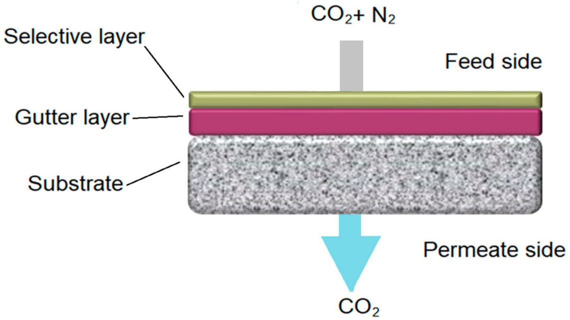
Enhanced weathering, meanwhile, “has been demonstrated in the laboratory and in small scale field trials, but has yet to be demonstrated at scale”.

Direct air capture and storage is currently limited by its large energy requirements and by cost; the technology is at a “medium readiness level”.

Direct Air Capture is hard: Can ML make it better?

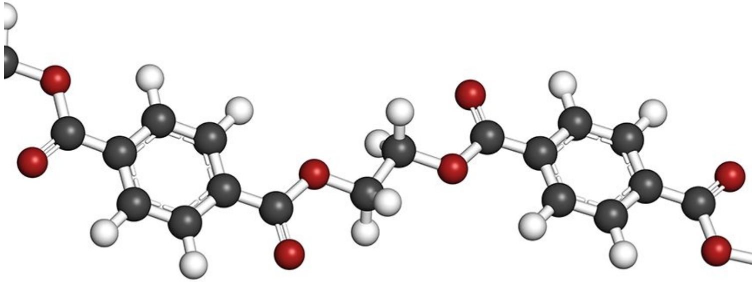


We need materials that can cheaply filter out CO2.



Direct Air Capture is hard: Can ML make it better?

“Polymer membranes” need to be selective (only let CO_2 pass) and permeable (let a lot of CO_2 pass)



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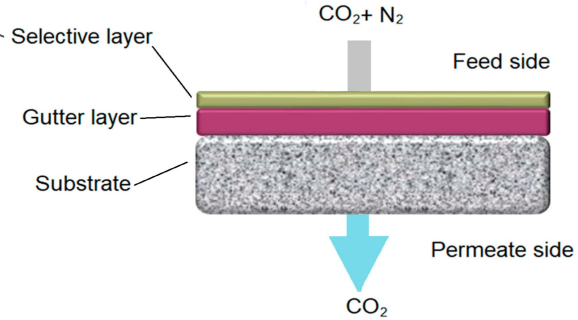

Direct Air Capture is hard: Can ML make it better?

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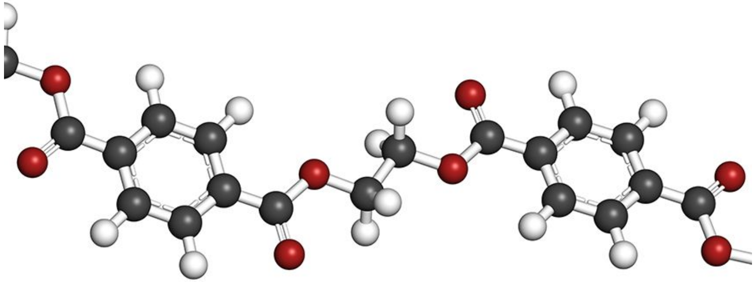


Can ML design better polymers?

Topics we've already talked about that are mentioned in this week's paper:

Elasticnet

Ensemble methods

XGBoost

Feed forward neural networks

Emulators

Reinforcement Learning

Pareto fronts

Graph neural networks

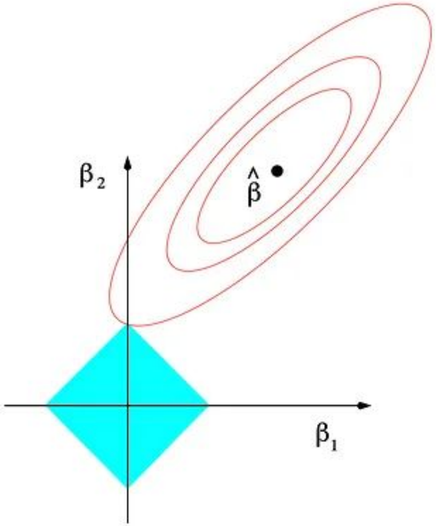
Transformers

Unsupervised learning

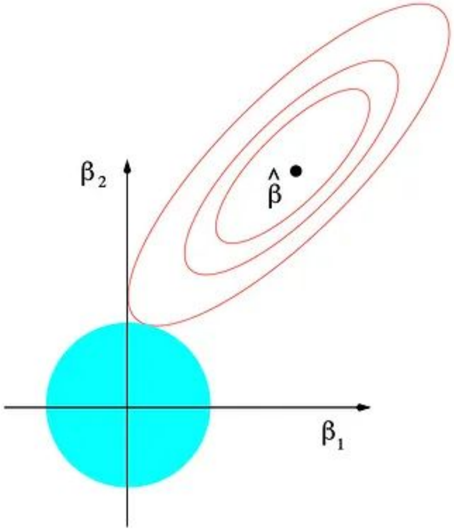
Cross validation

Hyper parameter tuning

ElasticNet: Regularized Linear Regression



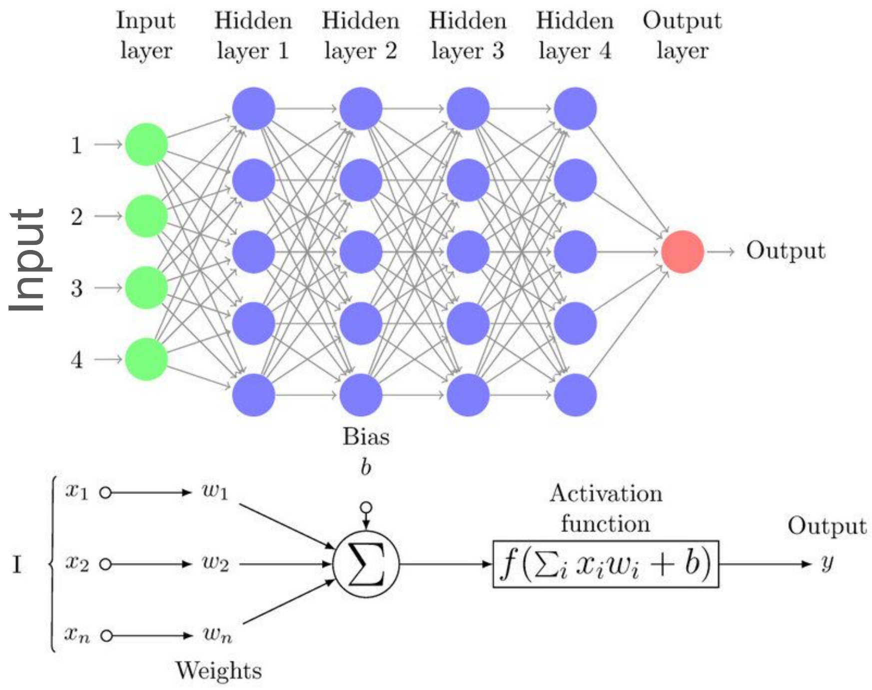
Lasso



Ridge

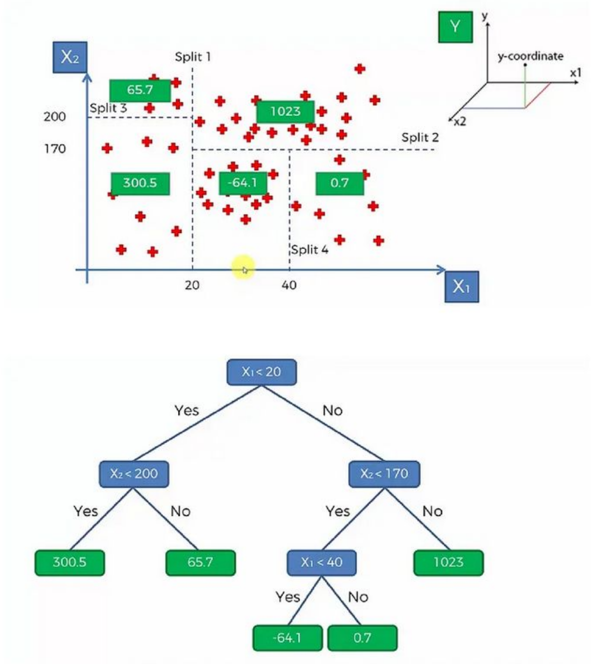
Lasso + Ridge = “ElasticNet”

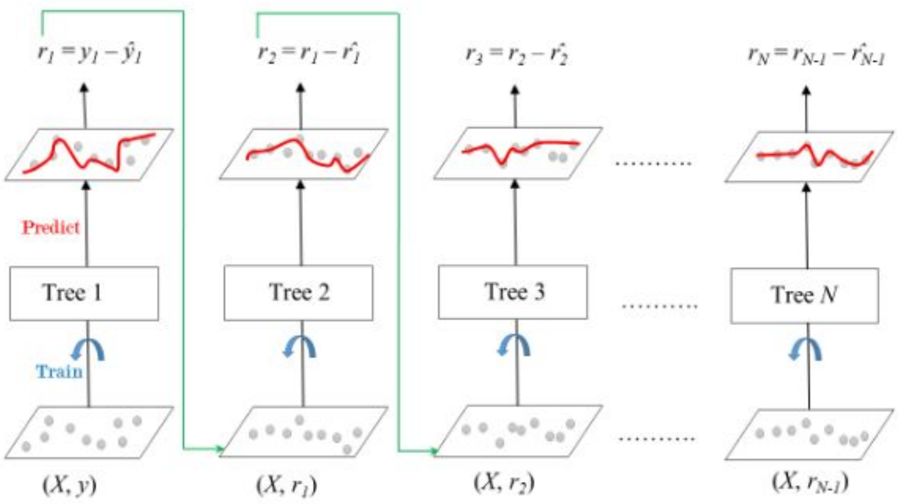
Basic Feedforward Neural Network



XGBoost

Gradient Boosted Trees (also an ensemble method)





Each tree predicts and subtracts the errors of the one before

Topics we’ve already talked about that are mentioned in this paper:

Elasticnet

Ensemble methods

XGBoost

Feed forward neural networks

Emulators

Reinforcement Learning

Pareto fronts

Graph neural networks

Transformers

Unsupervised learning

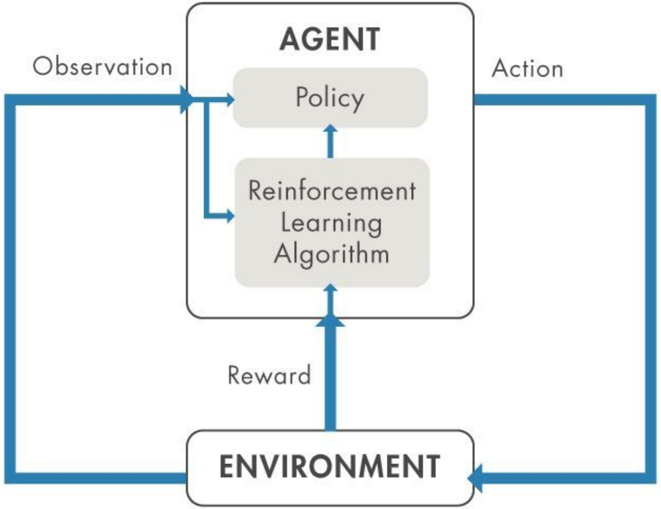
Cross validation

Hyper parameter tuning

Reinforcement learning

When using reinforcement learning to solve a control problem, the aim is to develop a **policy** that controls an **agent** to maximize **reward**.

The policy is a function that takes in a **state observation** and produces an **action**.



https://www.mathworks.com/company/newsletters/articles/reinforcement-learning-a-brief-guide.html

Topics we've already talked about that are mentioned in this paper:

Elasticnet

Ensemble methods

XGBoost

Feed forward neural networks

Emulators

Reinforcement Learning

$\boxed{\text{Pareto fronts}}$

Graph neural networks

Transformers

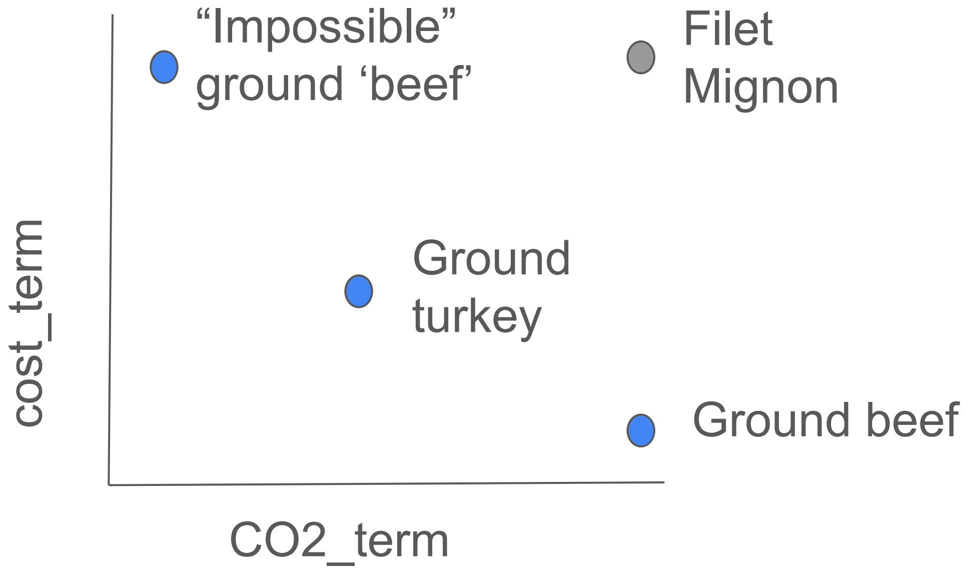
Unsupervised learning

Cross validation

Hyper parameter tuning

The pareto front is the result of trade-offs in the various objective terms

Trying to minimize:



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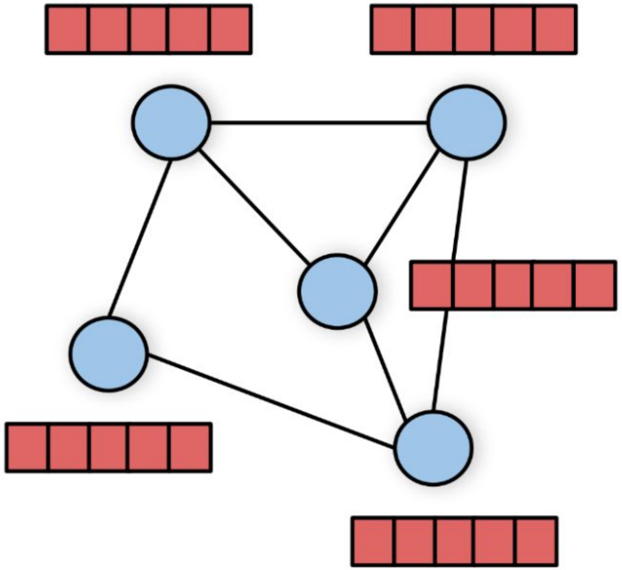
Graph Neural Networks (GNNs)

GNNs are artificial neural networks that can take *graphs* as input.

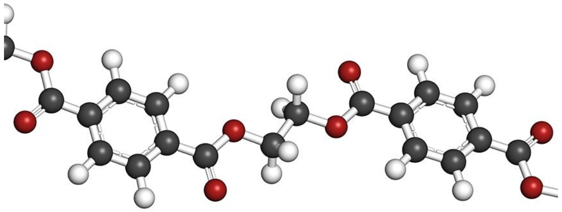
The graphs are represented by their adjacency matrix and any values needed to provide information about each node or edge.

The neural network learns how to combine information across nodes using a *message passing* algorithm.



Graph Neural Networks for molecules

Molecules are naturally represented as graphs!



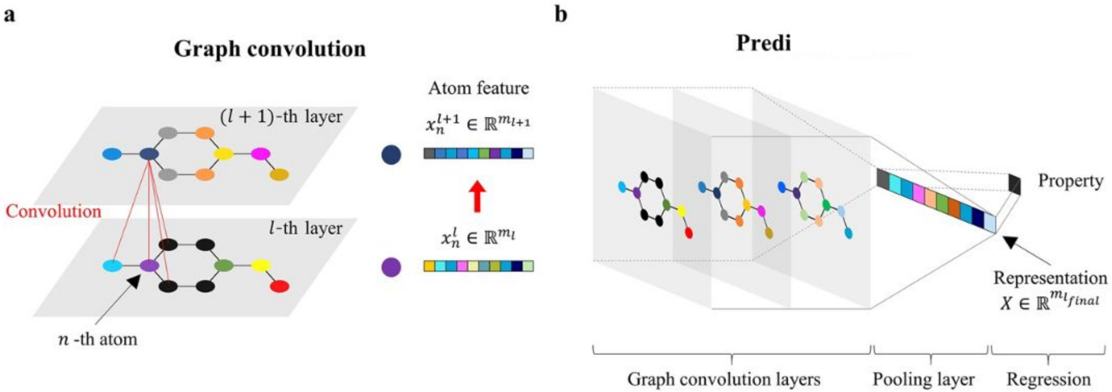


Figure 2. Property prediction model based on the GCN. (a) Feature vector of n-th atom x_n^l is updated iteratively through the l-th convolutional layer by the graph convolution that aggregates the features of neighboring atoms. (b) Graph-level molecular representation vector X is obtained by the pooling layer that sums up the feature vectors of all the atoms at the final convolution layer. The vector X is input to the regression algorithms (linear regression (LR) only shown here) for the property prediction.

Park et al, 2022

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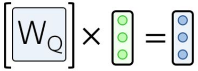
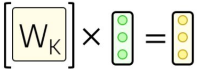
Transformer architecture

Each vector receives three representations ("roles")



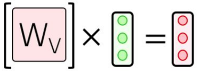
Query: vector **from** which the attention is looking

"Hey there, do you have this information?"



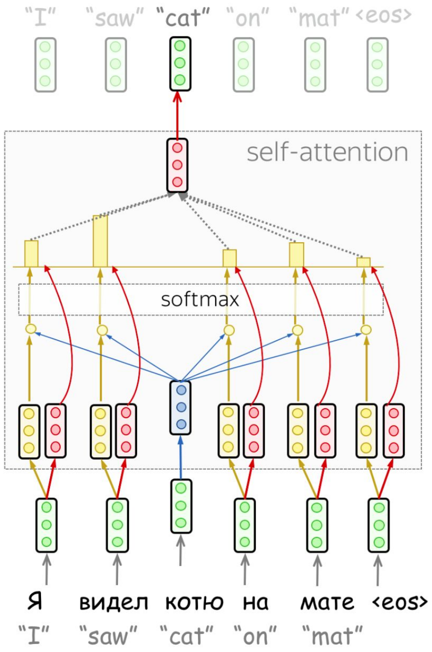
Key: vector **at** which the query looks to compute weights

"Hi, I have this information – give me a large weight!"



Value: their weighted sum is attention output

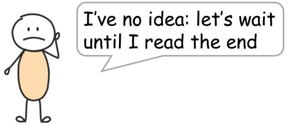
"Here's the information I have!"



Key insight: combine information across words. This is known as "self-attention".

I arrived at the bank after crossing the ... ...street? ...river?

What does **bank** mean in this sentence?



RNNs

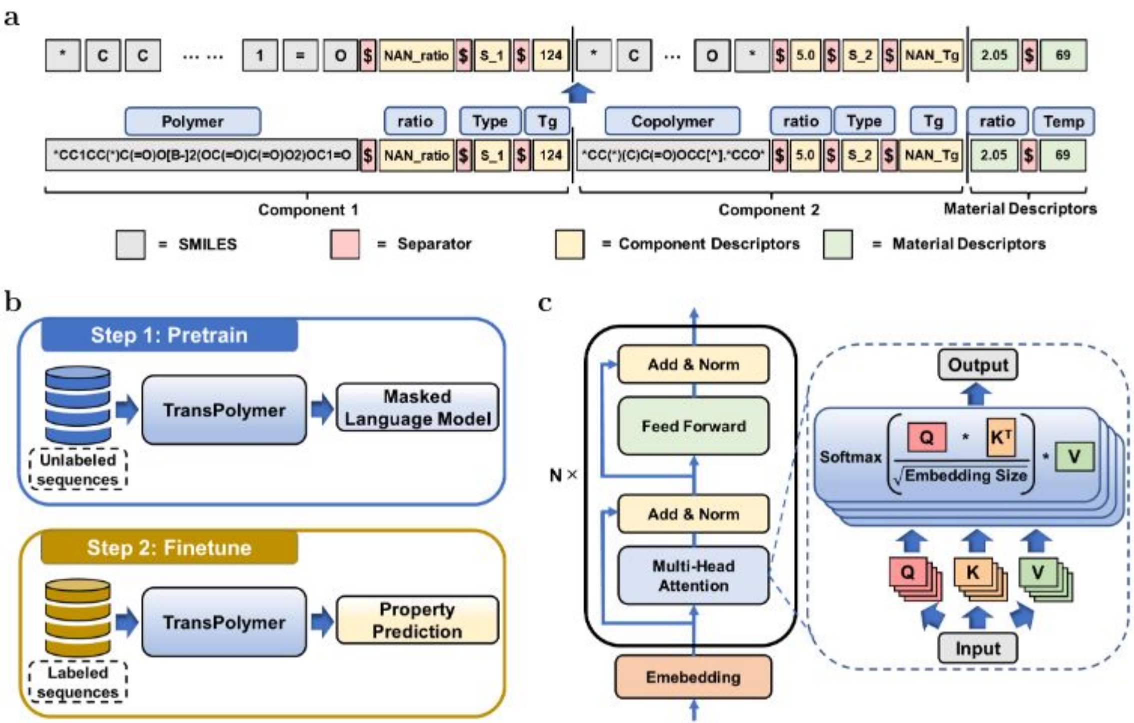
O(N) steps to process a sentence with length N

Transformer

Constant number of steps to process any sentence

Transformers for molecules

Need to represent the molecular structure as a sequence of characters



Xu et al, 2022

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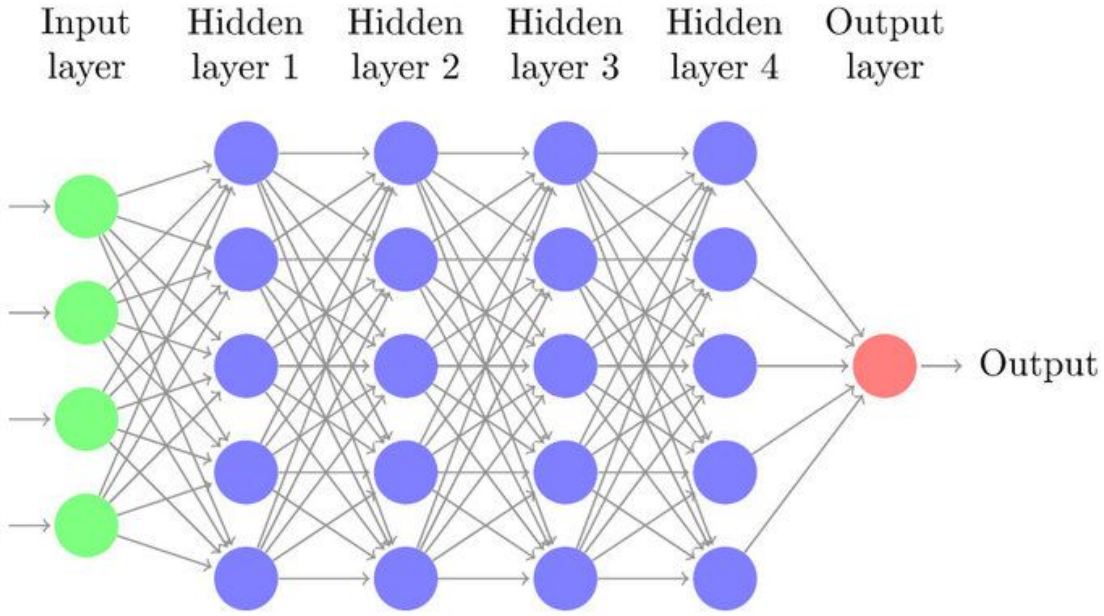
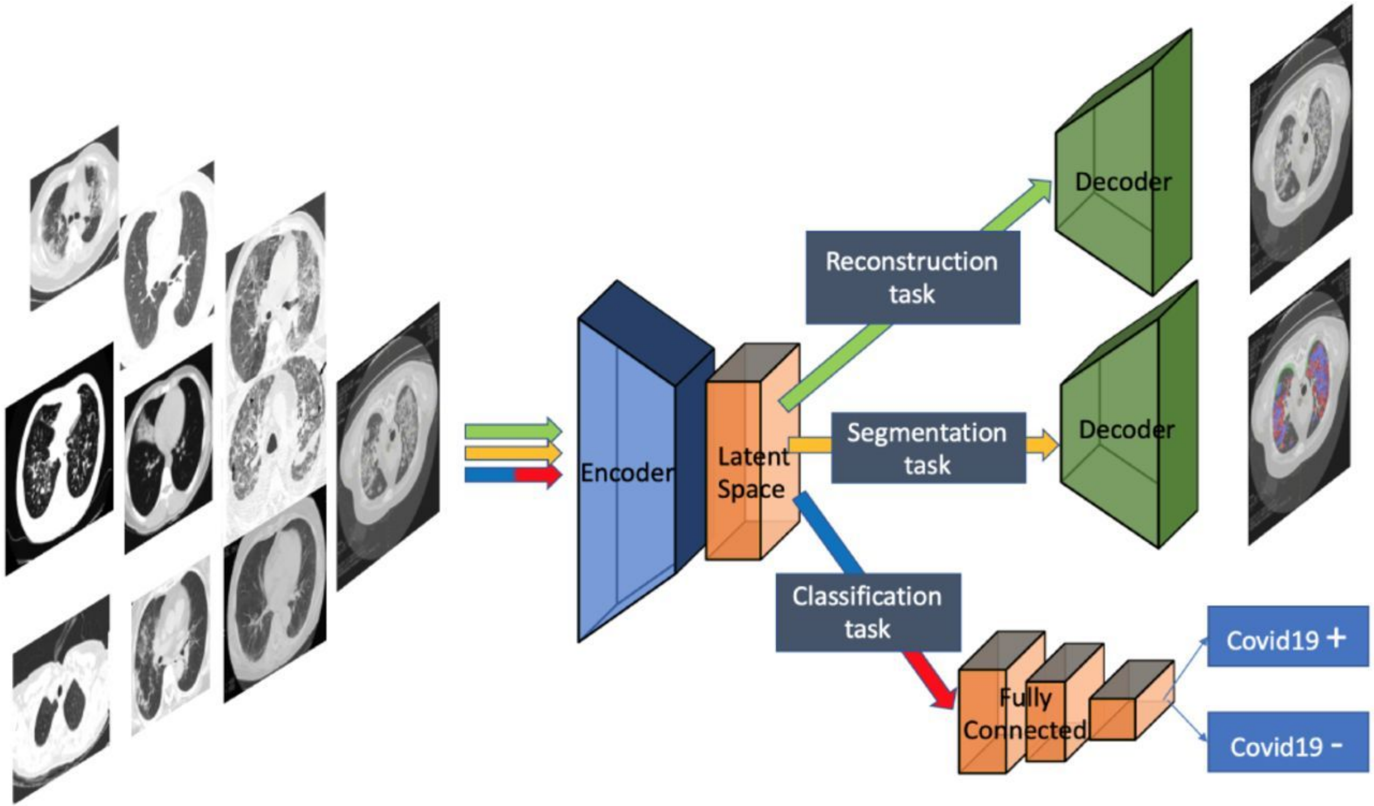
New topic: multi-task learning

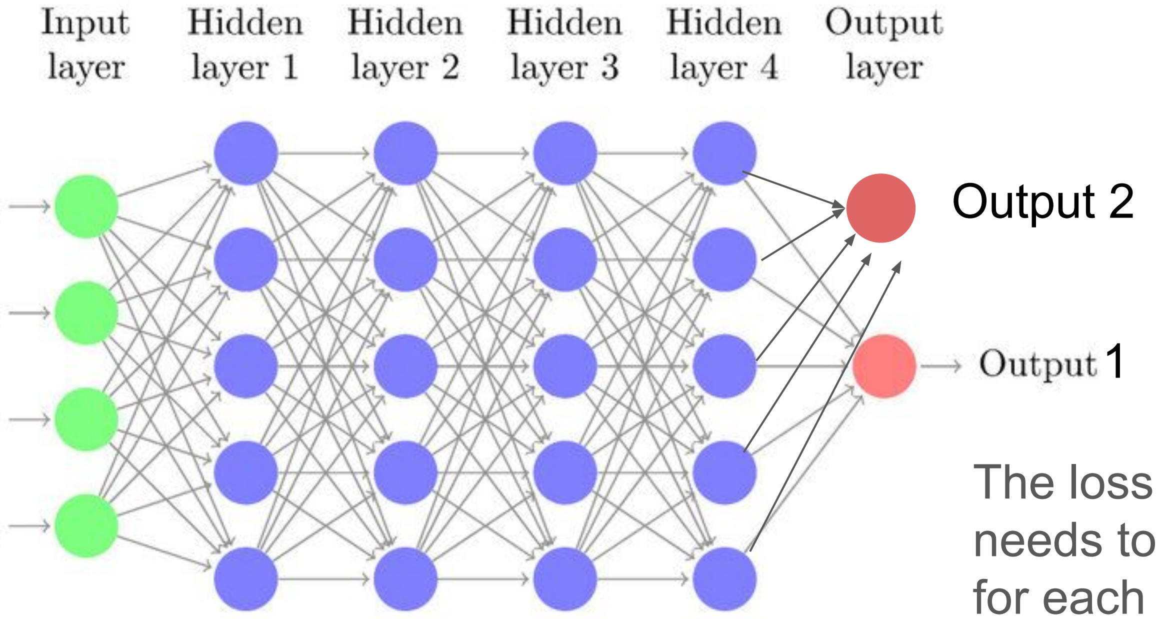
Multi-task learning: making a single model do multiple things





Amyar et al, 2020

Multi-task learning: making a single model do multiple things



The loss function needs to include terms for each output