Towards explainable message passing networks for predicting carbon dioxide adsorption in metal-organic frameworks

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Abstract

Metal-organic framework (MOFs) are nanoporous materials that could be used to capture carbon dioxide from the exhaust gas of fossil fuel power plants to mitigate climate change. In this work, we design and train a message passing neural network (MPNN) to predict simulated CO_2 adsorption in MOFs. Towards providing insights into what substructures of the MOFs are important for the prediction, we introduce a soft attention mechanism into the readout function that quantifies the contributions of the node representations towards the graph representations. We investigate different mechanisms for sparse attention to ensure only the most relevant substructures are identified.

1 Introduction

Anthropogenic carbon dioxide (CO_2) emissions are a major contributor to climate change and ocean acidification [1]. Carbon dioxide capture and storage [2] is among a concerted portfolio of approaches [3] to stabilize and eventually reduce our CO_2 emissions. In post-combustion carbon capture, CO_2 is separated from the combustion exhaust gas of fossil fuel power plants, at the point of emission, and then geologically sequestered [1]. Metal-organic frameworks (MOFs) [4] are nano-porous, crystalline materials that can selectively adsorb CO_2 [5, 6] and therefore could be used to capture CO_2 from the flue gas of fossil fuel power plants [7].

MOFs are acclaimed as "designer materials" [8] because the chemistry of the internal surface of the MOF can be (computationally) designed to target the adsorption of CO_2 [9]. MOFs are synthesized modularly, by linking organic molecules to metals/metal clusters to form an extended network. Due to the abundance of molecular building blocks and their post-synthetic modifiability, the space of MOFs is vast. Molecular models and simulations [10, 11] and machine learning [12, 13, 14] play an important role in navigating this vast space of MOFs to find a suitable/optimal MOF for energy-efficient CO_2 capture and release [15].

Here, we design and train a message passing neural network (MPNN) [16, 17] to predict the (simulated) amount of CO_2 adsorption in MOFs. As opposed to the traditional machine learning approach of human-engineering a feature vector to represent the structure of the MOF [18, 19, 20, 21, 22], the MPNN directly takes a graph representation of the MOF structure as input and automatically learns a vector representation of the MOF to use for the prediction task, in an end-to-end manner. This is achieved by iteratively passing information between neighboring nodes to learn hidden

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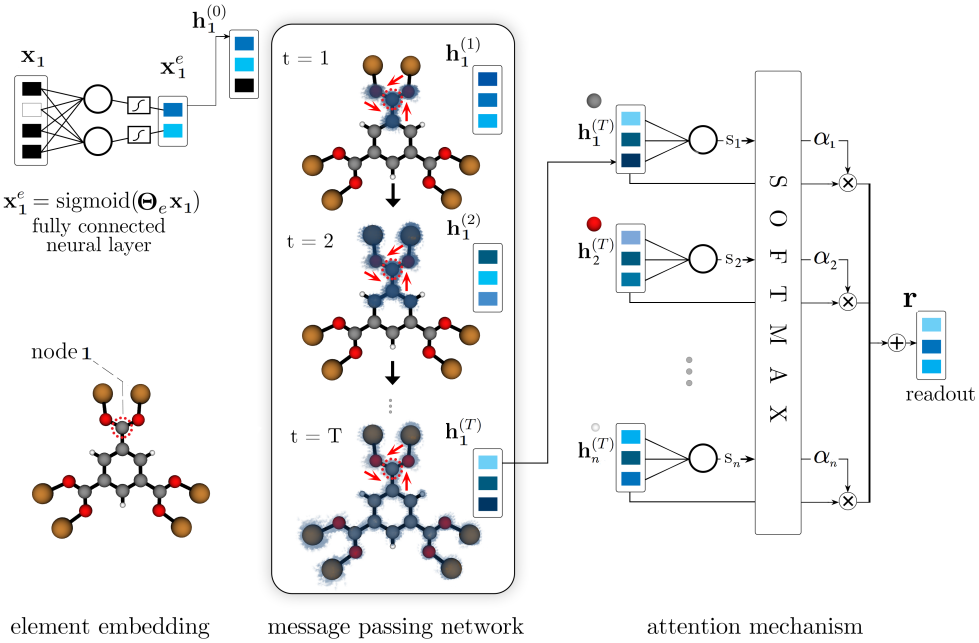


Figure 1: The architecture of our message passing neural network (MPNN).

representations of the local bonding environments within the MOFs, then, through a readout function, aggregating the local node representations into a graph representation used for the prediction task. In a step towards explaining the predictions of the MPNN by identifying important substructures in the graph, we incorporated an attention mechanism in the readout function of the MPNN that quantifies the contribution of each node's representation to the graph representation. Explainability is advantageous because it (i) can elucidate design rules and chemical intuition for synthesizing MOFs with desirable adsorption properties and (ii) build appropriate trust/skepticism of particular predictions based on the explanation.

MPNNs [16, 17] have been used to predict the properties of molecules and materials [23, 24, 25, 17, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35], as well as to generate molecules and materials with desired properties [36, 37]. There has been limited efforts in interpreting/explaining MPNNs or graph neural networks (GNNs) in general [29, 38, 39, 40, 41, 42].

2 Proposed framework

2.1 Problem overview

We aim to predict the equilibrium CO_2 adsorption in a MOF at a given temperature and pressure, $a \in \mathbb{R}^+$ [mmol/g]. Each MOF structure is represented as an undirected, node-labeled graph $G = (\mathcal{V}, \mathcal{E}, \mathbf{X})$, where $\mathcal{V}$ is the set of $n = |\mathcal{V}|$ nodes or vertices, representing atoms, $\mathcal{E}$ is the set of edges, representing bonds, and $\mathbf{X} \in \mathbb{R}^{d \times n}$ is the node feature matrix, whose columns are one-hot encodings of the chemical elements of the atoms (d possible elements). In a supervised manner, we aim to learn a function that maps a MOF to its predicted CO_2 adsorption: $f : G \mapsto f(G) = a$.

2.2 Converting a MOF crystal structure to a graph

We constructed the node-labeled graph G representing each MOF from its unit cell, the list of atoms in the unit cell, and the crystallographic coordinates of those atoms. A bijection exists between the nodes $\mathcal{V}$ and the atoms comprising the unit cell of the MOF. Two atoms are assigned an edge (bond) iff, as in Refs. [34, 43, 44], (i) they are less than a distance r apart, with r the sum of their covalent radii [45] (some metals modified) plus a 0.25 Å tolerance, and (ii) they share a Voronoi face in a

Voronoi diagram of the surrounding atoms. We used periodic distance in our calculations to include bonds across the periodic boundary of the unit cell.

2.3 Message passing neural network that represents f

Fig. 1 shows the architecture of our message passing neural network (MPNN) that includes an attention mechanism to construct the graph representation from the set of node representations.

Message passing. First, our MPNN operates on nodes and learns a vector representation of the local bonding environment of each node in the graph. This is achieved by a chemical element embedding followed by iterations of message passing.

The chemical element embedding layer maps the one-hot encoding of the chemical element of the node to a low-dimensional, dense representation:

$$\mathbf{x}_v^e = \texttt{sigmoid.}(\mathbf{\Theta}_e \mathbf{x}_v), \tag{1}$$

where $\mathbf{x}_v$ is column v of $\mathbf{X}$ and $\mathbf{\Theta}_e$ is a $r \times d$ learned matrix, with $r < d$.

Message passing is then used to learn a representation of each node encapsulating information about its local bonding environment. Let $\mathbf{h}_v^{(t)} \in \mathbb{R}^k$ be the hidden representation of node v at time step t, with $k \geq r$, initialized with the element embedding $\mathbf{x}_v^e$ padded with zeros. In each time step, every node receives information from its neighbors and updates its hidden representation accordingly, from an aggregated message, using a gated graph neural network (GGNN) [46]. The aggregated message received by node v is:

$$\mathbf{m}_v^{(t+1)} = \mathbf{\Theta}_m \sum_{u \in \mathcal{N}(v)} \mathbf{h}_u^{(t)} \tag{2}$$

where $\mathbf{\Theta}_m$ is a learned $k \times k$ matrix shared across all nodes and $\mathcal{N}(v)$ is the set of nodes that share an edge with node v. A Gated Recurrent Unit (GRU) (shared across all nodes) then updates the hidden representation of node v:

$$\mathbf{h}_v^{(t+1)} = \texttt{GRU}(\mathbf{h}_v^{(t)}, \mathbf{m}_v^{(t+1)}). \tag{3}$$

We conduct T time steps of message passing, after which $\mathbf{h}_v^{(T)}$ contains information about the bonding environment of node v within a graph-distance of T.

Readout and prediction. A readout function [47] maps the set of hidden node representations to a fixed-size vector representation of the entire graph. We use a soft attention mechanism [46] where the attention of node v, α_v, is computed from the hidden features via a `softmax`:

$$\alpha_v = \frac{e^{\boldsymbol{\theta}_s^\intercal \mathbf{h}_v^{(T)}}}{\sum_{u=1}^{n} e^{\boldsymbol{\theta}_s^\intercal \mathbf{h}_u^{(T)}}} \tag{4}$$

where $\boldsymbol{\theta}_s \in \mathbb{R}^k$ is a learned vector shared across all nodes. To introduce sparsity, we also try (1) the quasi-norm L(0.5) regularization of the attention scores and (2) `sparsemax` [48] in place of `softmax`. The attention score of node v then determines the contribution of its hidden representation $\mathbf{h}_v^{(T)}$ to the representation of the graph, $\mathbf{r}$:

$$\mathbf{r} = \sum_{v=1}^{n} \alpha_v \mathbf{h}_v^{(T)}. \tag{5}$$

Finally, a neural network predicts the CO_2 adsorption ($\hat{a}$) from the graph representation:

$$\hat{a} = \texttt{softplus}\left(\boldsymbol{\theta}_a^\intercal \left(\texttt{sigmoid.}\left(\mathbf{\Theta}_a \mathbf{r}\right)\right)\right) \tag{6}$$

where $\mathbf{\Theta}_a$ is a learned $z \times k$ matrix and $\boldsymbol{\theta}_a \in \mathbb{R}^z$ is a learned vector. The `softplus` ensures $a > 0$.

3 Results

As train, test, and validation data, we use simulated CO_2 uptake at 298 K and 0.15 bar from Ref. [49], taken from the Materials Cloud [50], in 6 103 computation-ready, experimental MOF structures [51].

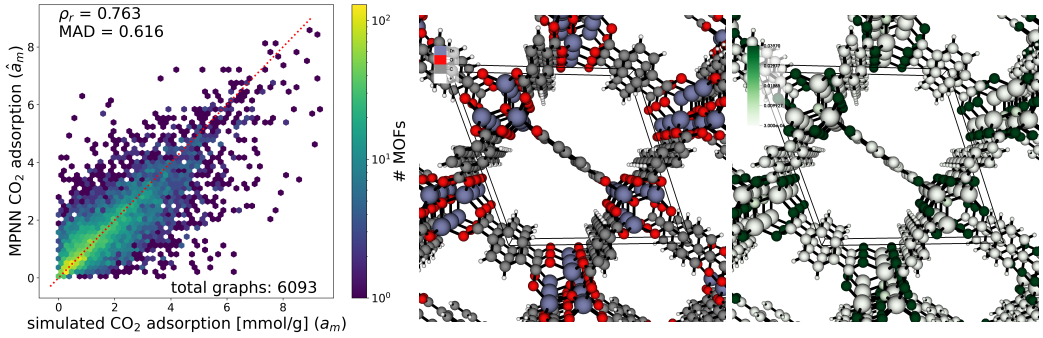
	mean (std)			
Method	**MAD**	**MSE**	ρ_r	Entropy (sparsity)
MPNN (softmax)	0.616 (0.03)	0.868 (0.10)	0.764 (0.02)	0.78 (0%)
MPNN (sparsemax)	0.666 (0.04)	1.000 (0.11)	0.732 (0.02)	0.45 (94%)
MPNN (L0.5, $\lambda = 0.001$)	0.645 (0.02)	0.933 (0.08)	0.743 (0.01)	0.72 (0%)
MPNN (L0.5, $\lambda = 0.05$)	0.737 (0.04)	0.1.174 (0.13)	0.684 (0.04)	0.32 (0%)

Table 1: Prediction performance and attention sparsity by different methods. Mean and standard deviation (std) over 10 folds.

We use the mean absolute deviation (MAD) loss function $\ell = \frac{1}{M}\sum_{m=1}^{M} ||\hat{a}_m - a_m||_1$ to train our network within $K = 10$-fold cross validation, where M is the total number of MOFs, $\hat{a}_m$ is the predicted CO_2 adsorption of MOF m predicted by the MPNN by eqn. 5, a_m is the simulated CO_2 adsorption (treated as ground truth) and $||\cdot||_1$ is the L1 norm. Through hyperparameter exploration, we settled on $r = 10$, $k = 70$, and $T = 4$. Tab. 1 summarizes the performance of our model using the mean absolute deviation (MAD), mean square error (MSE), Spearman's rank correlation coefficient, ρ_r, and normalized entropy of the attentions (1 for uniform attention across all nodes and 0 for all attention concentrating on one node). Vanilla `softmax` is able to achieve the best MAD performance. Fig. 2a shows a parity plot, using softmax, for the test MOFs during the cross-validation procedure. Sparsemax introduced substantial sparsity in the attention scores ($\%94$ of the attention scores are zero); however, there is no way to control the sparsity. Using Quasi-norm L(0.5) regularisation produces a less uniform attention distribution, but with a price of slightly higher MAD. The regularization parameter, λ, enables us to trade-off training set accuracy with sparsity. Smaller entropy ($\lambda = 0.001$ to 0.05) results in less accuracy (MAD = 0.645 to 0.737).

4 Discussion: towards explainability

We include the attention score α_v as a step towards an MPNN with explainable predictions. If α_v is large, the hidden representation of node v had a significant contribution to the graph representation $\mathbf{r}$ used to predict adsorption, a. Fig. 2c visualizes the attention of each node in a MOF as an example. The local bonding environments of the darker atoms contributed more to the final graph representation used for the prediction task than the lighter atoms.



(a) (b) (c)

Figure 2: (a) Parity plot for the MPNN (softmax), showing the MPNN-predicted vs. simulated CO_2 adsorption, including every MOF in the data set when it served as a test MOF in cross validation. Diagonal line shows equality. (b, c) Visualization of MOF IRMOF-1, where color indicates (b) the identity of the atom and (c) the attention score α_v on the atom using the MPNN (softmax). Black boxes = unit cell.

Our inspection of the attention scores across different MOFs did not yield any clear insight or chemically meaningful patterns. This leads us to believe that the attention score is not as meaningful as we have hoped for identifying important substructures. we further believe this is due to (i) $\mathbf{h}_v^{(T)}$ of node v is enriched with information from all nodes within T steps from node v via message

passing; (ii) neighboring nodes tend to have strong similarity; and (iii) the attention scores do not necessarily reflect the importance of node v for the predicted adsorption [52]. Therefore, we are currently working to redesign the MPNN to short-circuit message passing, isolate the individual contributions of the nodes, and rigorously lend more explainability of the prediction.

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