

Task 4: Discovering Future Solar Energy Materials

Pretraining feature representations

In lecture, you have learned about training neural network autoencoders. An autoencoder consists of an encoder f and a decoder g , which are jointly optimized to model the identity function:

$$\mathbf{x} \approx g(f(\mathbf{x}; \theta); \phi) \quad (1)$$

Because the vector $\mathbf{z} = f(\mathbf{x}; \theta)$ usually has a lower dimensionality than \mathbf{x} , the autoencoder learns an efficient lower dimensional *feature representation* for \mathbf{x} . This is an *unsupervised* technique because it allows learning from unlabelled data samples $\{\mathbf{x}_n\}$, e.g., images without their associated ground truth class label. The feature representation $f(\mathbf{x}; \theta)$ may prove useful in related tasks, where we work with the same inputs \mathbf{x} but need to predict a quantity y about \mathbf{x} .

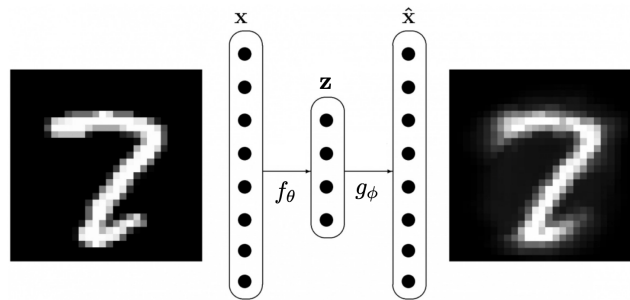


Figure 1: Unsupervised training of a feature representation $f(\mathbf{x}; \theta)$

In this task, we not only have access to an unlabelled data set $\{\mathbf{x}_n\}$ that we can leverage, for instance, using an autoencoder. Instead, we have *labeled* data $\{(\mathbf{x}_n, y_n)\}$, and while the quantity y is different from our quantity of interest y^* , it is highly related. Thus, a good feature representation for predicting y is likely also useful for predicting y^* , and more so than using only unlabelled data $\{\mathbf{x}_n\}$. For example, we can train an encoder f and a final predictor h to approximate y :

$$y \approx h(f(\mathbf{x}; \theta); \phi) \quad (2)$$

As with the autoencoder, we can use the *pretrained* feature extractor $f(\mathbf{x}; \theta)$ in a related task.

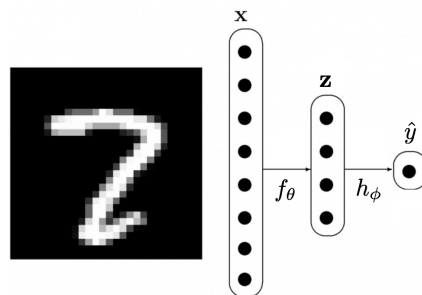


Figure 2: Supervised training of a feature representation $f(\mathbf{x}; \theta)$