HEP(e)xML

Introduction to Un- and Semi-Supervised Learning for Undergraduates

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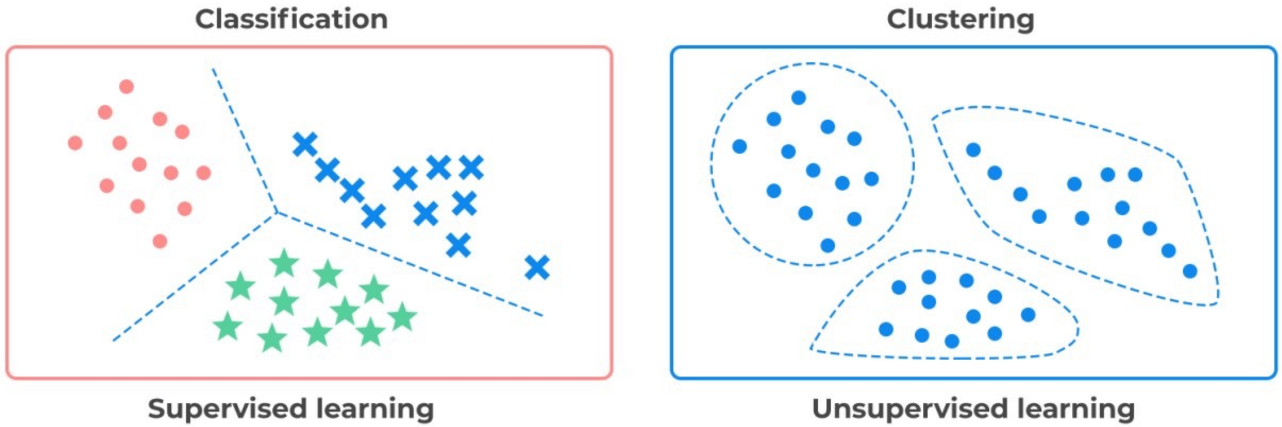
Overview

We'll go over a few key concepts in the lecture, including

- **Definitions** of un-supervised/semi-supervised learning
- **Examples** of tasks amenable to this type of learning
- **Implementations** of a few of the simplest algorithms

This lecture will assume you have attended and understood the previous series in the lectures!

Unsupervised Learning



- Unlike the ML we have done up to this point, unsupervised ML **does not use labels** in the learning process
- This means that it is most useful for unlabeled data, and is typically used for
  - **Dimensionality reduction** of a big dataset
  - **Clustering** of previously unorganized data points
  - **Association** of variables in a dataset

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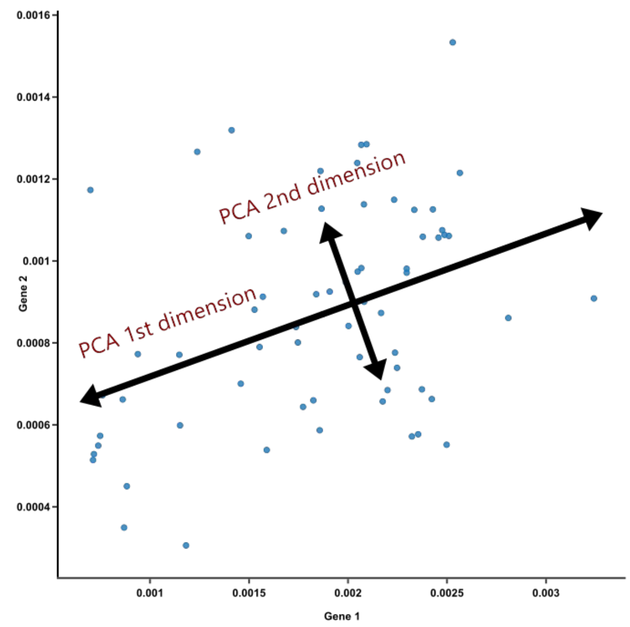
Unsupervised Learning: Dim. Reduction

- A host of non-neural dimensionality reduction techniques already exist
- These include **Principal Component Analysis**
  - This is done by projecting the dataset onto the **n** top eigenvectors of the covariance matrix, sorted by their total variance
  - This amounts to transforming the coordinates such that the greatest variance is on the 1st axis, second greatest on the 2nd, etc.
  - Then, the remaining vector may be truncated
- There is also **Singular Value Decomposition**, which uses a similarly non-neural method



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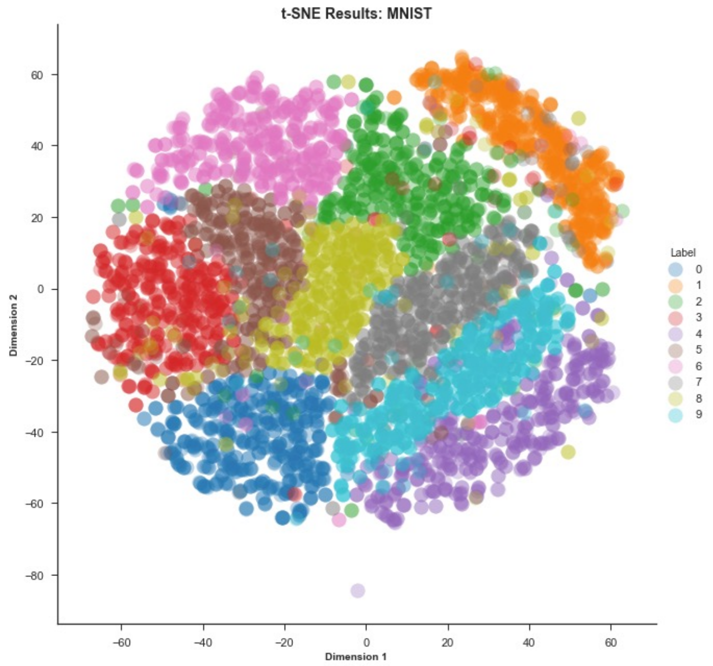
Unsupervised Learning: Dim. Reduction

- There are also neural approaches to dimensionality reduction
- One very popular method currently is **t-SNE**
  - This first estimates a probability distribution for the high dimensional samples
  - Then, defines a similar distribution for the points in the low-dimensional embedding
  - Lastly, minimizes KL-divergence between the distributions
- Figure at right shows the differences between MNIST figures for TSNE, which TSNE is very good at



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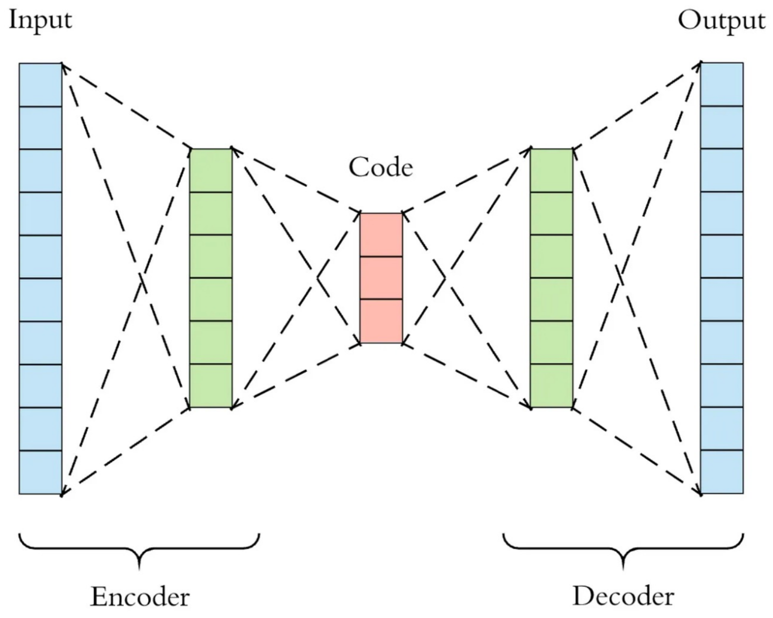
Unsupervised Learning: Autoencoders

- Autoencoders (AEs) also work well for dimensionality reduction
- Generally, AEs are a method of reconstructing the inputs, under the influence of some **constraint**
- For a neural autoencoder, this constraint is in the dimension of the bottleneck node



- These can be used for **anomaly detection** in physics by taking their **reconstruction error** (difference in input/output) and using this as an **anomaly score**

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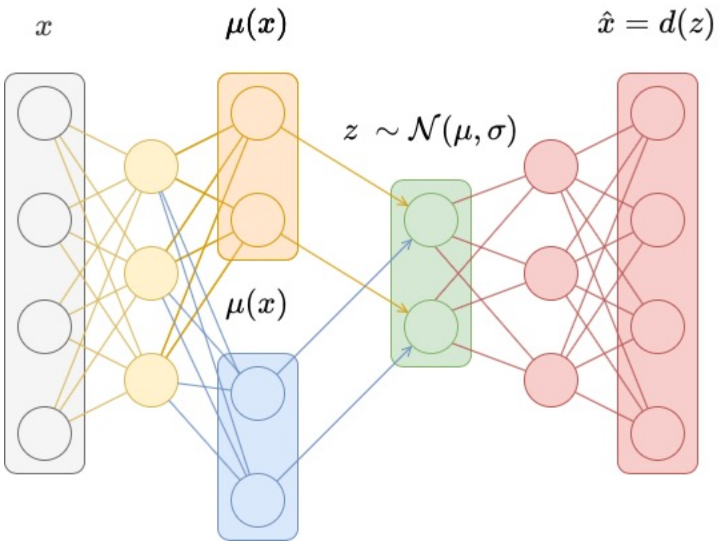
Unsupervised Learning: Variational AEs

- Variational AEs are similar to neural AEs, except that their bottleneck structure includes some **variational** component



- This means that the latent space is constructed by sampling from a **normal distribution** with parameters specified by the internal layers of the AE (z-layer in figure)
- Then, we include a term in the loss function of the AE which minimizes the difference in the latent space distribution from an N-dimensional unit gaussian
- We do this with the [Kullback-Leibler divergence]

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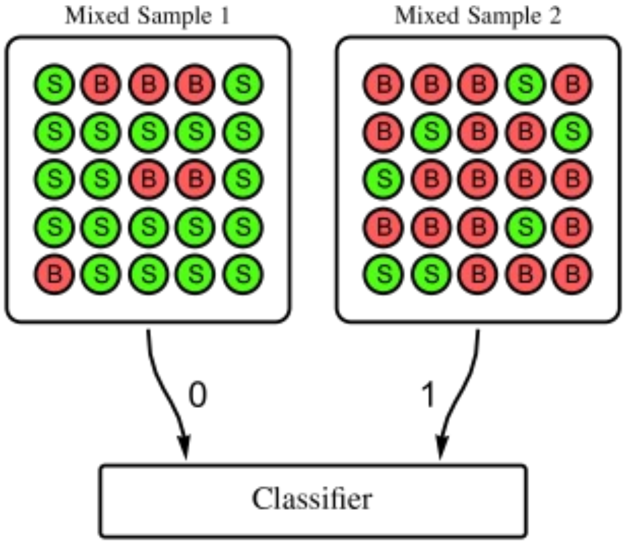
Semi-Supervised Learning: CWoLa

- For physics anomaly detection, we focus on semi-supervised algorithms which have the potential to find signals given weak constraints
- One algorithm which does this is Classification Without Labels (CWoLa)



- CWoLa works by training a classifier to distinguish between a signal region (SR) and a sideband region (SB)
- In the case where the SR has significant differences from the SB due to signal, CWoLa is effective at finding hard-to-detect signals

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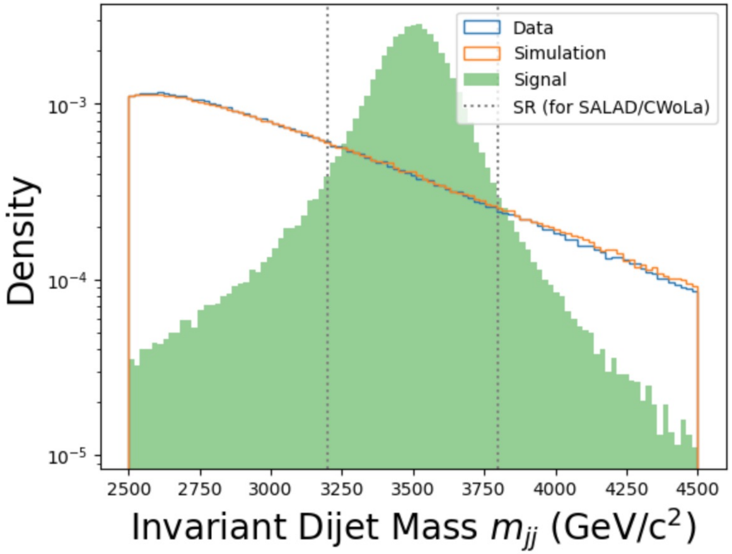
Semi-Supervised Learning: CWoLa

- In practice, this is done by identifying some **resonant feature**, typically mass-related
- Example: many new-physics signals may be resonant in the spectrum of their total mass (i.e. higgs)



- In this case an effective search could scan across the mass spectrum, training classifiers to distinguish between SR/SB
- If a signal doesn't exist in a given SR/SB region, nothing will be found
- If a signal does exist, CWoLa will find it! (ideally)

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Semi-Supervised Learning: CWoLa

- Such a search is referred to as "weakly-supervised," because we are specifying a mass resonance, but nothing else about the signal.
- The more precisely we specify the signal region, the stronger the supervision is.
- Eventually we will just reach supervised classification (i.e. all of our signal properties are specified, so we are training signal vs. background effectively)

Implementing CWoLa:

- During the tutorial, we will do this as an exercise!
- The algorithm is a **simple neural network**, but trained to tag SR vs SB region data.
- To evaluate, we use the truth tags of the data.

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Other models

- There are a slew of other unsupervised models used for new physics discovery
- Many of these have to do with modeling the **density** of a dataset, and identifying events which lie outside of this
- The **2020 LHC Olympics paper** provides an excellent overview of models and their new-physics search efficacy
- A few good ones:
  - **Normalizing flows** are excellent density estimators
  - **Reweighting** of simulation to data can be used to estimate exact SR features for data, improving CWoLa
  - Graph/convolutional autoencoders

Next: tutorial!

[Click here to be taken to the tutorial Colab]

[Solutions (boo)]