Unsupervised Learning

We have thus far focused on *Supervised Learning* where we are given training set

$$\langle \mathbf{X}, \mathbf{y} \rangle = [\mathbf{x^{(i)}}, \mathbf{y^{(i)}} | 1 \leq i \leq m]$$

and we wish to construct a function to map from arbitrary feature vectors $\mathbf{x}$ of length n to some target/label $\mathbf{y}$.

We now switch to *Unsupervised Learning* where we are given

$$\mathbf{X} = [\mathbf{x^{(i)}} | 1 \leq i \leq m]$$

That is: feature vectors *without* associated target/labels.

This may feel somewhat strange ? What can we do given only features ?

Quite a bit ! Learning relationships *between* features enables us to

- Make recommendations based on similarity to other examples
- Enables us to visualize the data and discover relationships among examples
- Filter out "noise" or low information features

For example: from the perspective of some companies **you** are a feature vector !

- Several thousand attributes that define your past behavior
    - Purchases
    - Books read, movies viewed (one feature per book/movie)
    - Music, food preferences
    - Activities, hobbies

- Sparse vector
    - You've seen only a small fraction of the thousands of possible movies (one feature per movie)
- "You may also like" recommendation
    - The relationship between features among the training examples
    - Supports an association between a subset of features that are defined for you
    - And other features (movies/products) that are not yet defined for you

Dimensionality reduction

Discovering the relationship among features can facilitate a more compact representation of feature vectors.

Let

$$\mathbf{x}_j = [\mathbf{x}_j^{(\mathbf{i})} \mid 1 \leq i \leq m] \text{ for } 1 \leq j \leq n$$

denote the values of feature j among the m examples in the training set.

- So $\mathbf{x}_j$ is a vector of length m.

Is it possible that many $(\mathbf{x}_j, \mathbf{x}_{j'})$ pairs are highly correlated ($j' \neq j$)?

Dimensionality reduction is the process of representing a dataset

- That has n raw features
- With $n' << n$ synthetic features
- While retaining *most* of the information

Examples

Color 3D object to Black/white still image

- Lose Depth, Color dimensions
  - Spatial dimensions $(1000 \times 1000 \times 1000)$
  - Color dimension: 3
  - $n = 1000 * 1000 * 1000 * 3$
  - $n' = 1000 * 1000 = \frac{n}{1000*3}$

For the purpose of recognizing the object, little information is lost

Equity time series

Consider an equity index (e.g., the S&P 500) of $n = 500$ stocks

- An example $\mathbf{x^{(i)}}$ is a vector of daily returns of length $n = 500$
- $\mathbf{x}_j^{(\mathbf{i})}$ is the daily return of stock j on day i
- $\mathbf{x}_j$ is the *timeseries* of daily returns of stock j
- $\mathbf{x}_j, \mathbf{x}_{j'}, j \neq j'$ can be correlated
    - All stocks in the "market" tend to move up/down together
    - Daily returns of stocks with similar characteristics tend to be more similar than for stocks with differing characteristics
        - Industry, Size

One way to interpret the high mutual correlation among equity returns

- There are *common influences (factors)* affecting many individual equities
- Pair-wise correlation of equity returns (i.e., features) arises through influence of the shared factors

We can write this mathematically:

Let $\tilde{\mathbf{x}}_{\text{index}}$ be the time series of daily returns of a factor ("the market") that affects *all* equities

$$\begin{aligned}
\mathbf{x}_1 &= \beta_1 * \tilde{\mathbf{x}}_{\text{index}} + \epsilon_1 \\
\mathbf{x}_2 &= \beta_2 * \tilde{\mathbf{x}}_{\text{index}} + \epsilon_2 \\
&\vdots \\
\mathbf{x}_{500} &= \beta_{500} * \tilde{\mathbf{x}}_{\text{index}} + \epsilon_{500}
\end{aligned}$$

The daily return of each of stock j in the index is decomposed into

- The daily return associated with factor $\tilde{\mathbf{x}}_{\text{index}}$: $\beta_j * \tilde{\mathbf{x}}_{\text{index}}$
- A daily return ϵ_j that is stock-specific

Note that we have actually *increased* the number of features

- From n
    - $\mathbf{x}_j$ for $1 \leq j \leq n$
- To $(n+1)$
    - $\tilde{\mathbf{x}}_{\text{index}}$
    - ϵ_j for $1 \leq j \leq n$

But, by adding a few more factors (similar to $\tilde{\mathbf{x}}_{\text{index}}$ but perhaps influencing the returns of a subset of equities)

- We can make the magnitude of the daily stock specific part ϵ_j approach 0
- To the point of that we can drop features ϵ_j for $1 \leq j \leq n$
- And have a model with only a handful of features: the factors

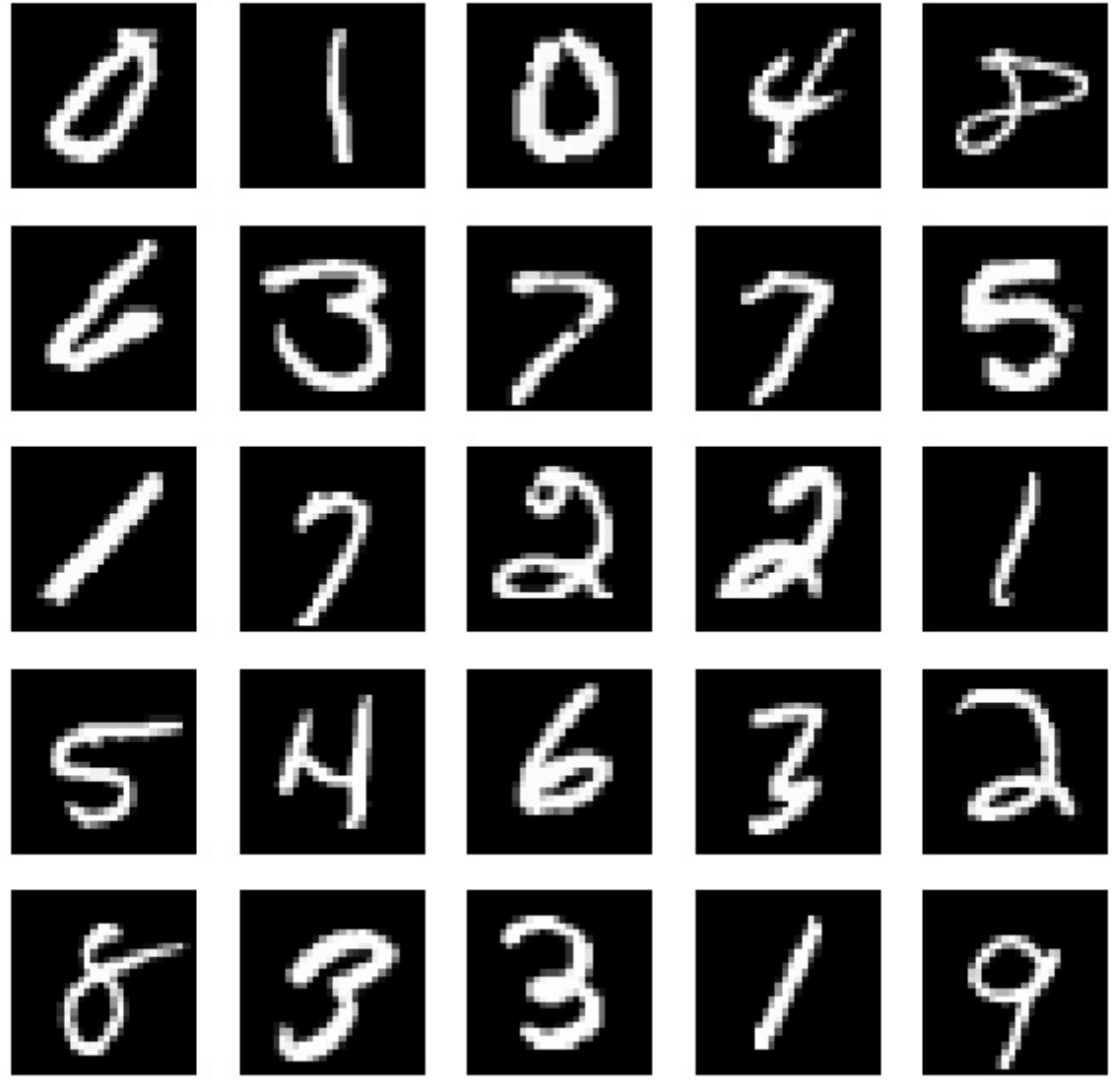
Representing MNIST digits with 20% of the information

We will subsequently show how to represent the MNIST digits ($n = 784$) with vectors of length $n' \approx 150$

Here's what happens when

- We encode the digits with vectors of length n'
- Perform the inverse mapping back to vectors of length n so we can display as a (28×28) image

PCA: reconstructed MNIST digits (95% variance)



The reconstructed images are a little blurry (compared to the originals) but still very recognizable.

So it *is possible* to represent the information of the raw 784 features with only 20% (≈ 150) as many synthetic features.

In other words: 80% of the pixels may be somewhat redundant.

Where are the correlated features in images of digits?

Consider the examples consisting of the (28×28) pixel grids representing the MNIST digit dataset.

Here are some cases to consider:

Let j, j' be indices of two pixels in one of the 4 corners of the (28×28) grid

- Most pixels in the corners are the same (background) colors so the correlation of $\mathbf{x}_j$ and $\mathbf{x}_{j'}$ is high

Let j, j' be indices of two pixels that lie in a vertical line in the center of the (28×28) grid

- They will be somewhat correlated because they have the same value in 10% of the images
    - Corresponding to images of digit "1"

Uses of dimensionality reduction

Feature Engineering

If n is large and many features are mutually correlated

- A reduced number $n' << n$ of synthetic features
- Obtained by dimensionality reduction techniques
- May result in better models
    - Some models, like Linear Regression, may be sensitive to correlated features (collinearity)

Clustering

Dimensionality reduction can facilitate an understanding of the structure of examples.

Consider: Are the m examples in the training set

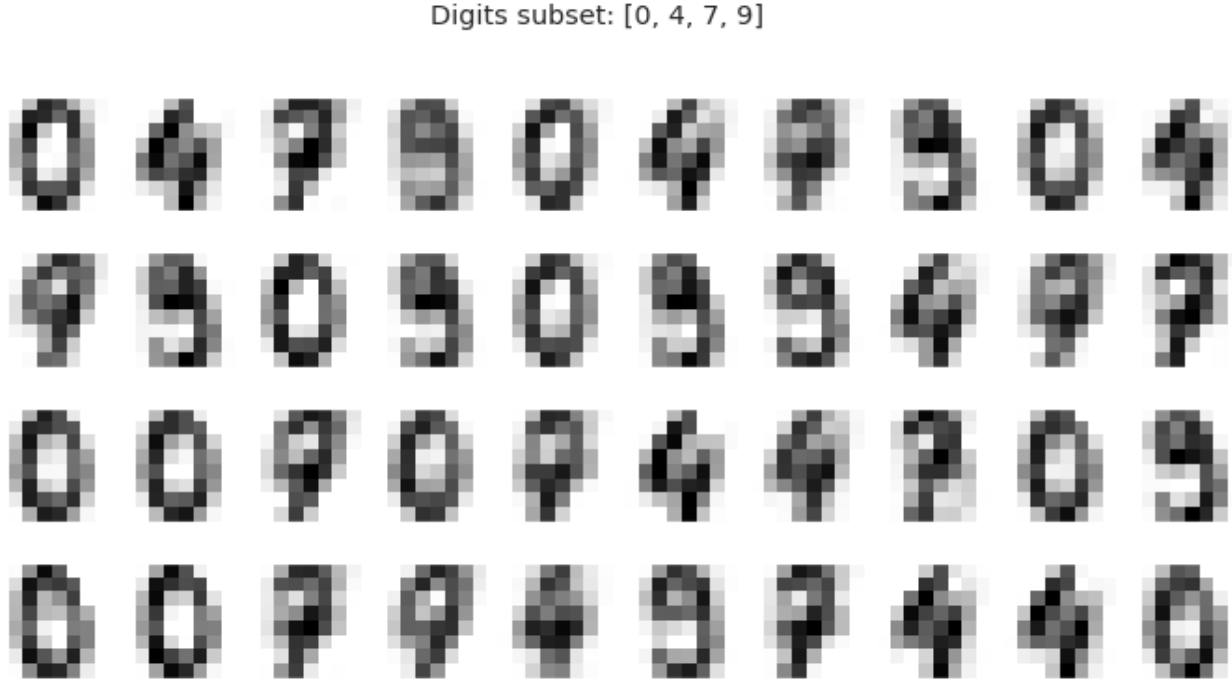
- Uniformly distributed across the n dimensional space ?
- Do they form *clusters* of examples with similar feature vectors ?

Unfortunately: it's hard to visualize n dimensions when n is large.

- By reducing the number of dimensions
- We may be able to visualize related examples
- In such a way that the reduced dimension examples don't lose too much information

Let's illustrate with a limited subset of the smaller (8×8) digits.

8 x 8 digits, subset



It would be difficult to visualize an example in $n = (8 * 8) = 64$ dimensional space.

By transforming each example to a smaller number ($n' = 2$) of synthetic features we *can* visualize

- Each example as a point in two dimensional space

8 x 8 digits, subset clusters

You can see that our $m \approx 700$ examples form 4 distinct clusters.

- The clusters were formed
    - Based solely on features

It turns out that the clusters correspond to examples mostly representing a single digit.

- The clusters organized themselves based on similarity of features
- This is unsupervised ! No targets were used in forming the clusters!
- We use the hidden target merely to color the point, not to form the clusters

This hints that dimensionality reduction may be useful for *supervised* learning as well

- Use commonality of features to reduce dimension
- Reduced dimensions more independent
    - Better mathematically properties (reduced collinearity)
    - More interpretable
- Under assumption that
    - Examples with similar features (i.e., in same cluster) have similar targets

Noise reduction

Consider

- The MNIST example, where we reduced n by 80% without losing visual information.
- The equity return example, where the stock specific return ϵ_j became increasingly small

Both examples suggest that there are many features

- With small significance
- Or that represent "noise" In the latter case, dropping features actually improves data quality by eliminating irrelevant feature.s

In [5]:
```
print("Done")
```

```
Done
```