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

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

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

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

(i.e., $\mathbf{X}_j$ denotes a column of $\mathbf{X}$; feature j across all examples)

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 2D 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 daily observations of all tickers in an equity index (e.g., the S&P 500) of $n = 500$ stocks

Dataset $\mathbf{X}$

- row dimension: date
    - $\mathbf{X}^{(\mathbf{i})}$ (Row i of $\mathbf{X}$) corresponds to one day of returns, across all n stocks
- column dimension: stock ticker
    - $\mathbf{X}_j$ is the *timeseries* of daily returns of stock j
- $\mathbf{x}_j^{(\mathbf{i})}$ is the daily return of stock j on day i

It is common to observe that the timeseries of two tickers j, j' are 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

Thus, $\mathbf{X}_j, \mathbf{X}_{j'}, j \neq j'$ are correlated

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 return timeseries $\mathbf{X}_j$ of each stock j in the index is decomposed into

- The return timeseries associated with factor $\tilde{\mathbf{X}}_{\text{index}}$: $\beta_j * \tilde{\mathbf{X}}_{\text{index}}$
- A return timeseries ϵ_j that is stock-specific
- the return of j at time i is
$$\mathbf{x}_j^{(\mathbf{i})} = \beta_j * \mathbf{x}_{\text{index}}^{(\mathbf{i})} + \epsilon_j^{(\mathbf{i})}$$

Note

We can obtain the β's via Linear Regression

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 another factor

- e.g., a "size" factor
- similar to $\tilde{\mathbf{X}}_\text{index}$ in that it influences all equities

$$
\begin{aligned}
\mathbf{X}_1 &= \beta_{1,\text{idx}} * \tilde{\mathbf{X}}_\text{index} + \beta_{1,\text{size}} * \tilde{\mathbf{X}}_\text{size} + \epsilon'_1 \\
\mathbf{X}_2 &= \beta_{2,\text{idx}} * \tilde{\mathbf{X}}_\text{index} + \beta_{2,\text{size}} * \tilde{\mathbf{X}}_\text{size} + \epsilon'_2 \\
\vdots \\
\mathbf{X}_{500} &= \beta_{500,\text{idx}} * \tilde{\mathbf{X}}_\text{index} + \beta_{500,\text{size}} * \tilde{\mathbf{X}}_\text{size} + +\epsilon'_{500}
\end{aligned}
$$

the magnitude of the stock-specific ϵ'_j *decreases* compared to the original ϵ_j

- some of the return previously attributed to ϵ_j
- has been explained by $\beta_{j,\text{size}} * \mathbf{X}_\text{size}$

As we add even more factors

- some may be specific to *sub-sets* of the universe
    - where $\beta_{j,\text{size}} = 0$ when ticker j is not part of the sub-set
    - e.g., industry factors
- the stock-specific ϵ series approaches 0

Once this occurs

- we can drop the ϵ
- and have a model with many fewer factors than n

We thus obtain an approximation of

- the effect of $n = 500$ features (i.e., 500 daily returns)
- using only n' features (the factors)
    - with $n \gg n'$

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)
    - more explainable (fewer factors) models

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 ?

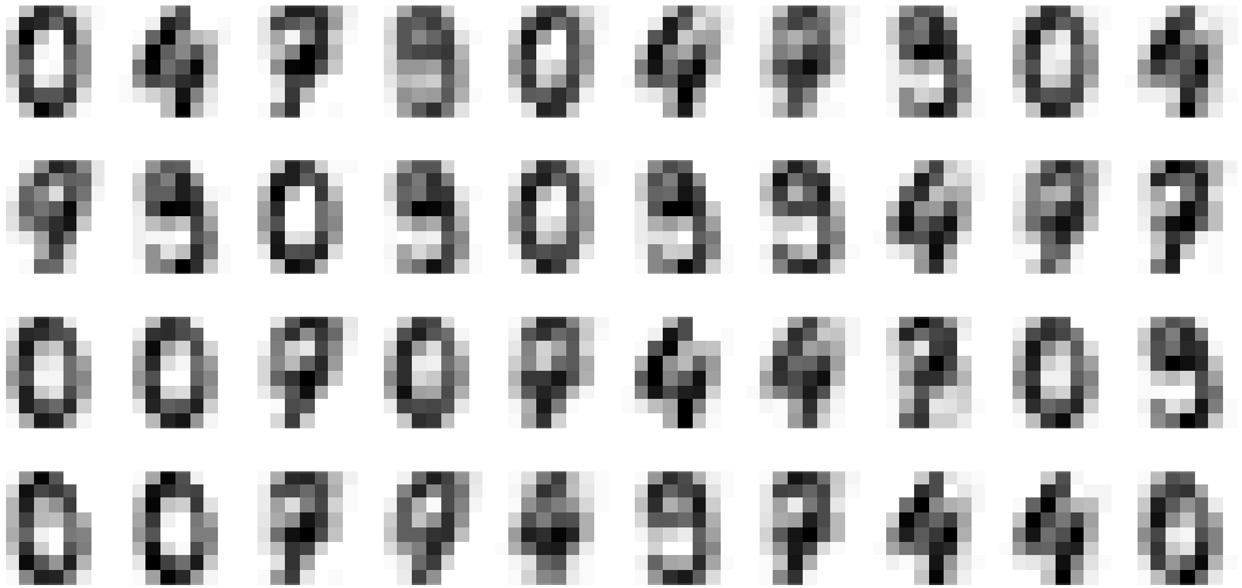
Unfortunately: it's hard to visualize n dimensions when n is large.

- 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

Digits subset: [0, 4, 7, 9]



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

We can only see this

- because we have reduced dimensionality from 64 to 2

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

The reduced dimensions may

- capture salient properties ("semantics") of the example
    - rather than surface properties (pixels, "syntax")

For example: notice that

- low values of Component 1 are associated with the digits 4 and 7
    - is there some property common to these digits ? Strong vertical section maybe ?
- interpreting the meaning of synthetic features will be discussed subsequently

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]:

```python
print("Done")
```

```
Done
```