Material Summary: Dimensionality Reduction

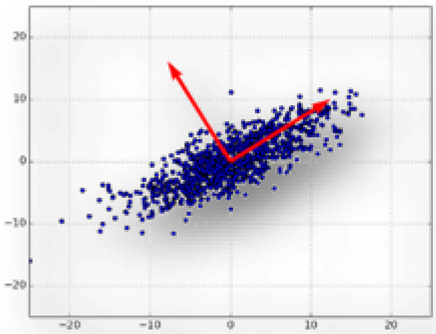
1. Dimensionality Reduction

1.1 Principal Component Analysis (PCA)

- A **non-parametric** technique for feature extraction
  - Transforms all variables so they are **linearly independent**
    - Note that this is a linear transformation
- The transformation is done to increase the explained variance in the data
- Number of principal components (PC): $p = \min(m, n)$
  - m – number of features, n – number of observations
  - Sorted from highest to lowest explained variance
  - Sorted from highest to lowest explained variance
- Most widely used practical application
  - Load a high-dimensional dataset with m features
  - Perform PCA, remove last k components
    - Result: dataset with $m - k$ features
    - Note that these **are not** $m - k$ of the original columns!

1.2 PCA Intuition

- There is a lot of math (and even physics) involved
- Intuitive explanation: casting a shadow
  - Projection into a lower-dimensional space
    - A nice *visualization* of PCA
- Example: 2D
  - The first principal component aligns with the axis of most variance in the data
  - The second is perpendicular to the first
    - **All components** are mutually orthogonal
      - I.e., linearly independent



- Result: The red arrows represent a new coordinate system
  - Also: if we drop the second coordinate, we've achieved dimensionality reduction without too much loss of information

1.3 Example: PCA in scikit-learn

- Reproduce the 2D example
  - Generate a blob
  - Use a shear transformation to make it look like a rotated ellipse
    - You can look up how to do this, for example in Wikipedia
  - Plot the original data, after the transformation
  - **Rescale the data**
    - This is **really important** in PCA, otherwise columns with large values will dominate in the PCs
  - Fit a PCA and apply the learned transformation to the original data

```
from sklearn.decomposition import PCA
pca = PCA().fit(data)
transformed_data = pca.transform(data)
```

  - Plot the transformed data
  - Plot the explained variance ratios of the various components

1.4 Kernel PCA

- As we saw, PCA only works for linear transformations

- We can obtain non-linear transformations using the "kernel trick"
  - Just like in SVMs
- This allows us to separate non-convex and non-linear data
  - Such as nested circles
  - As before, we need to set the gamma parameter
    - Width of the kernel (in the case of rbf)
    - If we don't know the exact value, we need to perform grid search
- *Docs* (note how linear PCA doesn't separate the data)
- Usage

```
from sklearn.decomposition import KernelPCA
pca = KernelPCA(kernel = "rbf", gamma = 5).fit(data)
transformed_data = pca.transform(data)
```

1.5 Linear Discriminant Analysis (LinDA)

- LinDA is a **supervised method** which tries to identify the attributes that account for the most variance between classes
  - Used in classification cases, with known class labels
  - Returns a transformation of the input data, like PCA
- *Comparison of 2-component PCA and LinDA* on the Iris dataset

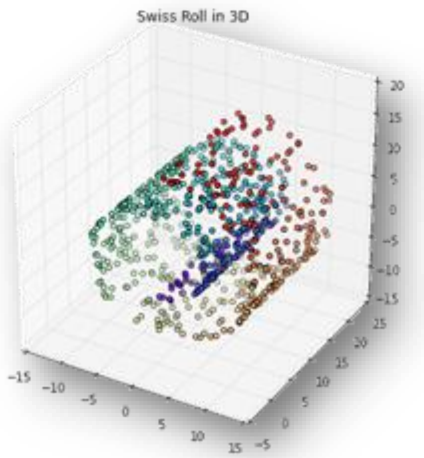
```
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
lda = LinearDiscriminantAnalysis(n_components = 2)
transformed_attributes = lda.fit(attributes, labels).transform(attributes)
```

- Linear Discriminant Analysis and Latent Dirichlet Allocation **have the same acronyms**, and are both used for dimensionality reduction / transformation
- They work in completely different ways

2. Manifold Learning

2.1 Problem Definition

- Manifold = surface / shape (not necessarily a plane)
- Idea
  - The dimensions are only artificially high
  - Even though there are many features, they can be expressed with a few parameters
    - "Low-dimensional manifold in a high-dimensional space"
    - Non-linear methods
- Example: "swiss roll" dataset
  - 2D "curled" shape in 3D
- Used not only for dimensionality reduction, it's a common way to visualize high-dimensional datasets
  - Especially for classification cases



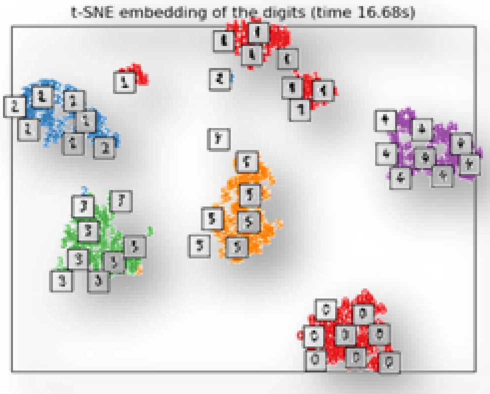
2.2 Isometric Mapping

- Seeks a lower-dimensional projection (embedding) which preserves distances between points
- Algorithm overview
  - Find the k nearest neighbors of each point (kNN)
  - Construct a connectivity graph
    - Two points are connected if they're neighbors (from the first step)
  - Compute shortest paths (Dijkstra, Floyd – Warshall)

- Perform projection on the graph
    - Similar to PCA
- High-level overview: project a manifold using nearest neighbors

```
from sklearn.manifold import Isomap
isomap = Isomap(n_neighbors = 5, n_components = 2)
transformed_data = isomap.fit_transform(data)
```

2.3t-SNE



- **t**-distributed **S**tochastic **N**eighbor **E**mbedding
    - Isomap tries to "unfold" a continuous structure
        - This is also true for other algorithms (*comparison*)
    - t-SNE looks for local clusters in the data
        - Useful for revealing clusters and structure
- Usual implementation: Barnes – Hut (2D or 3D only)
    - To preserve high-dimensional structure, we need to initialize it with PCA (instead of randomly)
    - It can be slow
    - Mainly used for **visualization** in image and text processing

```
from sklearn.manifold import TSNE
tsne = TSNE(n_components = 2, init = "pca")
transformed_data = tsne.fit_transform(data)
```

3. Real-World Examples

3.1 Example: Iris Dataset

- Perform PCA on the Iris dataset
    - Use the results to perform feature selection
- Compare the results to isometric mapping and 2D t-SNE
    - Visualize the first 2 components in all three cases
- Choose a classifier and score it before / after PCA
    - E.g., random forest
    - In most cases, first components will give a lower score but the algorithm will perform much faster (fewer variables)
    - Don't forget to transform new incoming data!
- Compare results on the raw dataset, and on the isomap transformation

3.2 Example: Eigenfaces

- Dataset: *Labeled Faces in the Wild*
    - Included in scikit-learn
- *Example*
    - Select only people with many images
        - In this case, ≥ 70
    - Use pixel values as raw inputs
    - Perform PCA to select the top 150 components (out of ~3000)
    - Use the PCA components to visualize "eigenfaces"

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Follow us:

```
eigenfaces = pca.components_.reshape((n_components, h, w))
# h, w are image height and width
```

    - I.e. to see each principal component as an image
  - Train and optimize an SVM
  - Perform classification

3.3 Example: Topics in Text

- Dataset: *20 Newsgroups*
  - Included in scikit-learn
- *Example* (LatDA and NMF)
  - LatDA – **Lat**ent **D**irichlet **A**llocation
    - Most widely-used algorithm for topic extraction
  - NMF – **N**on-negative **M**atrix **F**actorization
    - Simpler than LatDA, also used for topic extraction
- Preprocessing: counting words
  - "Bag of words" model
    - Matrix of how often each word occurs in each document
- Visualization of topics: top n words for each topic
- *LatDA and k-means clustering on the newsgroups*