Nonlinear Component Analysis as a Kernel Eigenvalue Problem

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  - PCA
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- Summary & Extension

PCA

- Invented by Karl Pearson, 1901*.
- Main idea
  - Convert a set of correlated variables linearly uncorrelated variables through orthogonal transformation
- Widely used for dimensionality reduction, feature extraction and data visualization

* https://en.wikipedia.org/wiki/Principal_component_analysis

PCA

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Algorithm 1 PCA in Feature Spaces

procedure PCA(X)
    given input: $X_{n \times m} \leftarrow \left[\mathbf{x}_1; \mathbf{x}_2; \cdots; \mathbf{x}_n\right]^T$
    de-mean (or standardize): $x_{ij} \leftarrow x_{ij} - \bar{x}_j \ or \ x_{ij} \leftarrow \frac{x_{ij} - \bar{x}_j}{s_j}$
    calculate covariance matrix: $Cov \leftarrow \frac{1}{n} X^T X$
    singular value decomposition (SVD): $[U, S, V] \leftarrow svd(Cov)$
    choose the first k eigenvectors: $E_{m \times k} \leftarrow \left[\mathbf{u}_1; \mathbf{u}_2; \cdots; \mathbf{u}_k\right]$
    project the test data $\mathbf{x}$: $\mathbf{p} \leftarrow E^T \mathbf{x}$
finish

* https://en.wikipedia.org/wiki/Principal_component_analysis

Kernel PCA

- Put forward by Scholkopf et al., 1998*
- Main idea
  - Expand the original feature space by non-linear transformations
  - Apply PCA in the transformed feature space
- Main drawback
  - Expanded feature space may have very high dimensions
  - Apply PCA is computationally expensive or even impossible
  - Solution -- Kernels

* Friedman, J., Hastie, T., & Tibshirani, R. *The elements of statistical learning.*

Expand the feature space

- Suppose we want to map $\vec{x}$ into a new space: $\phi(\vec{x})$
- $\vec{x}$ has d dimensions and $\phi(\vec{x})$ has m dimensions

$$m > d$$

- we need to calculate:
  - $\vec{x}\vec{x}^T$: complexity $O(d^2)$
  - $\phi(\vec{x})\phi(\vec{x})^T$: complexity $O(m^2)$
- What if $m \gg d$?
  - Solution: Kernels

“Kernel Trick”(1)

- **Example:**
  - $\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ and $\vec{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$
  - $\phi(\vec{x}) = \begin{bmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{bmatrix}$ and $\phi(\vec{y}) = \begin{bmatrix} y_1^2 \\ \sqrt{2}y_1y_2 \\ y_2^2 \end{bmatrix}$
  - Want to calculate: $\phi(\vec{x}) \cdot \phi(\vec{y}) = x_1^2y_1^2 + 2x_1x_2y_1y_2 + x_2^2y_x^2$
  - Define $\mathrm{k}(\vec{x}, \vec{y}) = (\vec{x} \cdot \vec{y})^2$
    - $\mathrm{k}(\vec{x}, \vec{y}) = x_1^2\, y_1^2 + 2x_1x_2y_1y_2 + x_2^2y_x^2 = \phi(\vec{x}) \cdot \phi(\vec{y})$

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- Important finding:
  - Complexity for $\mathrm{k}(\vec{x}, \vec{y})$ is still $O(d)$ instead of $O(m)$
- What’s next ?
  - Find some way to calculate $\mathrm{k}(\vec{x}, \vec{y})$ rather than $\phi(\vec{x})\phi(\vec{x})^T$

"Kernel Trick"(2)

- Covariance matrix:

$$C = \frac{1}{n}\sum_{i=1}^{m} \phi(\boldsymbol{x}_i)\phi(\boldsymbol{x}_i)^T$$

- Find eigenvalues and eigenvectors for:

$$\lambda \boldsymbol{v} = C\boldsymbol{v}$$

$$\lambda(\phi(\boldsymbol{x_k}) \cdot \boldsymbol{v}) = (\phi(\boldsymbol{x_k}) \cdot C\boldsymbol{v}) \text{ and } \boldsymbol{v} = \textstyle\sum_{i=1}^{n} \alpha_i \, \phi(\boldsymbol{x}_i)$$

- For kernel matrix K

$$K_{ij} = \left(\phi(\boldsymbol{x}_i) \cdot \phi(\boldsymbol{x}_j)\right)$$

$$n\lambda K\boldsymbol{\alpha} = K^2\boldsymbol{\alpha} \text{ or } n\lambda\boldsymbol{\alpha} = K\boldsymbol{\alpha}$$

- Projection for any given $\boldsymbol{x}$ on ith principal component

$$p_i(\boldsymbol{x}) = \sum_{j=1}^{n} \alpha_{ij} k(\boldsymbol{x}, \boldsymbol{x}_j)$$

Kernel PCA Algorithm

- Conclusion:
  - Only need to calculate the kernel matrix K
  - find the eigenvalues and eigenvectors for K

* Bishop, C. M. *Pattern Recognition and Machine Learning.*

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Algorithm 2 Kernel PCA

procedure K-PCA(X)

given input: $X_{n\times m} \leftarrow \left[\mathbf{x}_1; \mathbf{x}_2; \cdots; \mathbf{x}_n\right]^T$

calculate kernel matrix $K_{n\times n}: \ k_{ij} \leftarrow k(\mathbf{x}_i, \mathbf{x}_j)$

centralize $K : K' \leftarrow K - \mathbb{I}_n K/n - K\mathbb{I}_n/n + \mathbb{I}_n K \mathbb{I}_n/n^2$

calculate eigenvector $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \cdots, \boldsymbol{\alpha}_d$ according to: $n\lambda\boldsymbol{\alpha} = K'\boldsymbol{\alpha}$

normalize eigenvector according to: $n\lambda_i \boldsymbol{\alpha}_i^T \boldsymbol{\alpha}_i = 1$

project the test data $\mathbf{x}: \ p_i(\mathbf{x}) \leftarrow \sum_{j=1}^{n} \alpha_{ij} k(\mathbf{x}, \mathbf{x}_j)$

finish

Note: $\mathbb{I}_n$ stands for $n \times n$ matrix with all values equal to 1.

* Bishop, C. M. *Pattern Recognition and Machine Learning.*

Commonly Used Kernels*

- Polynomial kernel

$$K(x, y) = (\gamma x^T y + c_0)^d$$

- Radial basis function kernel (Gaussian or RBF kernel)

$$K(x, y) = \exp(-\gamma \|x - y\|^2)$$

- Sigmoid kernel

$$K(x, y) = \tanh(\gamma x^T y + c_0)$$

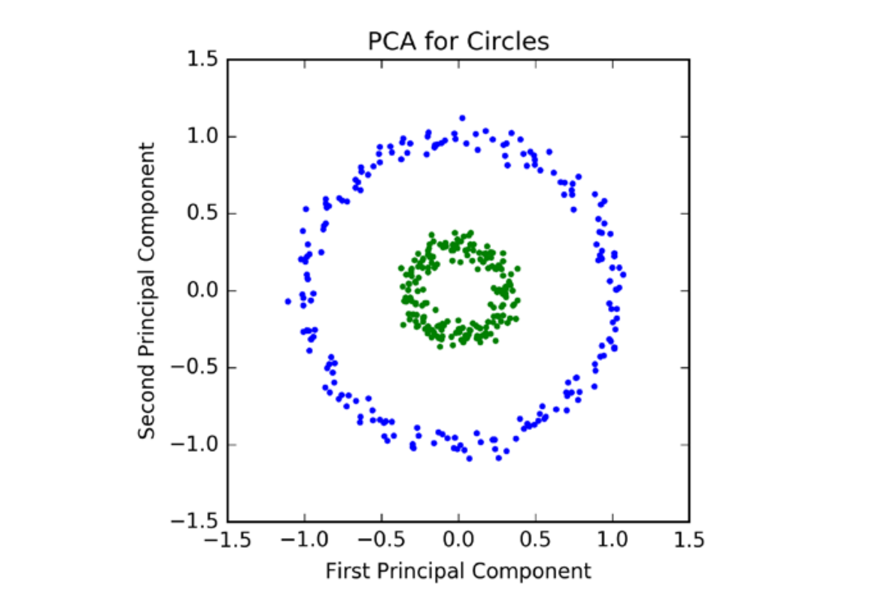
- Laplacian kernel

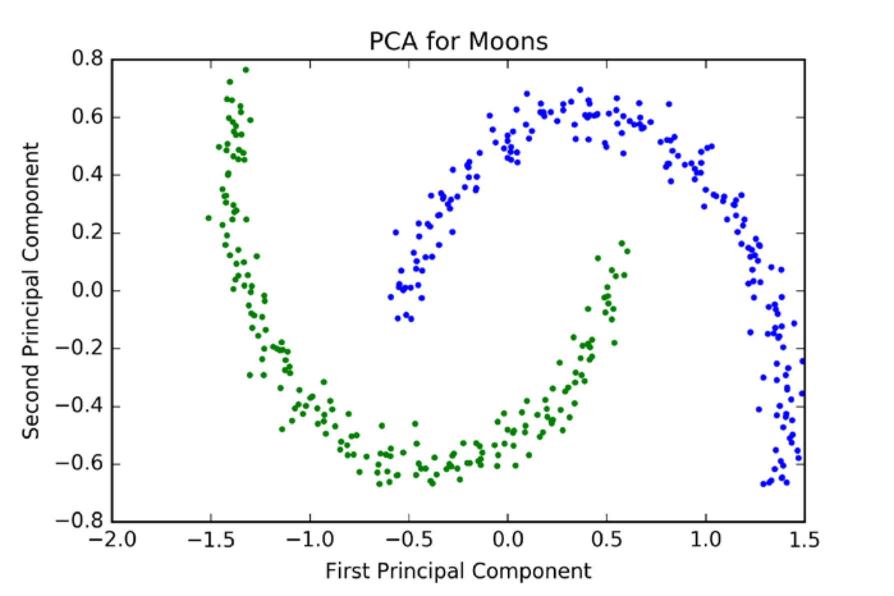
$$K(x, y) = \exp(-\gamma \|x - y\|_1)$$

- And so on.

* http://scikit-learn.org/stable/modules/metrics.html#metrics

Toy Examples





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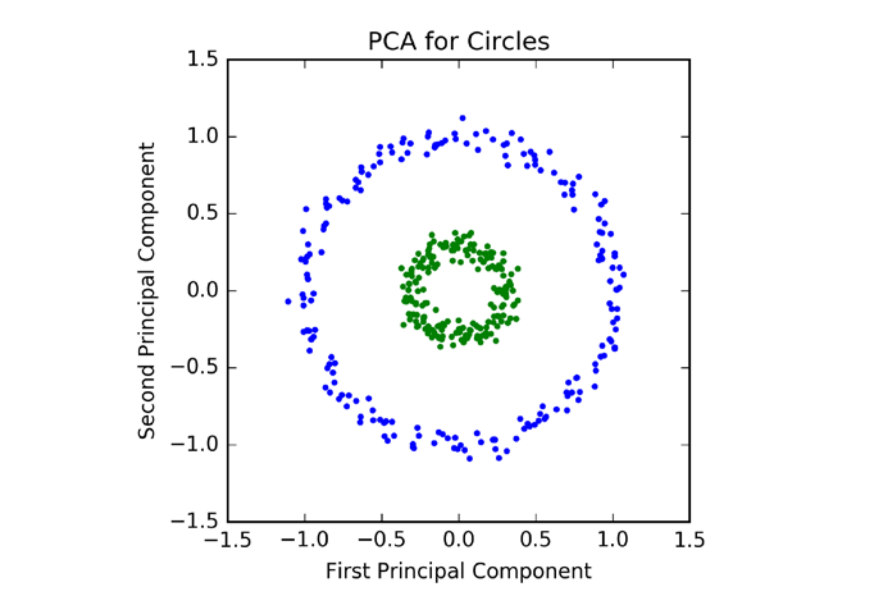
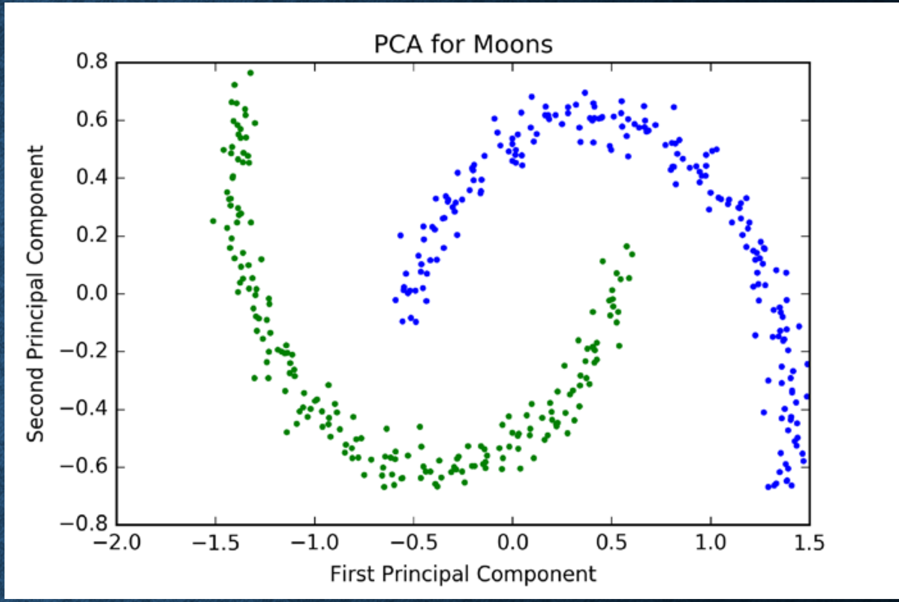
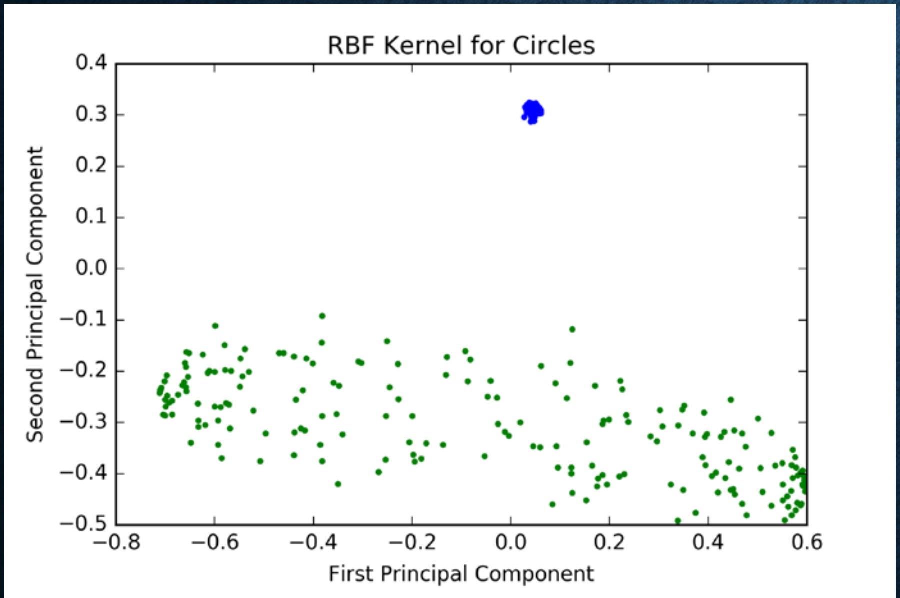
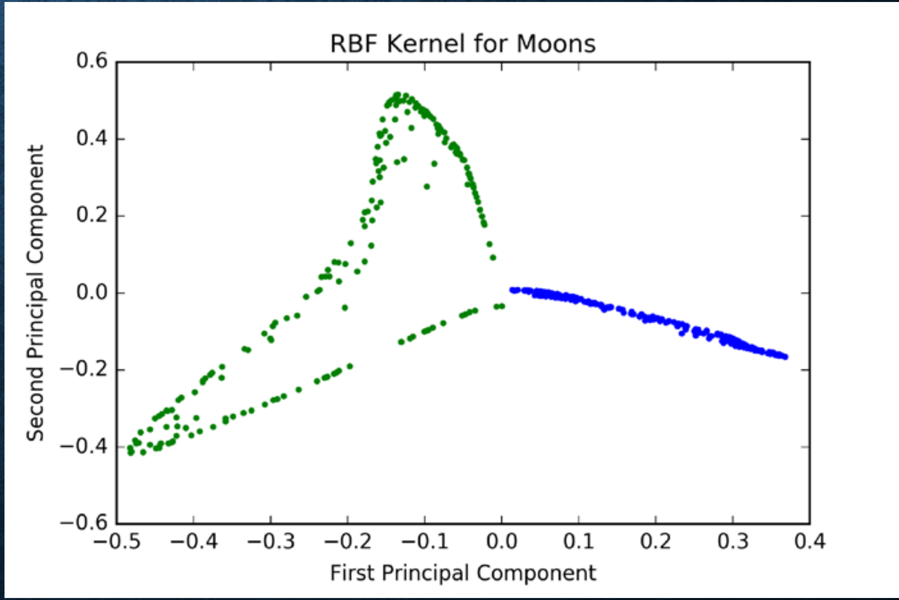






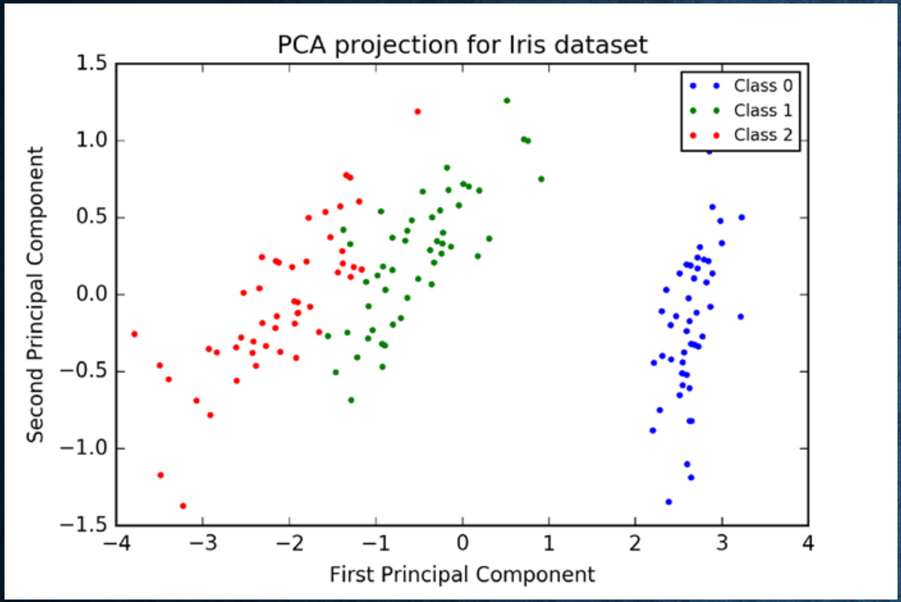


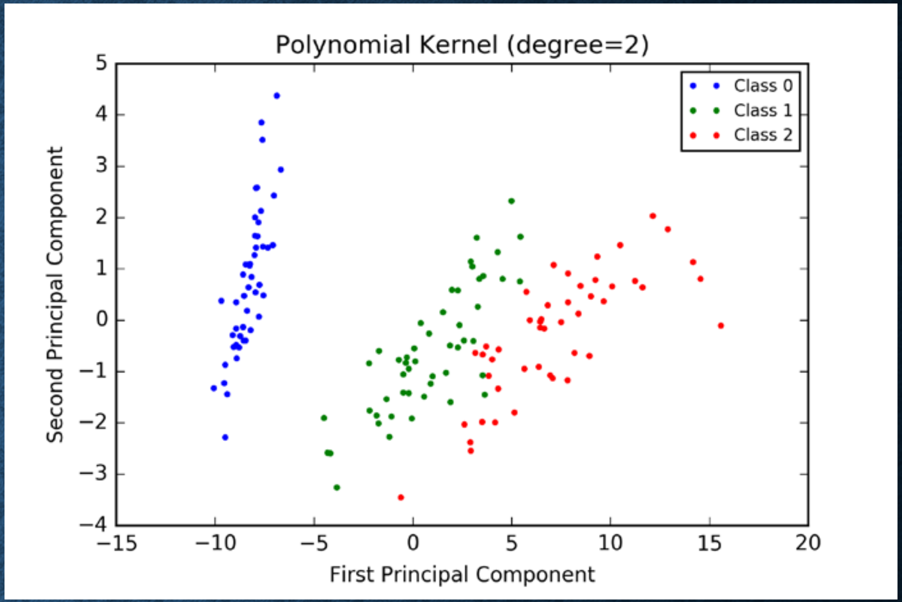
Iris Dataset – Introduction

- Iris flower dataset is introduced by Ronald Fisher (1936)*
- It contains 3 different types of irises (Setosa, Versicolor, and Virginica)**.
- The dataset has 150 records and each has 4 features:
  - Sepal Length
  - Sepal Width
  - Petal Length
  - Petal Width.

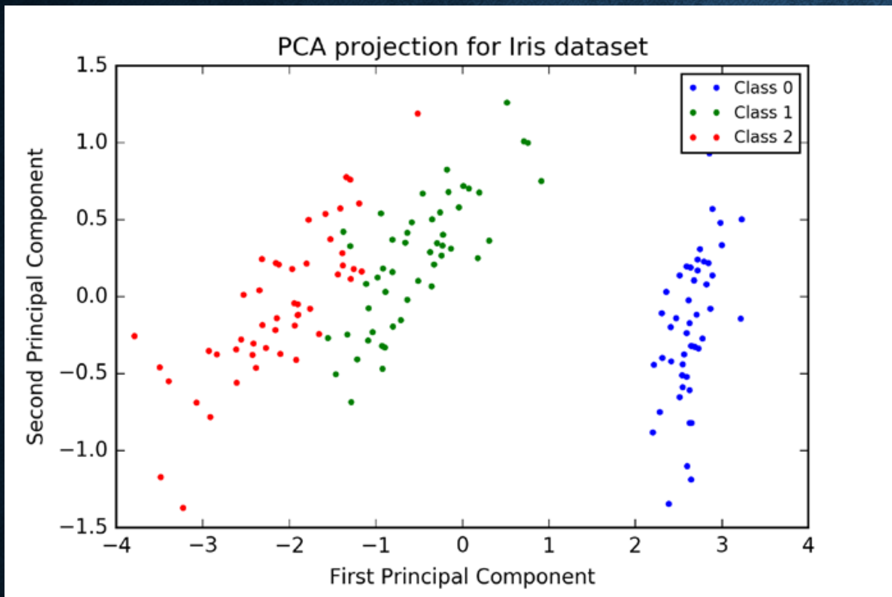
* https://en.wikipedia.org/wiki/Iris_flower_data_set
** http://scikit-learn.org/stable/auto_examples/datasets/plot_iris_dataset.html

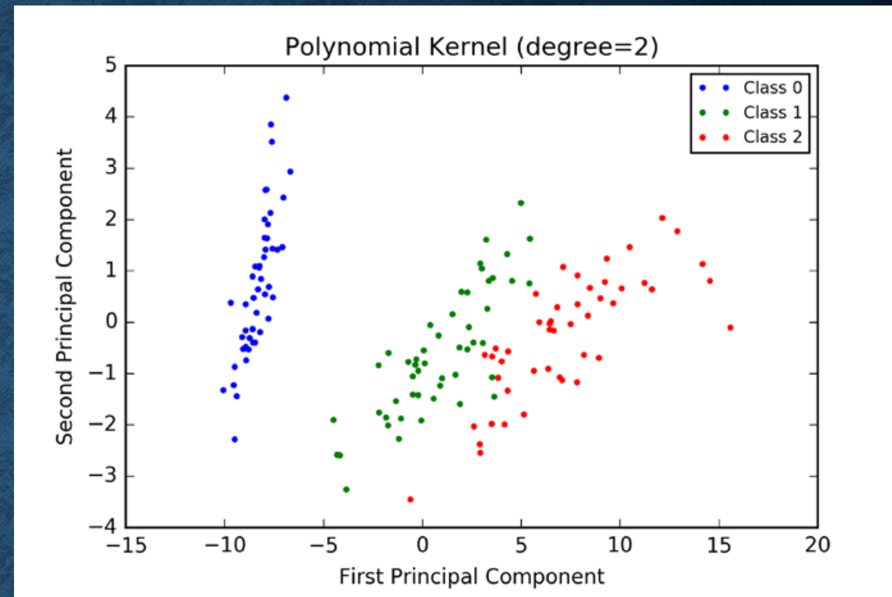
Iris Dataset – PCA vs. K-PCA

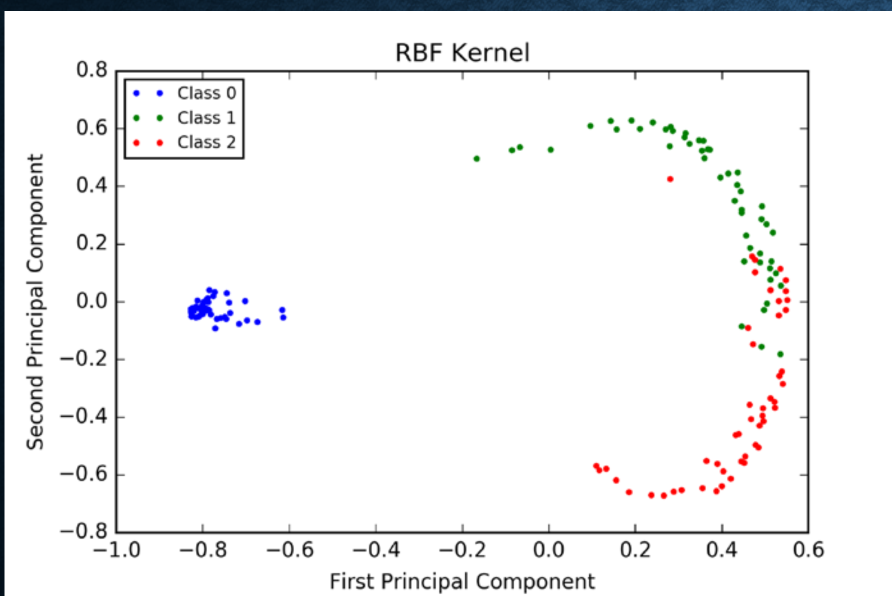


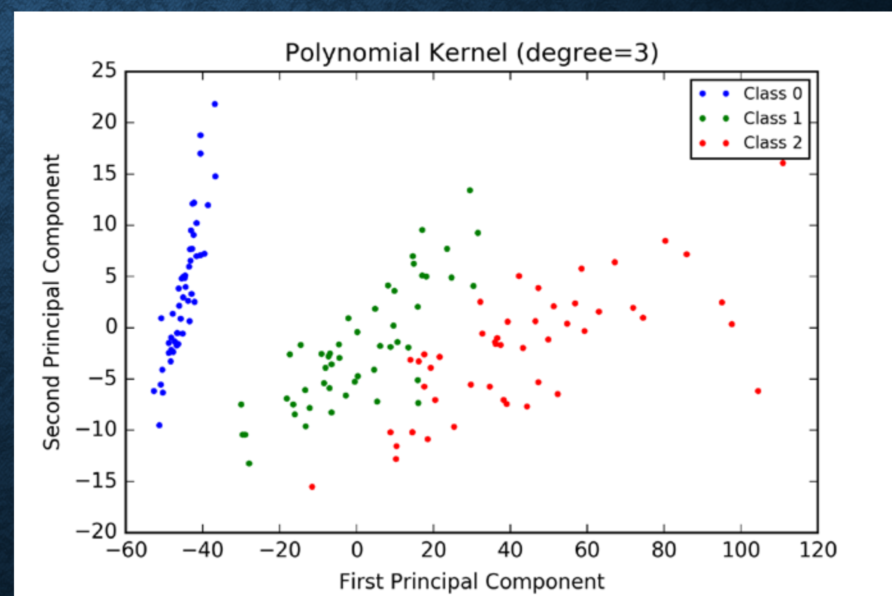


Iris Dataset – PCA vs. K-PCA









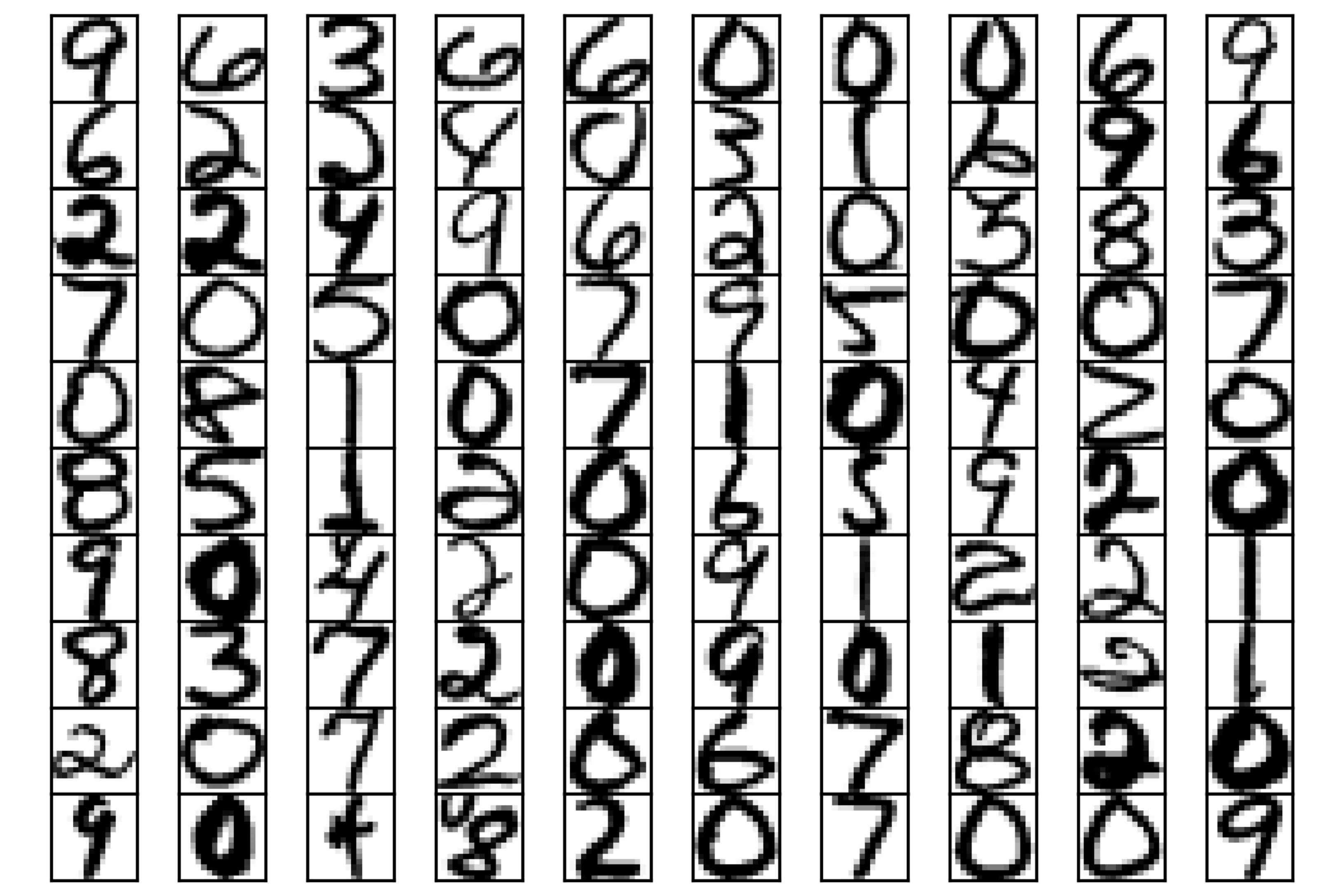
Digits Dataset – Introduction

- Normalized handwritten digits, automatically scanned from envelops by the U.S. Postal Service*.
- All the images have been processed into 16×16 grayscale images (256 features).
- The dataset has 10 classes (0-9). There are 7291 training observations and 2007 test observations.

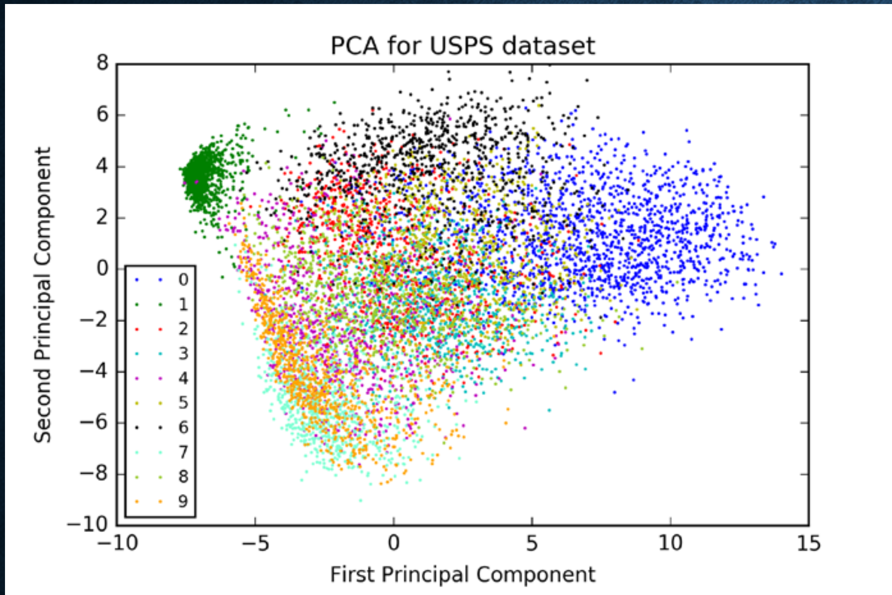
Class	0	1	2	3	4	5	6	7	8	9	Total
Train	1194	1005	731	658	652	556	664	645	542	644	7291
Test	359	264	198	166	200	160	170	147	166	177	2007

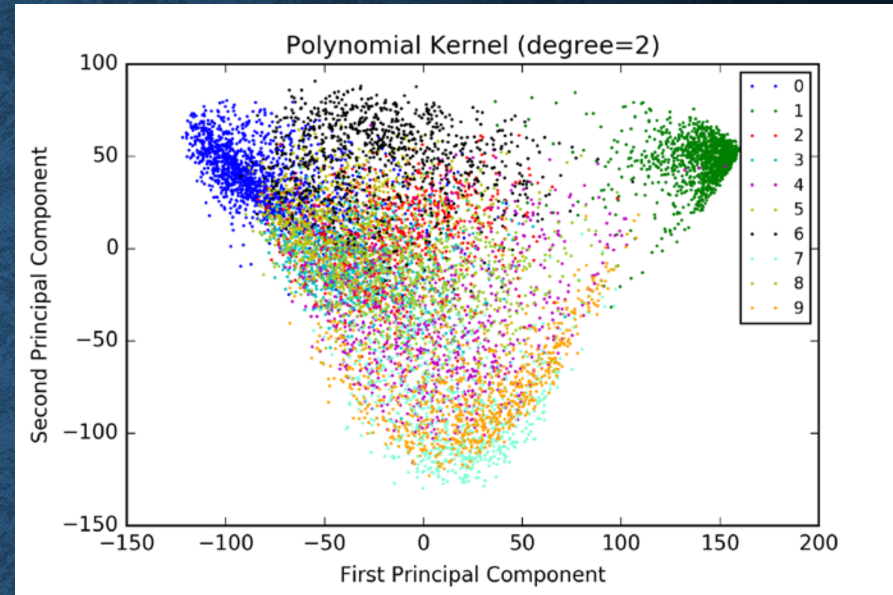
* http://statweb.stanford.edu/~tibs/ElemStatLearn/datasets/zip.info.txt
** http://scikit-learn.org/stable/auto_examples/datasets/plot_iris_dataset.html

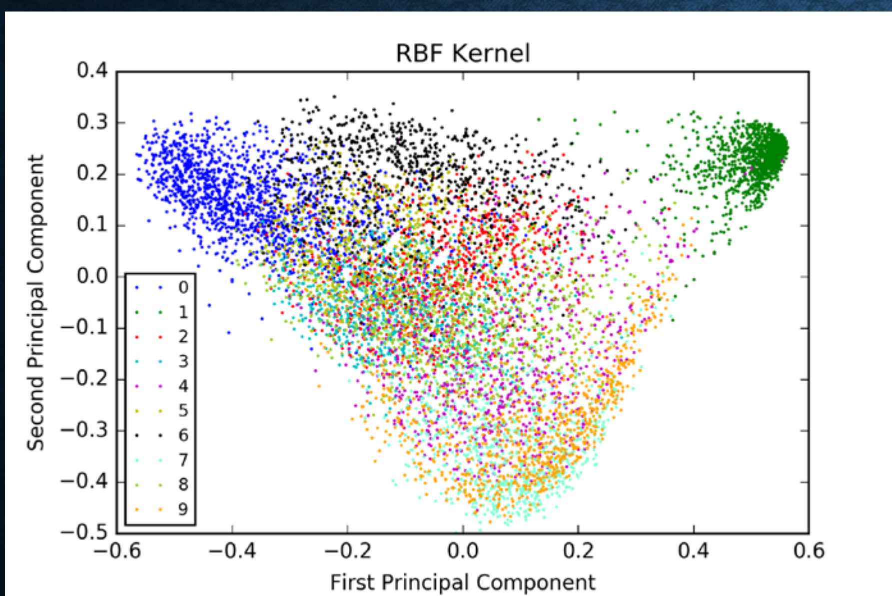
Digits Dataset – Introduction

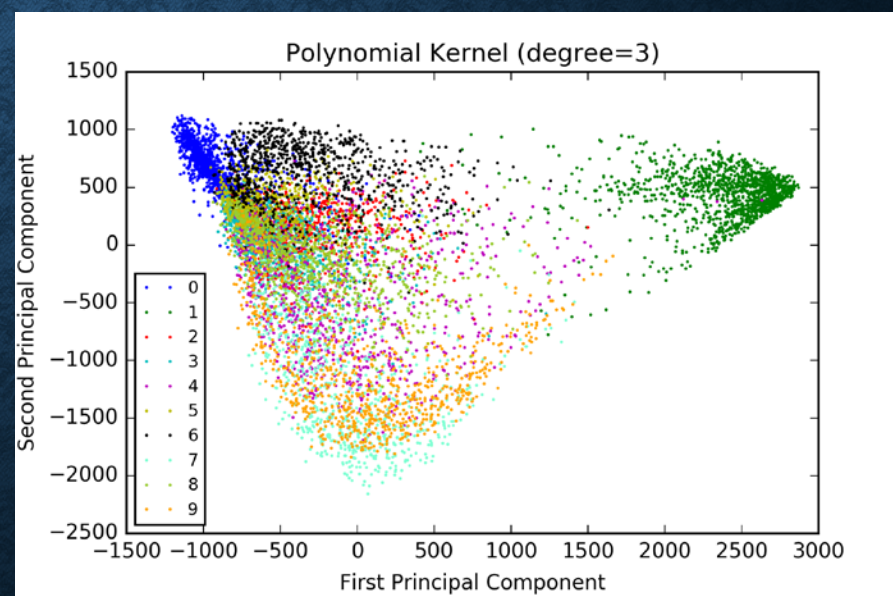


Digits Dataset – PCA vs. K-PCA



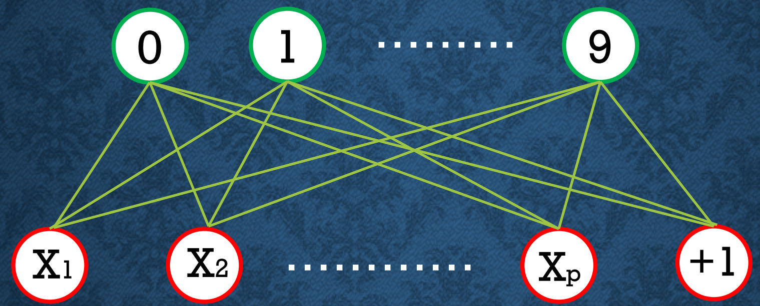






Digits Dataset – Classification

- Train a 10-way multi-class neural network for classification



- Training accuracy and testing accuracy

Inputs	Raw image	PCA	Polynomial Kernel (degree=2)	Polynomial Kernel (degree=3)	RBF Kernel
Feature Number	256	128	512	1024	1024
Training Accuracy	95.52%	94.94%	99.99%	98.51%	93.58%
Test Accuracy	90.98%	90.23%	94.42%	93.92%	88.14%

Summary

- Kernel PCA takes advantage of kernels to avoid huge computations
- Kernels PCA can work better than PCA
- Need to note:
  - Kernel matrix K has dimension of $n \times n$. It may need time to find eigenvectors when n is large
  - Using kernels, the parameters like d, γ, c_0 need to be determined by users

Extension

- There are a lot of methods for dimensionality reduction
    - Independent Component Analysis (ICA)
    - Non-negative Matrix Factorization (NMF)
    - Isometric Feature Mapping (ISOMAP)
    - Locality Sensitive Hashing (LSH)
    - Latent Semantic Analysis (LSA)
    - Restricted Boltzmann Machine (RBM)
    - Auto-encoder
    - And so on

Questions?

- All source codes are available in GitHub
  - https://github.com/JifuZhao/UIUC_Courses/tree/master/UIUC_IE529/project/code

- Thank you.