Kernel PCA and de-noising in feature spaces by S. Mika et al.

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Outline

Introduction

- **Kernel PCA** for data reconstruction and de-noising
- Approximate **pre-images** using **Gaussian Kernels**.

Kernel PCA

Consider the data set $\mathcal{X} = \{x_1, \ldots, x_\ell\}$ with $x_i \in \mathbb{R}^N$.

- Kernel PCA maps $\mathcal{X}$ into a higher dimensional feature space $\mathbf{F}$, i.e.

$$\mathbf{\Phi} : \mathbb{R}^N \to \mathbf{F}.$$

  $\mathbf{\Phi}(\boldsymbol{x}_i)$ is known as the $\mathbf{\Phi}$-image of $\boldsymbol{x}_i$.

- It then performs linear PCA in $\mathbf{F}$ using a projection operator onto the first n principal components in $\mathbf{F}$ as $\mathrm{P_n}$.

Reconstruction

Given the test point $\boldsymbol{t} \in \mathbb{R}^N$

- We reconstruct its $\boldsymbol{\Phi}$-image as $\mathrm{P_n}\boldsymbol{\Phi}(\boldsymbol{t})$.
- We then find its **pre-image** $\boldsymbol{z} \in \mathbb{R}^N$, such that $\boldsymbol{\Phi}(\boldsymbol{z}) \approx \mathrm{P_n}\boldsymbol{\Phi}(\boldsymbol{t})$ by minimizing

$$||\boldsymbol{\Phi}(\boldsymbol{z}) - \mathrm{P_n}\boldsymbol{\Phi}(\boldsymbol{t})||^2.$$

The Kernel Trick

- Using the **Kernel Trick** we can avoid working in high dimensional spaces
- Using **Gaussian kernels** it is possible to devise an iterative scheme to obtain an approximate pre-image.

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{\Phi}(\boldsymbol{x}_i) \cdot \boldsymbol{\Phi}(\boldsymbol{x}_j). = \exp(-||\boldsymbol{x}_i - \boldsymbol{x}_j||^2/c)$$

Toy example: 11 Gaussians

- 11 spherical gaussians with random centers in $[-1, 1]^{10}$
- Sample 100 points from each for training data
- Sample 33 points from each for test data
- Denoise the test data using kernel and linear PCA trained on training data

Results

σ	$n = 1$	2	3	4	5	6	7	8	9
0.05	2058.42	1238.36	846.14	565.41	309.64	170.36	125.97	104.40	92.23
0.1	10.22	31.32	21.51	29.24	27.66	23.53	29.64	40.07	63.41
0.2	0.99	1.12	1.18	1.50	2.11	2.73	3.72	5.09	6.32
0.4	1.07	1.26	1.44	1.64	1.91	2.08	2.22	2.34	2.47
0.8	1.23	1.39	1.54	1.70	1.80	1.96	2.10	2.25	2.39

Table: Their results

σ	$n = 1$	2	3	4	5	6	7	8	9
0.05	496.24	1614.73	1816.32	1598.64	972.89	623.70	364.37	153.05	90.50
0.1	178.33	752.52	803.60	586.85	396.99	259.77	152.16	104.50	89.89
0.2	37.65	63.62	18.41	5.16	3.35	2.82	2.73	2.30	3.43
0.4	6.03	4.06	1.77	1.78	1.87	2.08	5.49	9.24	9.54
0.8	0.62	0.98	1.25	1.54	1.83	1.80	1.75	1.57	1.53

Table: Our results

Greater than 1: Kernel PCA performs better

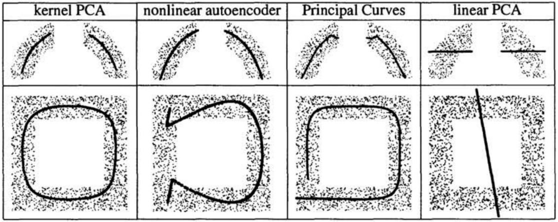
Toy example: De-noising

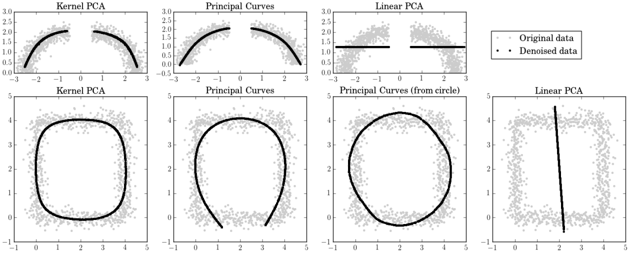
Figure: Noisy shapes in two dimensional plane

The intention is to compare de-noising results using Kernel PCA and other algorithms.

- Synthetic data is generated starting from different shapes in the plane and adding noise.
- Using two-dimensional data allows for a simple subjective analysis of the results by visual inspection.

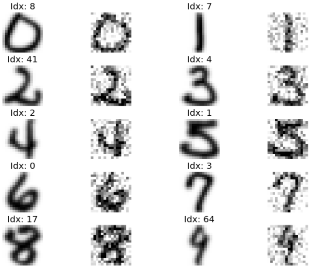
Results


kernel PCA
nonlinear autoencoder
Principal Curves
linear PCA


Kernel PCA
Principal Curves
Linear PCA
Original data
Denoised data
Kernel PCA
Principal Curves
Principal Curves (from circle)
Linear PCA

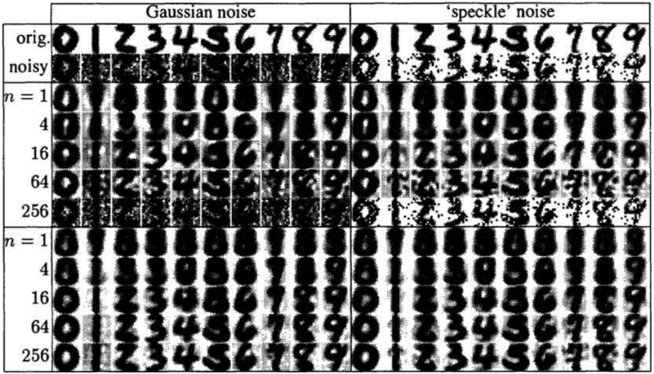
USPS Data set

- 16x16 labeled images of handwritten digits
- Scanned by the U.S. Postal Service
- A total of 9298 observations:
  - 7291 for training
  - 2007 for testing
- Deslanted and size-normalized
- Downloaded through `scikit-learn`
- Manually added noise:
  - Gaussian noise ($\mu = 0, \sigma = 0.5$)
  - Speckle noise ($p = 0.4$)



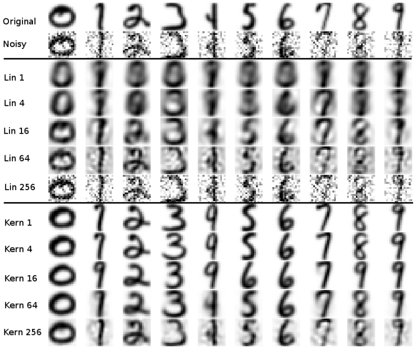
The first occurrence of each digit and its noisy version

Denoising: Linear vs Kernel PCA (their results)

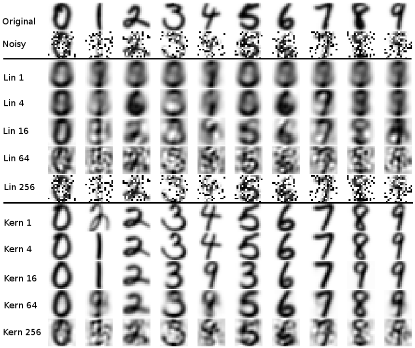


- For each digit select 300 "clean" samples
- Run Linear PCA and Kernel PCA on the noisy test classes with a variable number components for reconstruction

Denoising: Linear vs Kernel PCA (our results)

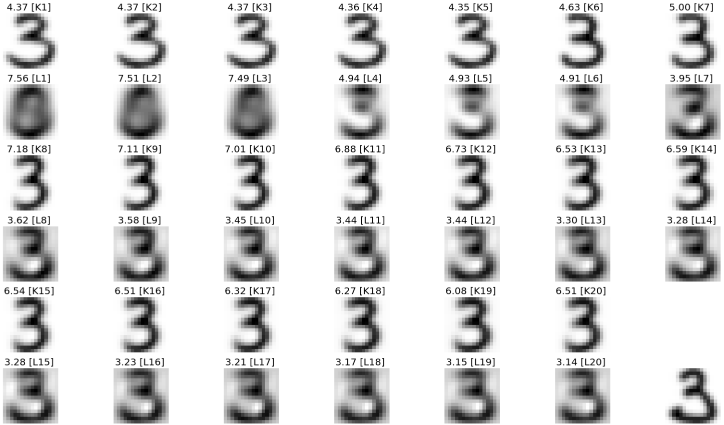


Linear and Kernel based denoising of Gaussian noise



Linear and Kernel based denoising of Speckle noise

Reconstruction: Linear vs Kernel PCA



- Number of features in the range [1,20]
- Euclidean distance from the target (bottom right)

Conclusion

- The results obtained by Mika *et al.* were reproduced with minor divergences
- Kernel PCA works well for extracting non-linear features
- Overhead when compared to Linear PCA:
  - Time complexity: needs to compute $k(t, x_i)\ \forall i$
  - Spatial complexity: need to store all training data

Thank you

References

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