Remember:

$N >> p$

Rank $r = p$

$\boxed{\text{SVD and PCA}}$

$$\underbrace{X_{N\times p} = Y^T_{N\times p}} = \begin{pmatrix} \vec{y}_1^{\,T} \\ \vdots \\ \vec{y}_N^{\,T} \end{pmatrix} \qquad \vec{y}_i \in \mathbb{R}^p$$

$$\tilde{Y}^T_{N\times p} = \left(I - \frac{1}{N} 1 1^T\right) Y^T$$

centered data matrix

$$\sum_{j=1}^{p} \sigma_j \vec{u}_j \vec{v}_j^{\,T} = \tilde{Y}^T_{N\times p} = U_{N\times p} \Sigma_{p\times p} V^T_{p\times p}$$

SVD

$$U = (\vec{u}_1, \dots, \vec{u}_p)_{N\times p}$$

SVD provides a new orthonormal basis $\{\vec{V}_j\}_{j=1}^{p}$

$$V = (\vec{v}_1, \dots, \vec{v}_p)_{p\times p}$$

$\boxed{\text{our new basis}}$

$\downarrow$ E-Y

Closest approximation of rank k

For a given k:

$$\hat{\tilde{Y}}^T_{N\times p} = \Big[\underbrace{\left[U_k \Sigma_k\right]}_{N\times k} V^T_{k\times p}\Big]$$

$$\left\{ \begin{array}{l} (Y_{PCA}) = \left[U_k \Sigma_k\right]_{N\times k} \\ \text{coordinates of the} \\ V_k = (\vec{v}_1, \dots, \vec{v}_k) \quad \vec{v}_i \in \mathbb{R}^p \end{array} \right\}$$

where $\Sigma_k = \mathrm{diag}\begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{pmatrix}$

$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_k$

ordered singular values.

Examples overleaf $\longrightarrow$

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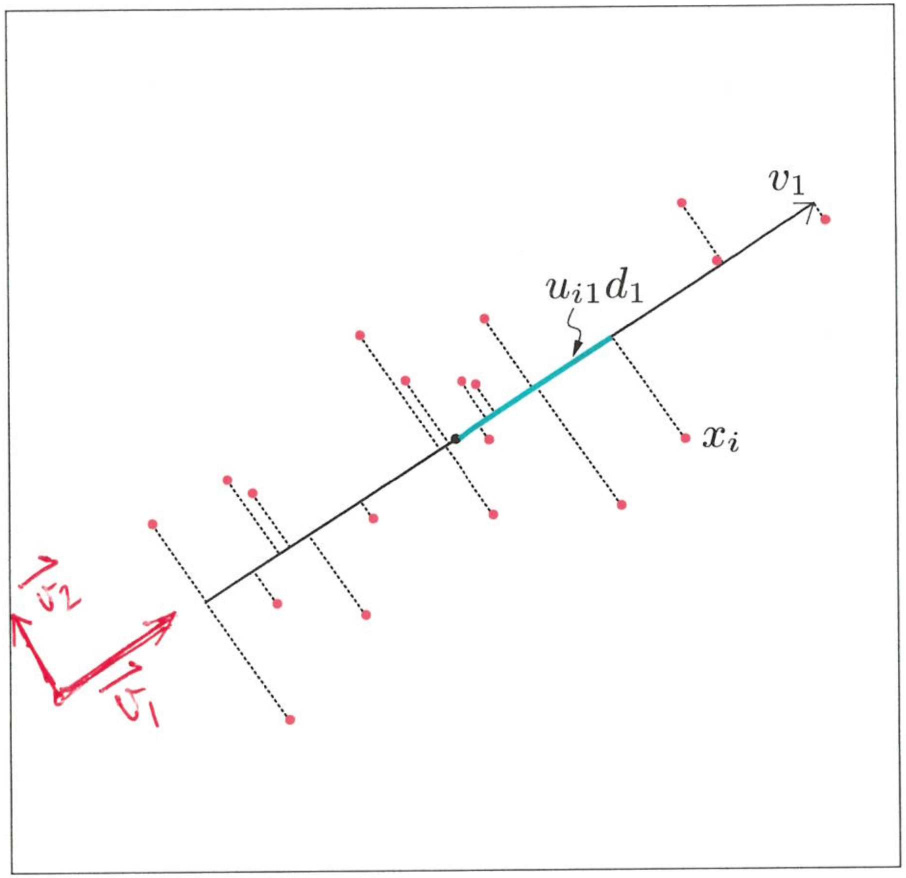
Illustration of PCA and SVD

$\vec{v}_1$ captures maximum variability



From the SVD:

$V = (\vec{v}_1 \ \vec{v}_2)$

$\boxed{\text{New basis}}$

$\vec{y}_i \in \mathbb{R}^2$

$i = 1, \dots, N$

$\vec{y}_i = \alpha_1^{(i)} \vec{v}_1 + \alpha_2^{(i)} \vec{v}_2$

$= \sigma_1 u_{i1} \vec{v}_1 + \sigma_2 u_{i2} \vec{v}_2$

$= (\vec{v}_1^T \cdot \vec{y}_i)\, \vec{v}_1 + (\vec{v}_2^T \cdot \vec{y}_i)\, \vec{v}_2$

If we approximate by first component, we minimize the sum of perpendicular errors.

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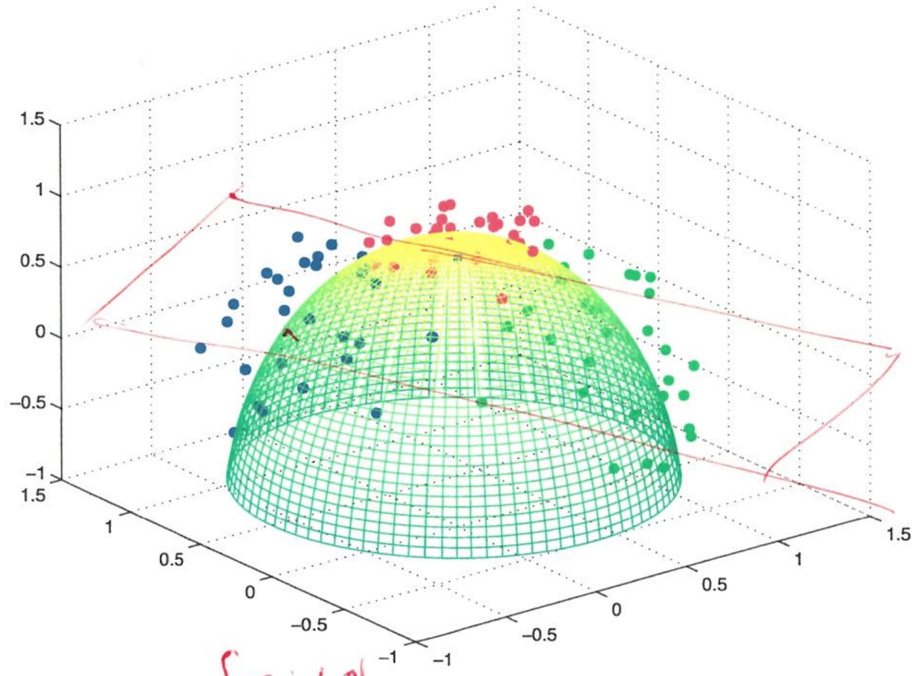
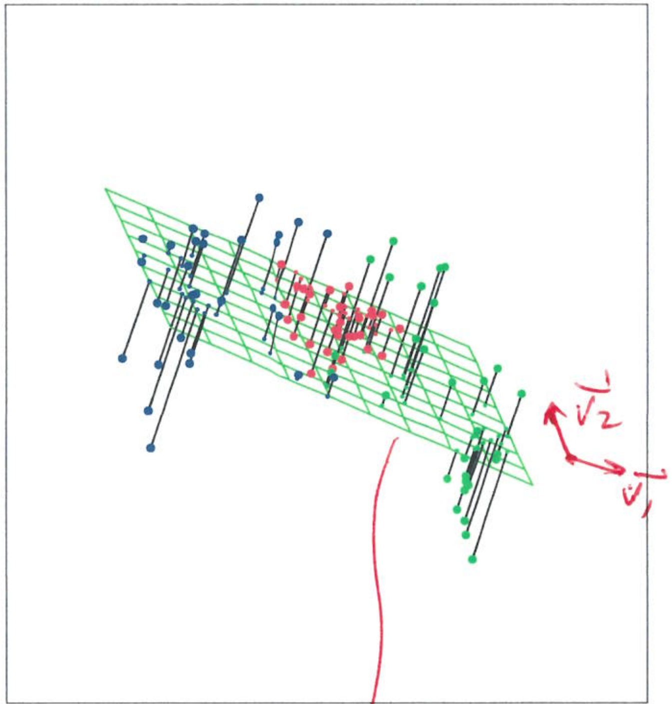
Illustration of PCA and SVD

$\vec{y}_i \in \mathbb{R}^3$



$\{\vec{y}_i\}_{i=1}^{N}$



Best approximation given by hyperplane $(\vec{v}_1, \vec{v}_2)$

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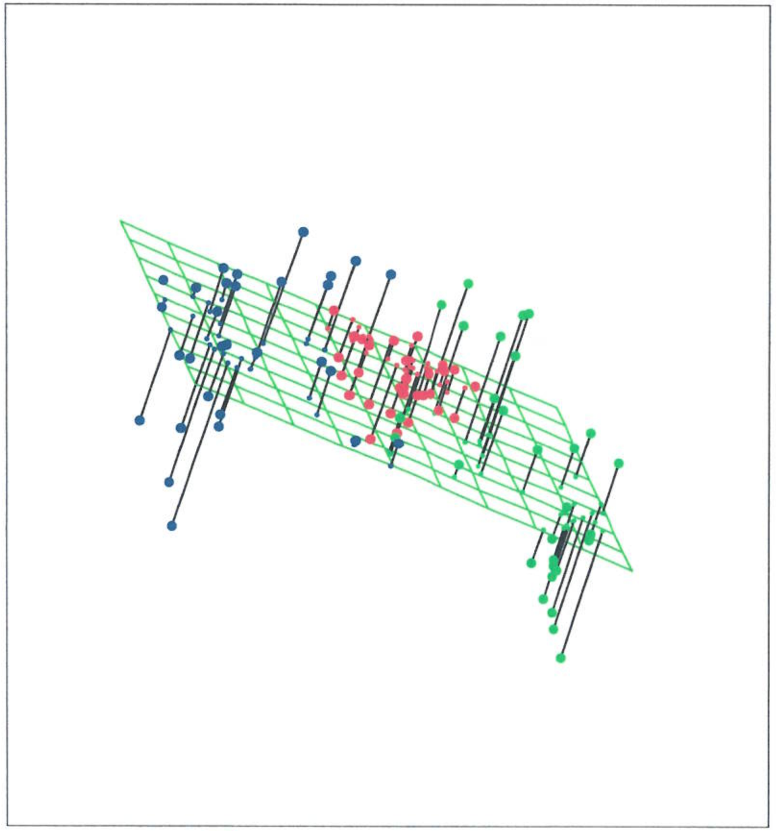
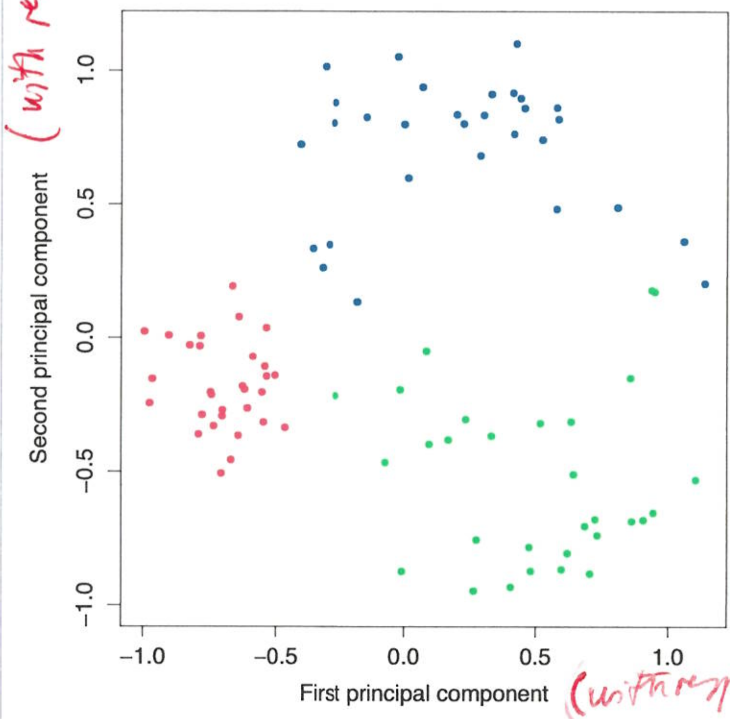
Illustration of PCA and SVD

$p=3$



$\tilde{y}^T_{N\times p}$

mapped to



(with respect to $\vec{v}_2$)

(with respect to $\vec{v}_1$)

$(y_{PCA})_{N\times 2}$ = coordinates in $(\vec{v}_1, \vec{v}_2)$

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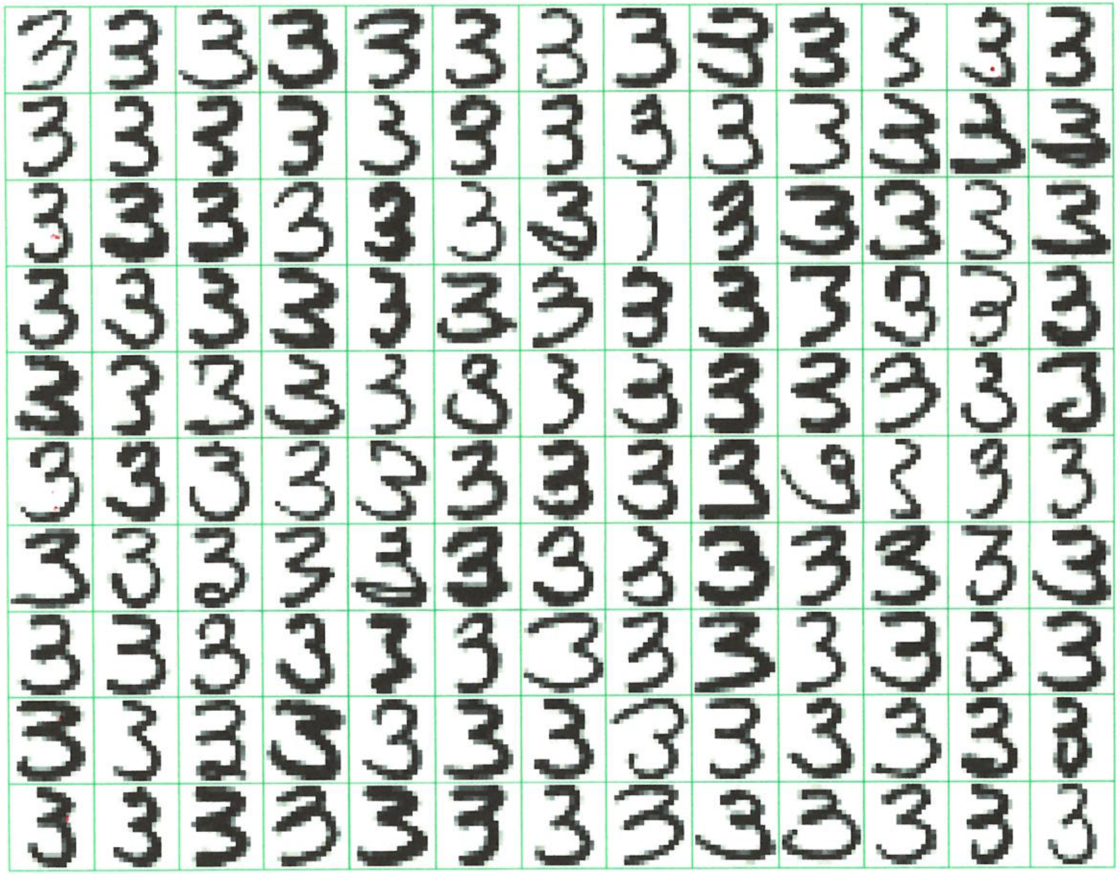
Illustration of PCA and SVD



Sample:

$\{\vec{y}_i\}_{i=1}^{130}$

$N = 130$ images

vectors:

$\vec{y}_i \in \mathbb{R}^{16 \times 16}$

Each $\vec{y}_i$ contains the grayscale of the images with 256 pixels.

Illustration of PCA and SVD

vectors expressed in terms of the first two $\vec{v}_i$

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 \vec{v}_1 + \lambda_2 \vec{v}_2$$

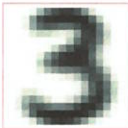
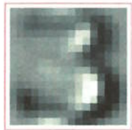
=  $+ \lambda_1 \cdot$  $+ \lambda_2 \cdot$  .

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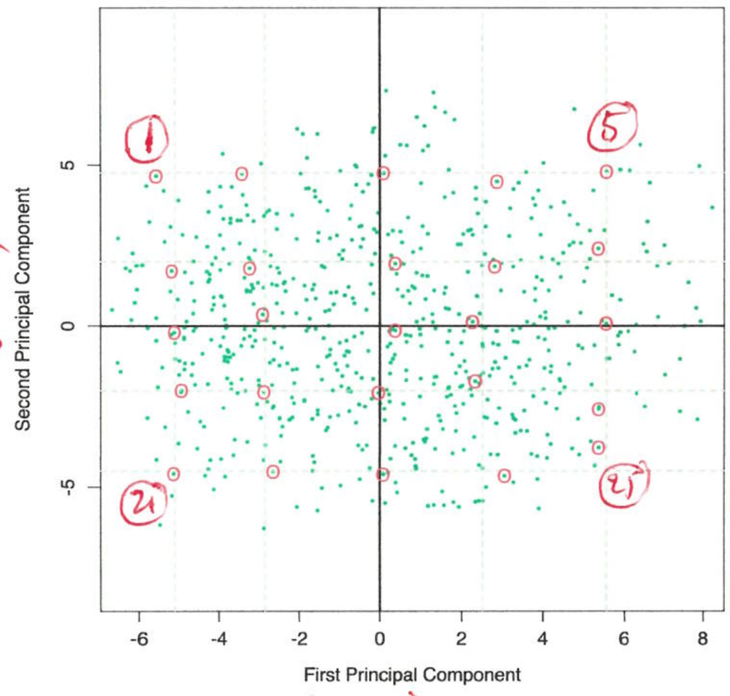
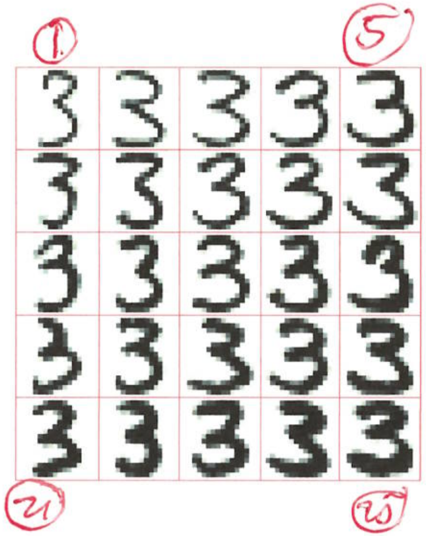
Illustration of PCA and SVD



(λ_2)

(λ_1)



PC2

The 3 becomes less thick

PC1

(The bottom part of the 3 becomes more curved)

First extension:

1. PCA is about linear projections that minimize a quadratic. How do we extend?

(1) "Nonlinearity": Kernel PCA

$$(\tilde{Y}^T\tilde{Y})_{ij} = (\vec{\tilde{y}}_i^T \cdot \vec{\tilde{y}}_j)$$

PCA was about eigenvalues of $\tilde{Y}^T\tilde{Y}$ and $\tilde{Y}\tilde{Y}^T$

which are "Kernel" matrices.

If we assume a kernel function

$$K_{ij} = K(\vec{\tilde{y}}_i, \vec{\tilde{y}}_j)$$

positive definite, etc. (see SVMs)

Then Eigendecomposition of K (kernel matrix)

e.g. $K(\vec{x}_i, \vec{x}_j) = e^{-\frac{\|\vec{x}_i - \vec{x}_j\|^2}{c}}$

Radial Kernel

Example overleaf

We can do spectral analysis of the kernel (which is nonlinear in the original coordinates)

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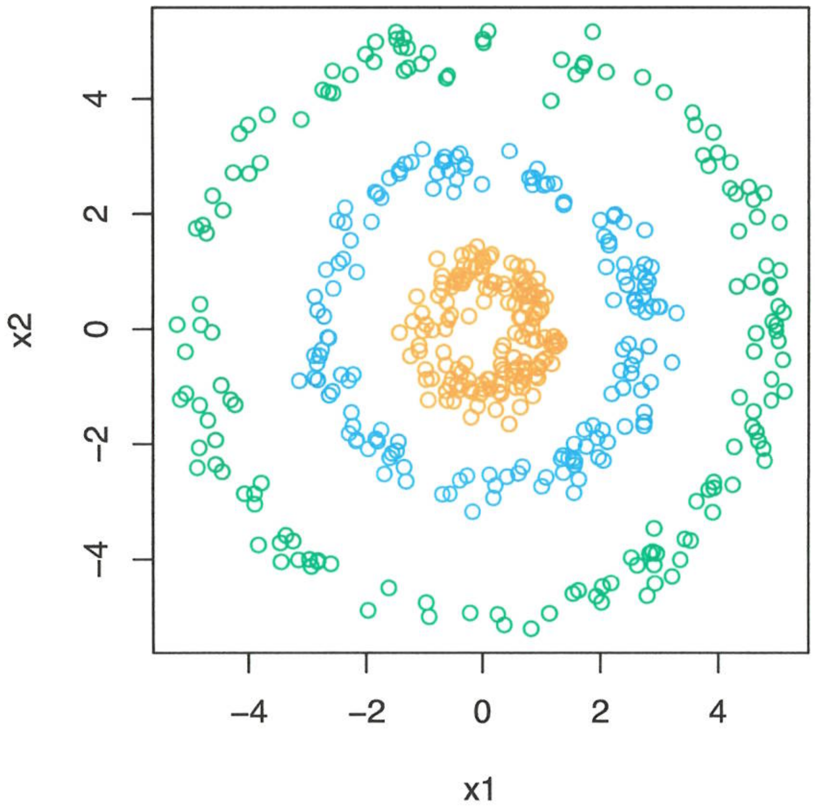
Representing these data in terms of standard PCA does not lead to a good mapping.



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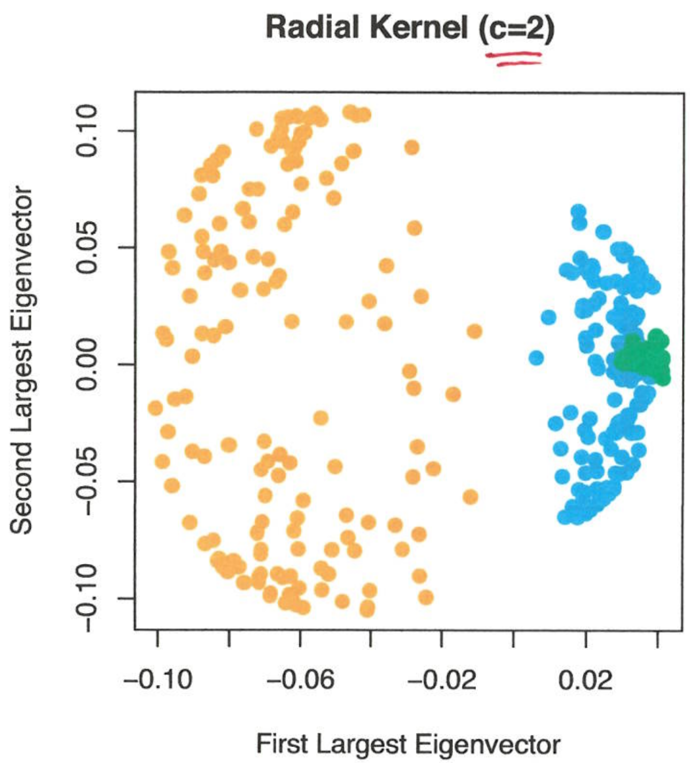
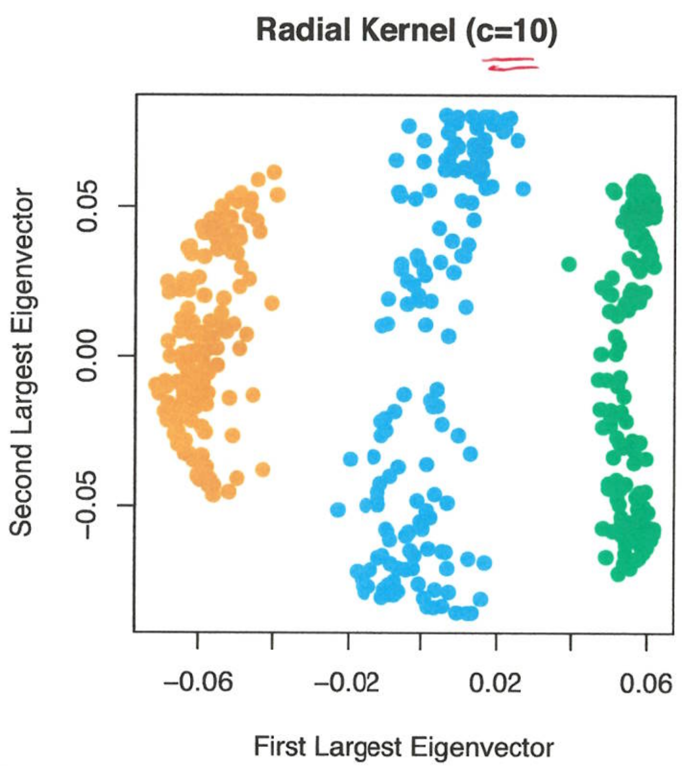
Kernel PCA

Increasing the hyperparameter c





Second extension: Interpretability through sparsity.

Sparse PCA

Our description from standard PCA was of the form:

$$(y_{PCA})_{N\times K} = (U_K \Sigma_K)_{N\times K}$$

coordinates in terms of

$$V_K = (\vec{v}_1 \dots \vec{v}_K)_{p\times K}$$

The basis V is Non sparse in terms of our original descriptors

i.e. V is not a sparse matrix.

This leads to diminished interpretability

Original PCA:

$\vec{v} \in \mathbb{R}^p$

This is an alternative description of PCA

$$\left\{ \begin{array}{l} \max\limits_{\vec{v}} \; \vec{v}^T (\tilde{Y}\tilde{Y}^T)\vec{v} \\ \text{such that } \vec{v}^T\vec{v} = 1 \end{array} \right\}$$

$\boxed{\text{Sparser}}$ by adding extra constraints.

$$\sum_{j=1}^{p} |v_j| \leq t$$

Similar to LASSO

$$\underbrace{\{\vec{v}_{j,L}\}_{j=1}^{p}}_{\text{SVD LASSO basis}}$$

Find a basis that tries to minimize the quadratic error under sparsity constraints.

If we find a description in terms of a few vectors that are sparse then the description is closer to identifying the important combinations of descriptors.

$$\hat{\vec{y}} = \hat{f}(\lambda) = \sum_{j=1}^{k} \lambda_j \underbrace{\vec{v}_{j,L}}$$

$k <<$ from LASSO.

Then the matrix V will be sparser and the $\vec{v}_j$ will contain more zeros

$$\vec{v}_{j,L} = \begin{pmatrix} \blacksquare \\ 0 \\ 0 \\ 0 \\ \blacksquare \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{array}{l} \to \text{coordinate for } x_1 \\ \\ \\ \\ \to \text{coordinate for } x_j \\ \\ \\ \\ \end{array}$$

Third extension: Interpretability through non-negativity

Non-negative matrix factorisation (NNM)

Standard PCA/SVD

$$\underset{N\times p}{\hat{\tilde{y}}^T} = \underset{N\times K}{(U_K \Sigma_K)} \underset{K\times p}{V_{K:}^T}$$

↓ the same matrix

$$\cancel{X} = \underbrace{(U_K \Sigma_K)}_{N\times K} \underbrace{V_{K:}^T}_{K\times p}$$

NNM:

Generalise to a factorisation:

$$X = \underset{N\times K}{W} \; H^T_{K\times p}$$

where we require positivity

$$w_{ij} \geq 0 \quad \forall \; i,j$$

$$h_{ij} \geq 0 \quad \forall \; i,j$$

It can be shown to be equivalent to:

$$\max_{W,H} \; L(W,H) = \sum_{i=1}^{N} \sum_{j=1}^{K} \left[X_{ij} \log (WH)_{ij} - (WH)_{ij} \right]$$

$X_{ij} \sim \text{Poi}$ with mean $(WH)_{ij}$

What does ~~it~~ NNM give?

See over →

for an example with images

Non negative matrix factorisation

$\{\vec{y}_i\}_{i=1}^{N}$ $\vec{y}_i \in \mathbb{R}^p$

Setup:

- Each $\vec{y}_i$ is an image 19x19 pixels, which is vectorized into a 361-dimensional vector.
- Number of images in sample $N=2429$

N=2429

p=381=19x19
k=49

$H^T_{49\text{x}381}$ picks the basis "features" of images

Each of the squares is a 381-dimensional vector

$\vec{W}_i^T$ (original) 1x49

all positive

VQ = K-means

The 49 faces closest to "Original"

This whole set of squares is the $(V_K)_{p \times k}$ matrix

Each of the squares is a $\vec{v}_j \in \mathbb{R}^{381}$

$\vec{u}_i$ (original) 1x49