

EE-559 – Deep learning

2.5. Basic clustering and embeddings

François Fleuret

<https://fleuret.org/ee559/>

Fri Oct 5 22:30:20 UTC 2018

Deep learning models combine embeddings and dimension reduction operations.

They parametrize and re-parametrize multiple times the input signal under more invariant and interpretable forms.

Deep learning models combine embeddings and dimension reduction operations.

They parametrize and re-parametrize multiple times the input signal under more invariant and interpretable forms.

To get an intuition of how this is possible, we consider here two standard algorithms:

- K -means, and
- Principal Component Analysis (PCA).

Deep learning models combine embeddings and dimension reduction operations.

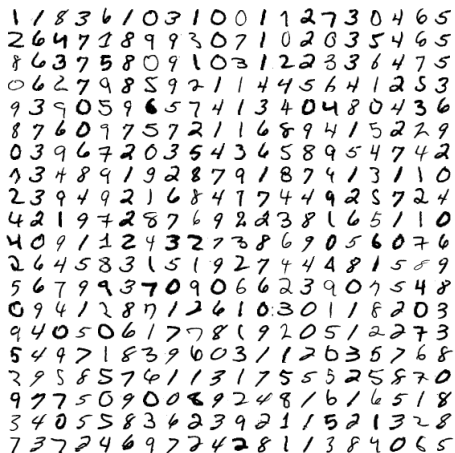
They parametrize and re-parametrize multiple times the input signal under more invariant and interpretable forms.

To get an intuition of how this is possible, we consider here two standard algorithms:

- K -means, and
- Principal Component Analysis (PCA).

We will illustrate these methods on our two favorite data-sets.

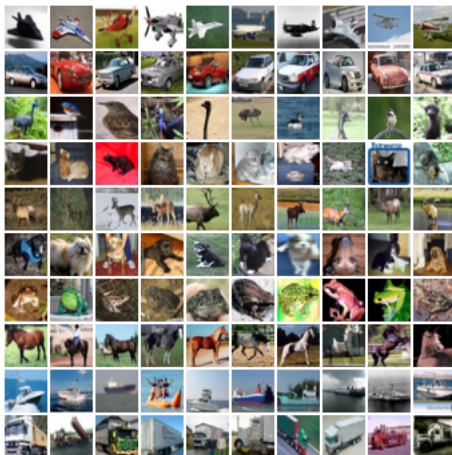
MNIST data-set



1 1 8 3 6 1 0 3 1 0 0 1 1 2 7 3 0 4 6 5
2 6 4 7 1 8 9 9 3 0 7 1 0 2 0 3 5 4 6 5
8 6 3 7 5 8 0 9 1 0 3 1 2 2 3 3 6 4 7 5
0 6 2 7 9 8 5 9 2 1 1 4 4 5 6 4 1 2 5 3
9 3 9 0 5 9 6 5 7 4 1 3 4 0 4 8 0 4 3 6
8 7 6 0 9 7 5 7 2 1 1 6 8 9 4 1 5 2 2 9
0 3 9 6 7 2 0 3 5 4 3 6 5 8 9 5 4 7 4 2
1 3 4 8 9 1 9 2 8 7 9 1 8 7 4 1 3 1 1 0
2 3 9 4 9 2 1 6 8 4 7 7 4 4 9 2 5 7 2 4
4 2 1 9 7 2 8 7 6 9 2 2 3 8 1 6 5 1 1 0
4 0 9 1 1 2 4 3 2 7 3 8 6 9 0 5 6 0 7 6
2 6 4 5 8 3 1 5 1 9 2 7 4 4 4 8 1 5 8 9
5 6 7 9 9 3 7 0 9 0 6 6 2 3 9 0 7 5 4 8
0 9 4 1 2 8 7 1 2 6 1 0 3 0 1 1 8 2 0 3
9 4 0 5 0 6 1 7 7 8 1 9 2 0 5 1 2 2 7 3
5 4 4 7 1 8 3 9 6 0 3 1 1 2 6 3 5 7 6 8
2 9 5 8 5 7 6 1 1 3 1 7 5 5 5 2 5 8 7 0
9 7 7 5 0 9 0 0 8 9 2 4 8 1 6 1 6 5 1 8
3 4 0 5 5 8 3 6 2 3 9 2 1 1 5 2 1 3 2 8
7 3 7 2 4 6 9 7 2 4 2 8 1 1 3 8 4 0 6 5

28 × 28 grayscale images, 60k train samples, 10k test samples.

CIFAR10 data-set



32 × 32 color images, 50k train samples, 10k test samples.

(Krizhevsky, 2009, chap. 3)

Given

$$x_n \in \mathbb{R}^D, \quad n = 1, \dots, N,$$

and a fixed number of clusters $K > 0$, K -means tries to find K “centroids” that span uniformly the training population.

Given

$$x_n \in \mathbb{R}^D, \quad n = 1, \dots, N,$$

and a fixed number of clusters $K > 0$, K -means tries to find K “centroids” that span uniformly the training population.

Given a point, the index of its closest centroid is a good coding.

Formally, [Lloyd's algorithm for] K -means (approximately) solves

$$\operatorname{argmin}_{c_1, \dots, c_K \in \mathbb{R}^D} \sum_n \min_k \|x_n - c_k\|^2.$$

Formally, [Lloyd's algorithm for] K -means (approximately) solves

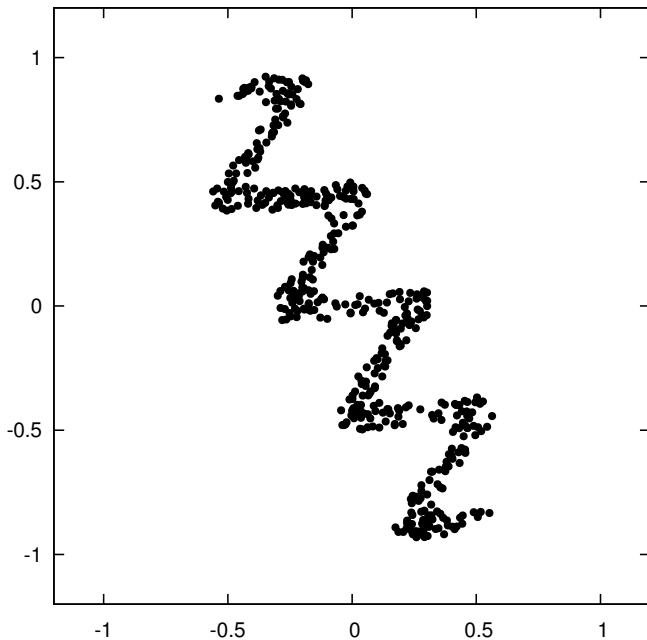
$$\operatorname{argmin}_{c_1, \dots, c_K \in \mathbb{R}^D} \sum_n \min_k \|x_n - c_k\|^2.$$

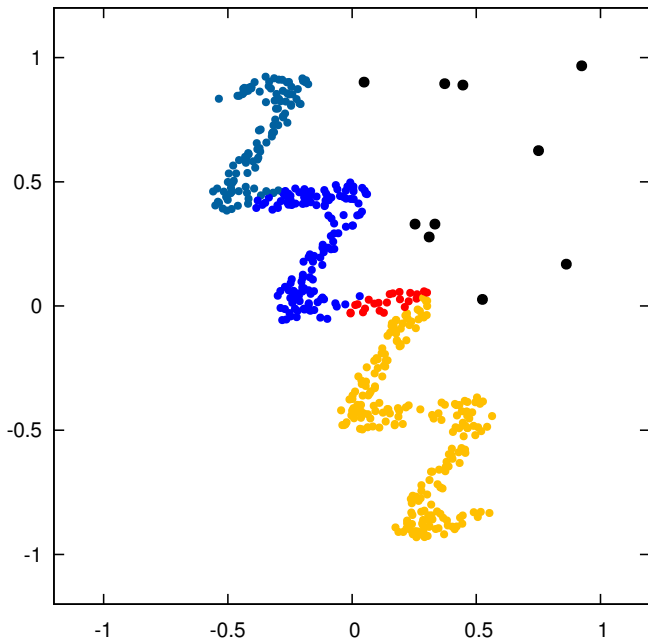
This is achieved with a random initialization of c_1^0, \dots, c_K^0 followed by repeating until convergence:

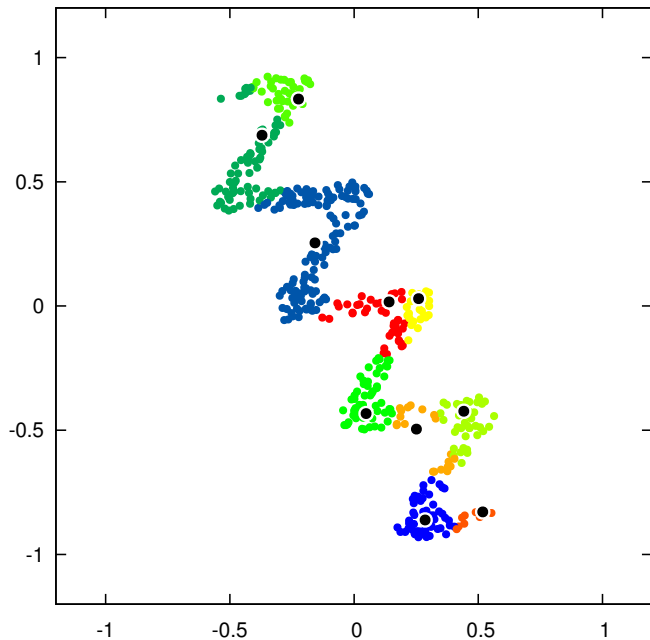
$$\forall n, k_n^t = \operatorname{argmin}_k \|x_n - c_k^t\| \quad (1)$$

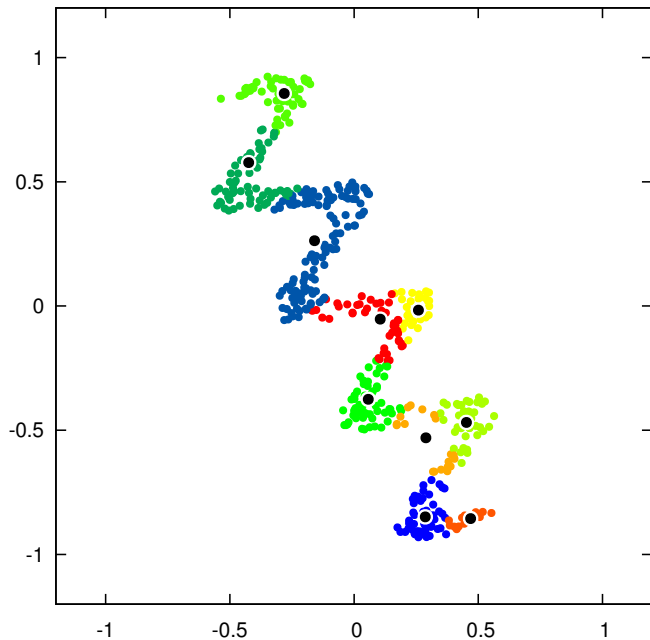
$$\forall k, c_k^{t+1} = \frac{1}{|n : k_n^t = k|} \sum_{n: k_n^t = k} x_n \quad (2)$$

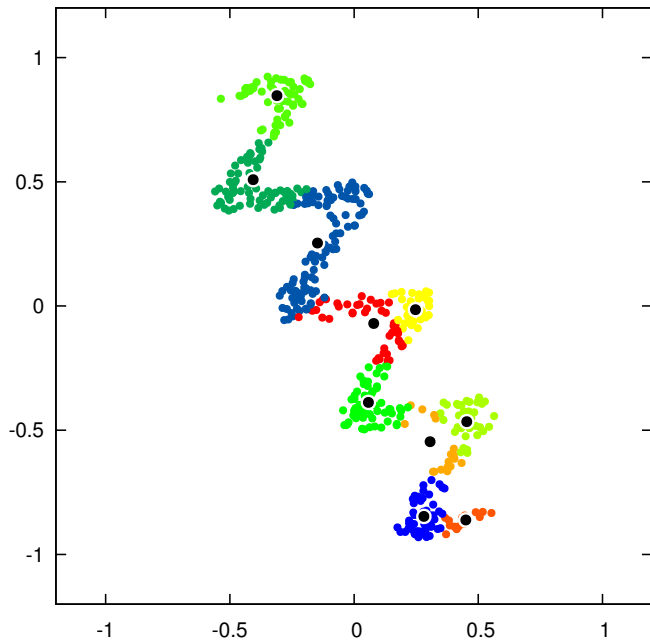
At every iteration, (1) each sample is associated to its closest centroid's cluster, and (2) each centroid is updated to the average of its cluster.

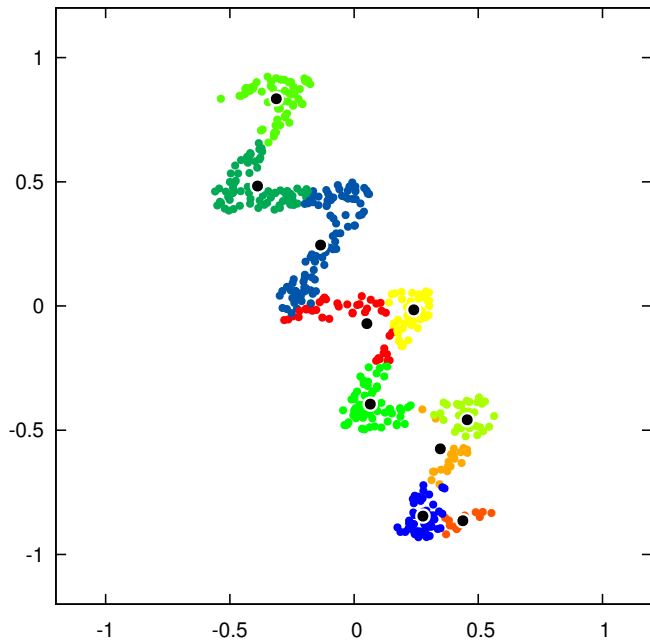


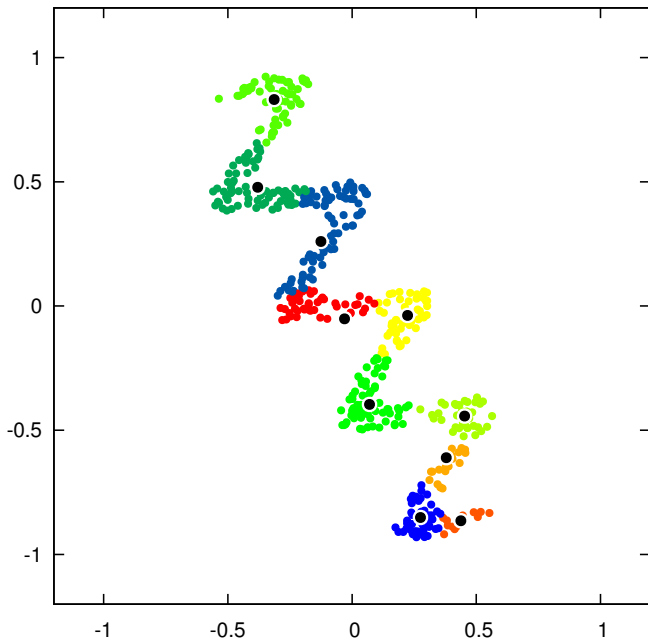


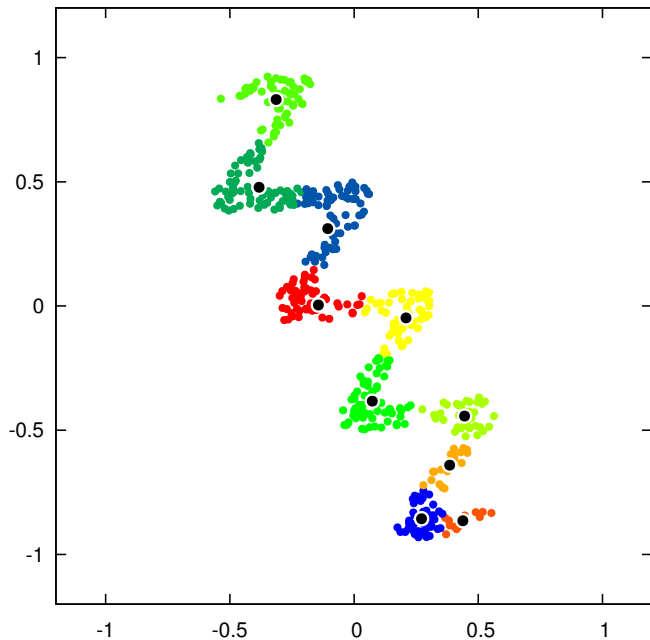


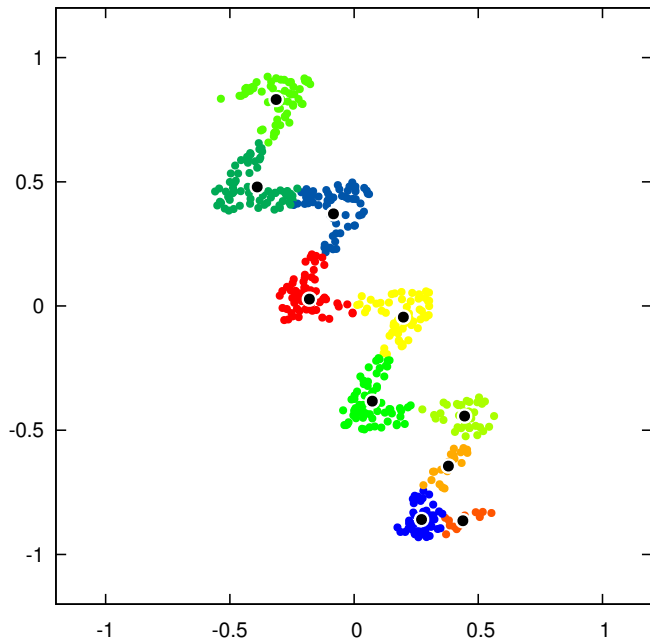


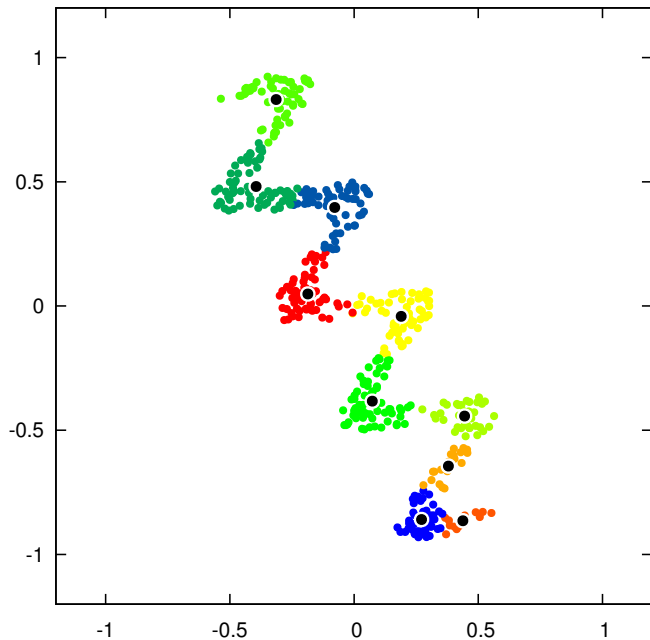


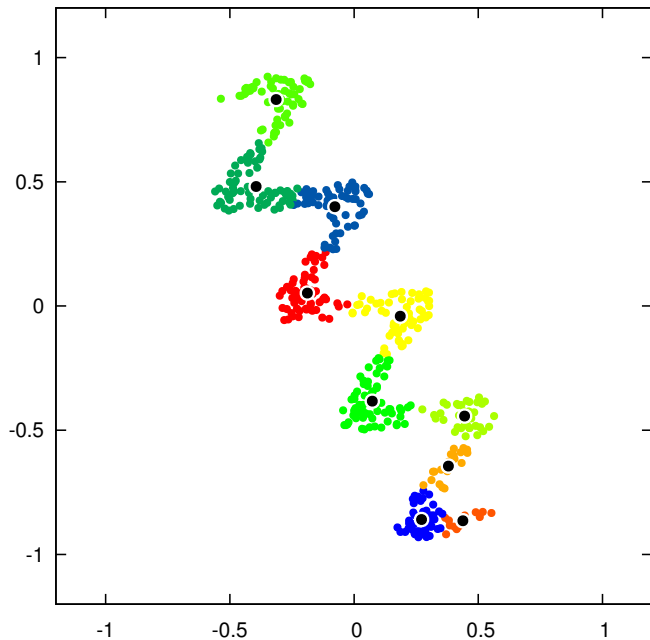


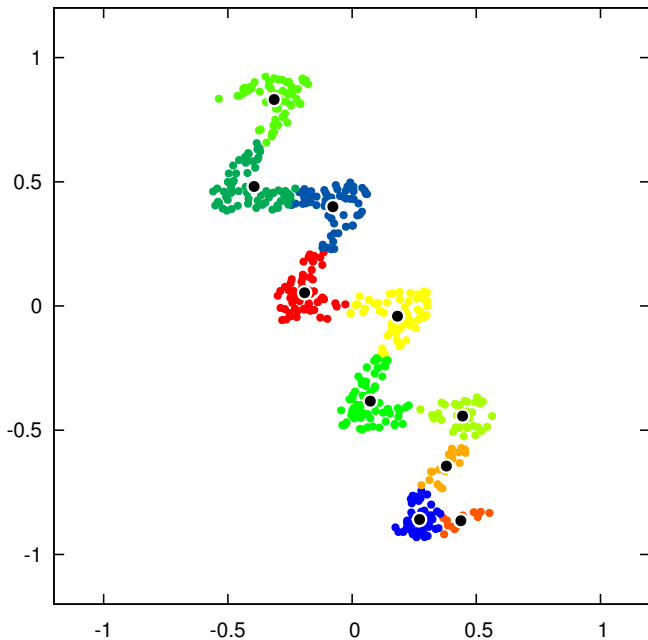












We can apply that algorithm to images from MNIST ($28 \times 28 \times 1$) or CIFAR ($32 \times 32 \times 3$) by considering them as vectors from \mathbb{R}^{784} and \mathbb{R}^{3072} respectively.

Centroids can similarly be visualized as images.

Clustering can be done per-class, or for all the classes mixed.

0
1
2
3
4
5
6
7
8
9
0

$K = 1$

00
11
22
33
44
55
66
77
88
99
00

$K = 2$

0000
1111
2222
3333
4444
5555
6666
7777
8888
9999
0901

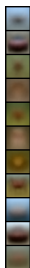
$K = 4$

00000000
11111111
22222222
33333333
44444444
55555555
66666666
77777777
88888888
99999999
96098231

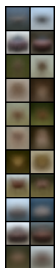
$K = 8$

0000000000000000
1111111111111111
2222222222222222
3333333333333333
4444444444444444
5555555555555555
6666666666666666
7777777777777777
8888888888888888
9999999999999999
6321017305986792

$K = 16$



$K = 1$



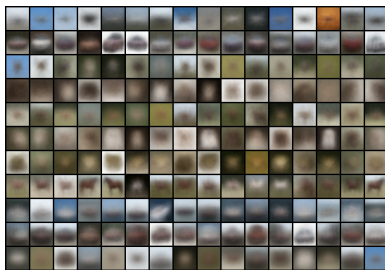
$K = 2$



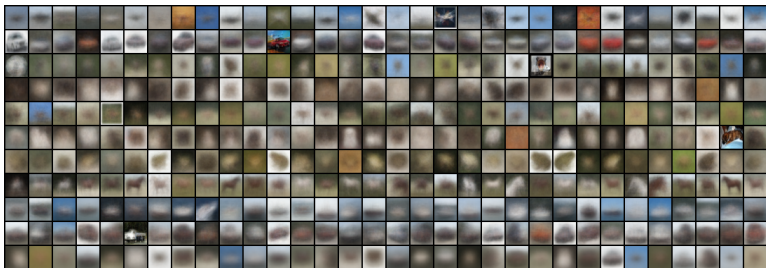
$K = 4$



$K = 8$



$K = 16$



$K = 32$

The Principal Component Analysis (PCA) aims also at extracting an information in a L^2 sense. Instead of clusters, it looks for an “affine subspace”, *i.e.* a point and a basis, that spans the data.

Given data-points

$$x_n \in \mathbb{R}^D, \quad n = 1, \dots, N$$

(A) compute the average and center the data

$$\bar{x} = \frac{1}{N} \sum_n x_n$$

$$\forall n, x_n^{(0)} = x_n - \bar{x}$$

The Principal Component Analysis (PCA) aims also at extracting an information in a L^2 sense. Instead of clusters, it looks for an “affine subspace”, *i.e.* a point and a basis, that spans the data.

Given data-points

$$x_n \in \mathbb{R}^D, \quad n = 1, \dots, N$$

(A) compute the average and center the data

$$\bar{x} = \frac{1}{N} \sum_n x_n$$

$$\forall n, x_n^{(0)} = x_n - \bar{x}$$

and then for $t = 1, \dots, D$,

(B) pick the direction and project the data

$$v_t = \operatorname{argmax}_{\|v\|=1} \sum_n \left(v \cdot x_n^{(t-1)} \right)^2$$

$$\forall n, x_n^{(t)} = x_n^{(t-1)} - \left(v_t \cdot x_n^{(t-1)} \right) v_t.$$

Although this is a simple way to envision PCA, standard implementations rely on an eigendecomposition. With

$$X = \begin{pmatrix} - & x_1 & - \\ & \vdots & \\ - & x_N & - \end{pmatrix}$$

we have

$$\sum_n (v \cdot x_n)^2$$

Although this is a simple way to envision PCA, standard implementations rely on an eigendecomposition. With

$$X = \begin{pmatrix} - & x_1 & - \\ & \vdots & \\ - & x_N & - \end{pmatrix}$$

we have

$$\sum_n (v \cdot x_n)^2 = \left\| \begin{pmatrix} v \cdot x_1 \\ \vdots \\ v \cdot x_N \end{pmatrix} \right\|_2^2$$

Although this is a simple way to envision PCA, standard implementations rely on an eigendecomposition. With

$$X = \begin{pmatrix} - & x_1 & - \\ & \vdots & \\ - & x_N & - \end{pmatrix}$$

we have

$$\begin{aligned} \sum_n (v \cdot x_n)^2 &= \left\| \begin{pmatrix} v \cdot x_1 \\ \vdots \\ v \cdot x_N \end{pmatrix} \right\|_2^2 \\ &= \|vX^T\|_2^2 \end{aligned}$$

Although this is a simple way to envision PCA, standard implementations rely on an eigendecomposition. With

$$X = \begin{pmatrix} - & x_1 & - \\ & \vdots & \\ - & x_N & - \end{pmatrix}$$

we have

$$\begin{aligned} \sum_n (v \cdot x_n)^2 &= \left\| \begin{pmatrix} v \cdot x_1 \\ \vdots \\ v \cdot x_N \end{pmatrix} \right\|_2^2 \\ &= \|vX^T\|_2^2 \\ &= (vX^T)(vX^T)^T \end{aligned}$$

Although this is a simple way to envision PCA, standard implementations rely on an eigendecomposition. With

$$X = \begin{pmatrix} - & x_1 & - \\ & \vdots & \\ - & x_N & - \end{pmatrix}$$

we have

$$\begin{aligned} \sum_n (v \cdot x_n)^2 &= \left\| \begin{pmatrix} v \cdot x_1 \\ \vdots \\ v \cdot x_N \end{pmatrix} \right\|_2^2 \\ &= \|vX^T\|_2^2 \\ &= (vX^T)(vX^T)^T \\ &= v(X^T X)v^T. \end{aligned}$$

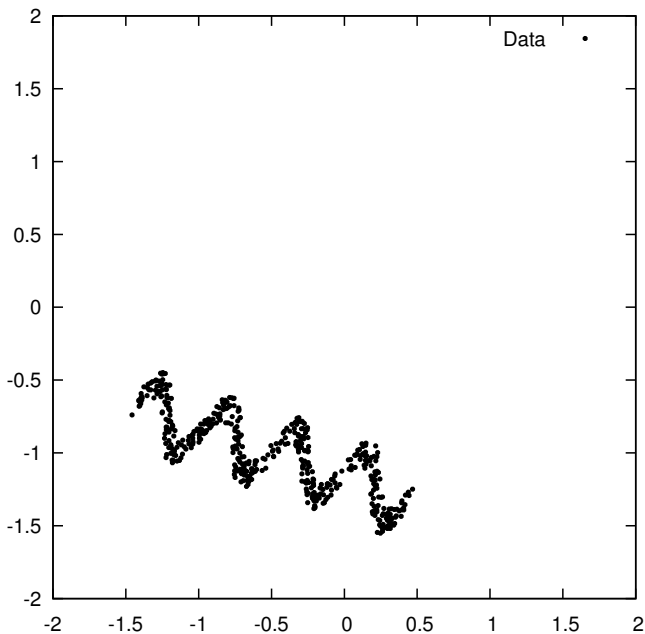
Although this is a simple way to envision PCA, standard implementations rely on an eigendecomposition. With

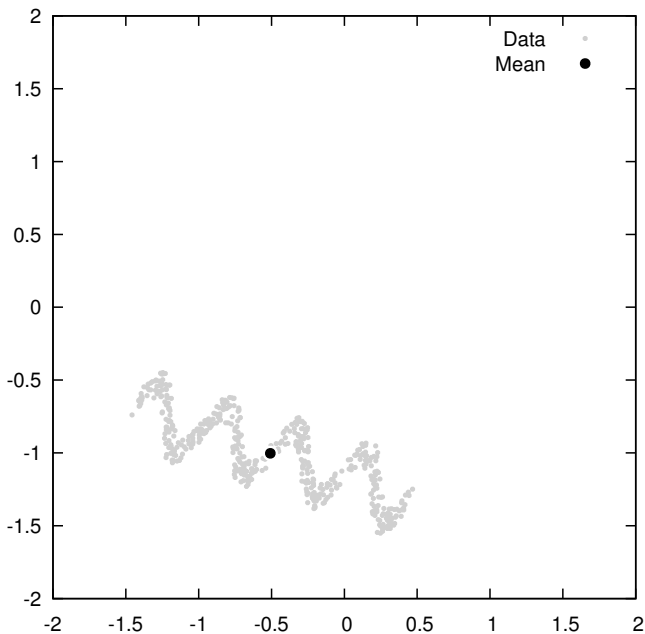
$$X = \begin{pmatrix} - & x_1 & - \\ & \vdots & \\ - & x_N & - \end{pmatrix}$$

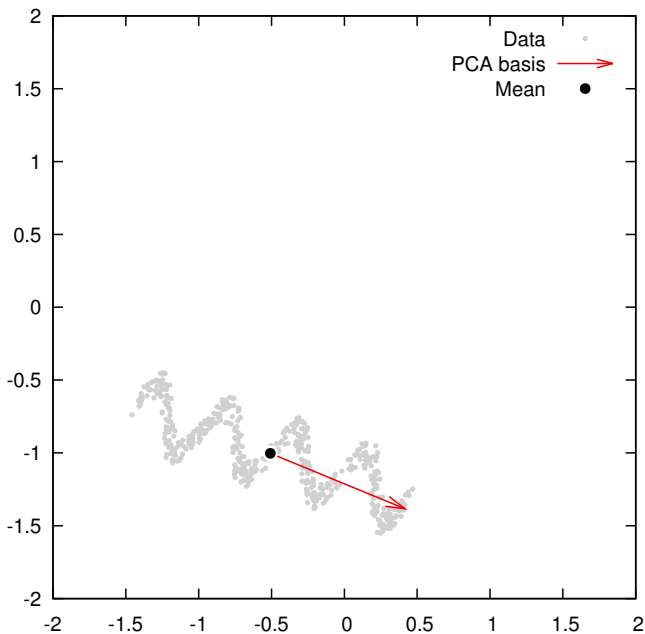
we have

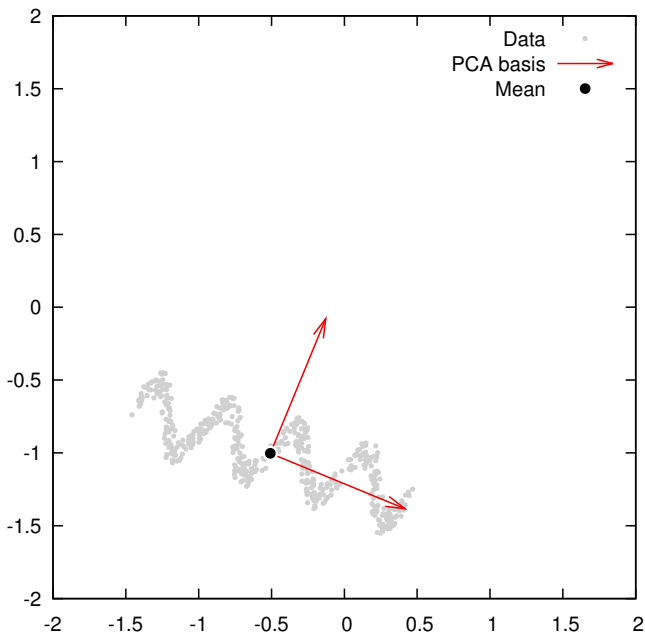
$$\begin{aligned} \sum_n (v \cdot x_n)^2 &= \left\| \begin{pmatrix} v \cdot x_1 \\ \vdots \\ v \cdot x_N \end{pmatrix} \right\|_2^2 \\ &= \|vX^T\|_2^2 \\ &= (vX^T)(vX^T)^T \\ &= v(X^T X)v^T. \end{aligned}$$

From this we can derive that v_1, v_2, \dots, v_D are the eigenvectors of $X^T X$ ranked according to [the absolute values of] their eigenvalues.





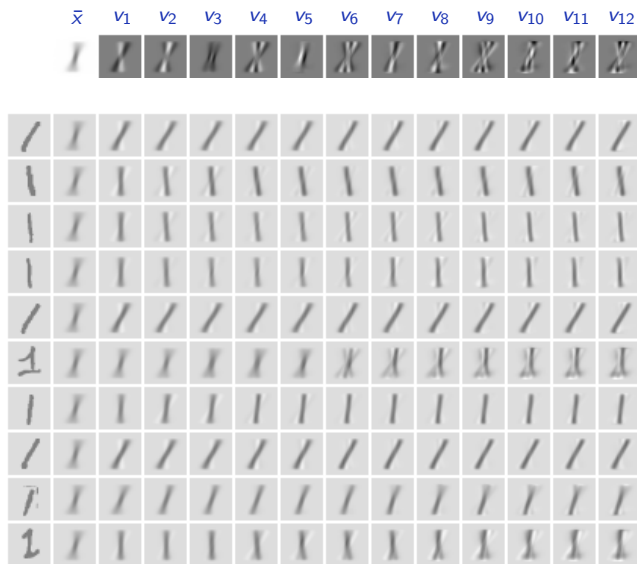


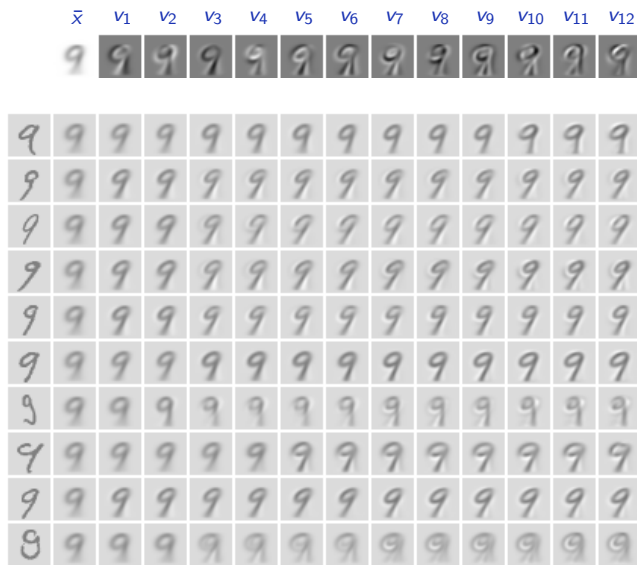


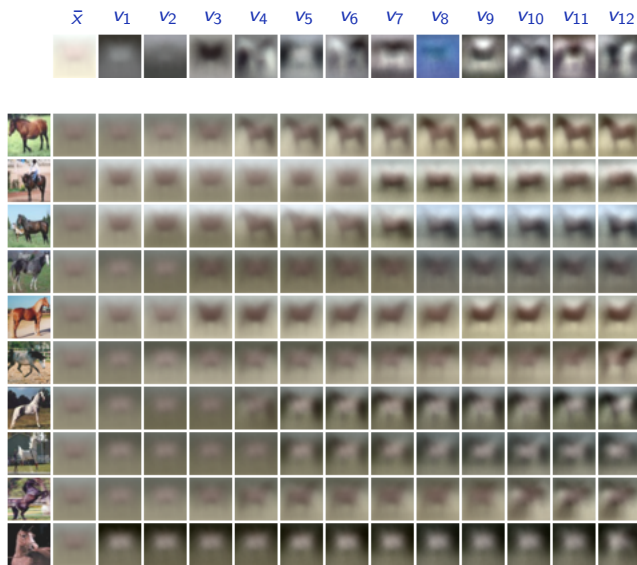
As for K -means, we can apply that algorithm to images from MNIST or CIFAR by considering them as vectors.

For any sample x and any T , we can compute a reconstruction using T vectors from the PCA basis, *i.e.*

$$\bar{x} + \sum_{t=1}^T (v_t \cdot x) v_t.$$









These results show that even crude embeddings capture something meaningful. Changes in pixel intensity as expected, but also deformations in the “indexing” space (*i.e.* the image plan).

However, translations and deformations damage the representation badly. “Composition” (*e.g.* object on background) is not handled at all.

These strengths and shortcomings provide an intuitive motivation for “deep neural networks”, and the rest of this course.

We would like

- to use many encoding “of these sorts” for small local structures with limited variability,
- have different “channels” for different components,
- process at multiple scales.

Computationally, we would like to deal with large signals and large training sets, so we need to avoid super-linear cost in one or the other.

The end

References

- A. Krizhevsky. Learning multiple layers of features from tiny images. Master's thesis, Department of Computer Science, University of Toronto, 2009.