Deep learning

2.5. Basic clusterings and embeddings

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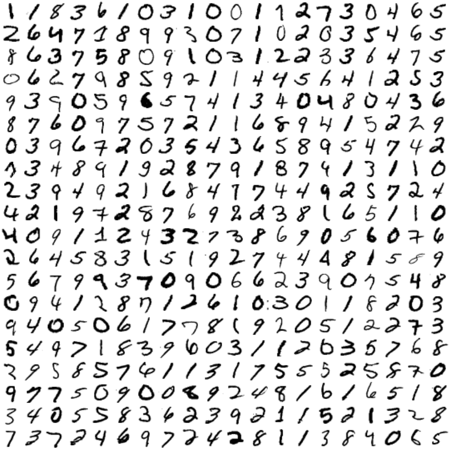
- K-means, and
- Principal Component Analysis (PCA).

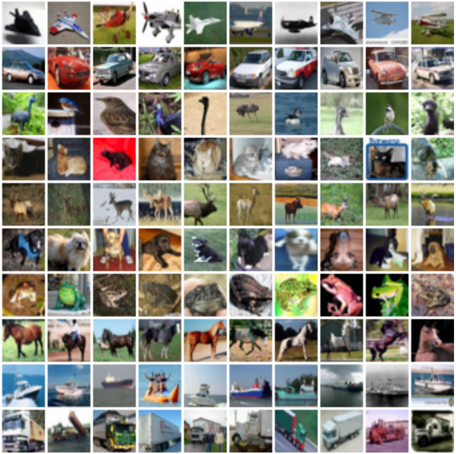
We will illustrate these methods on our two favorite data-sets.

MNIST data-set



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)

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

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

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

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

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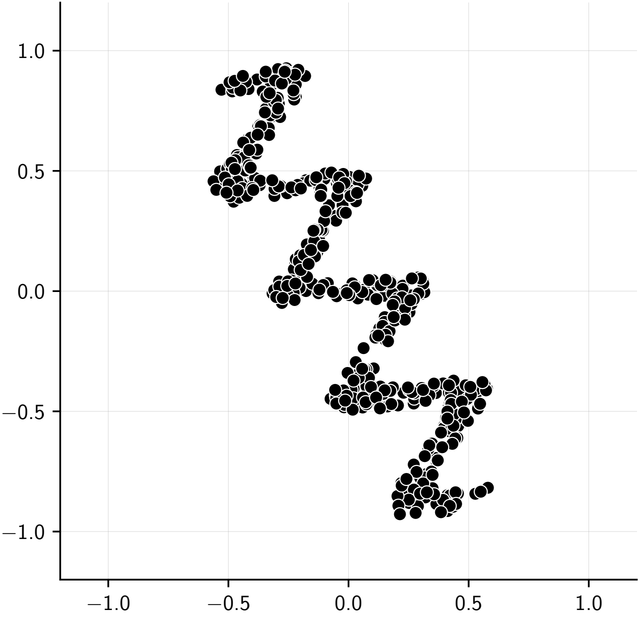
$$\underset{c_1,\dots,c_K \in \mathbb{R}^D}{\operatorname{argmin}} \sum_n \min_k \|x_n - c_k\|^2.$$

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

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

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

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.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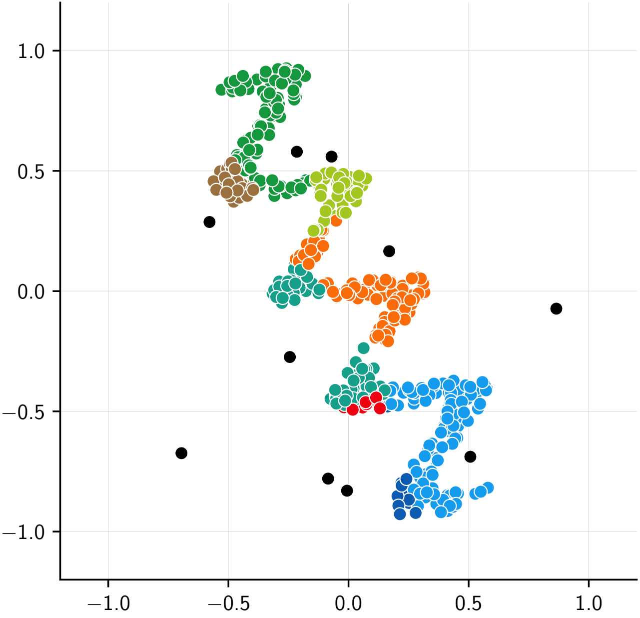

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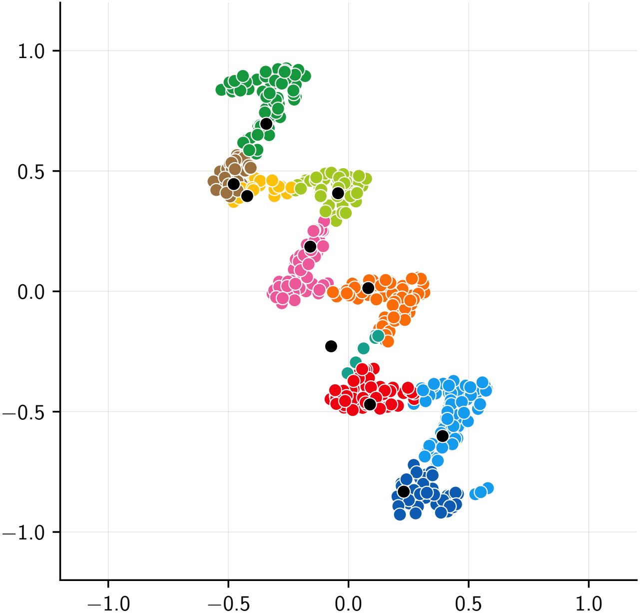
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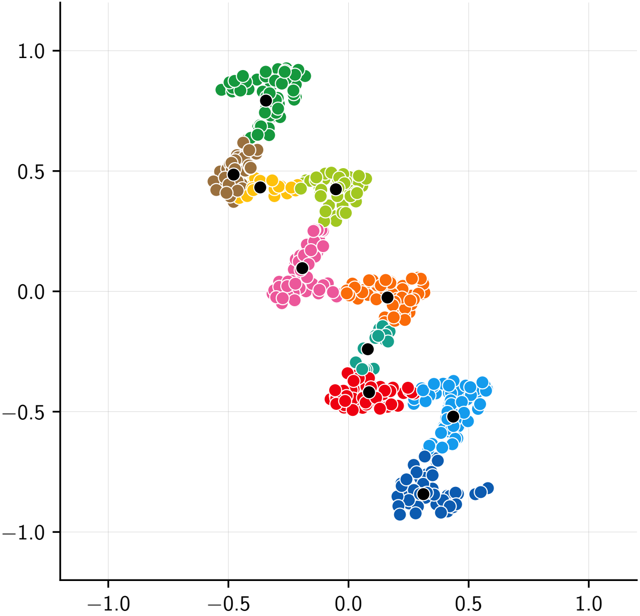
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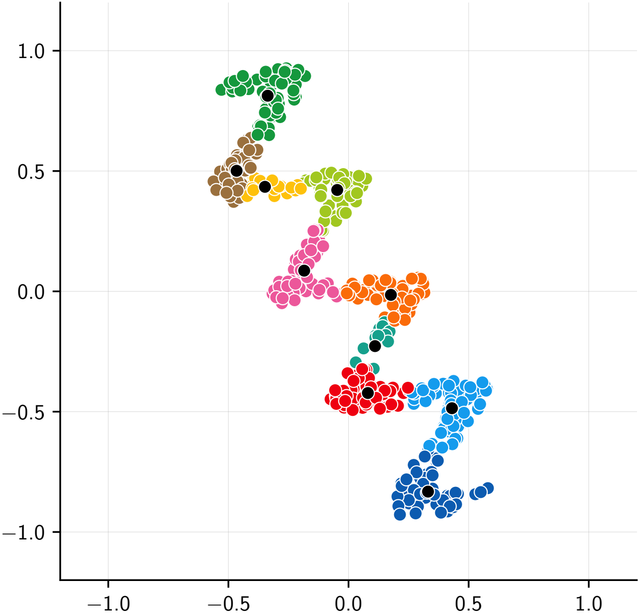

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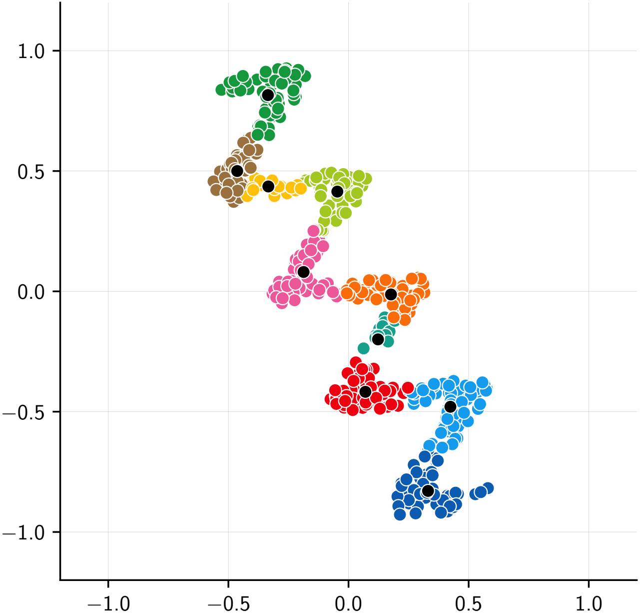
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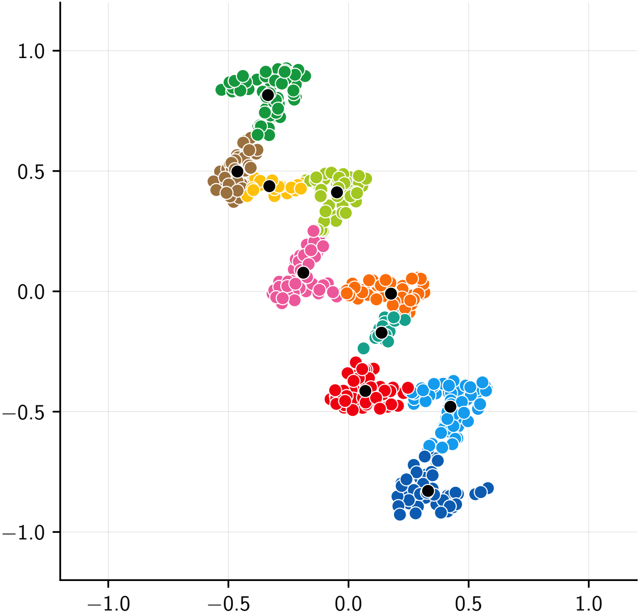

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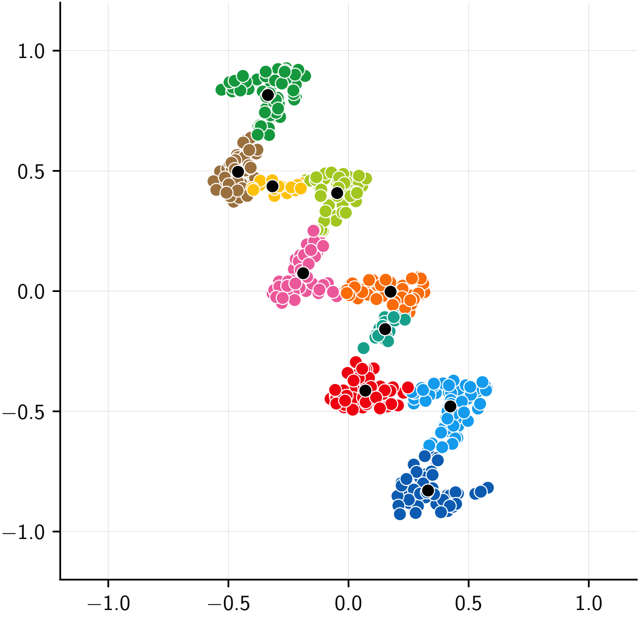

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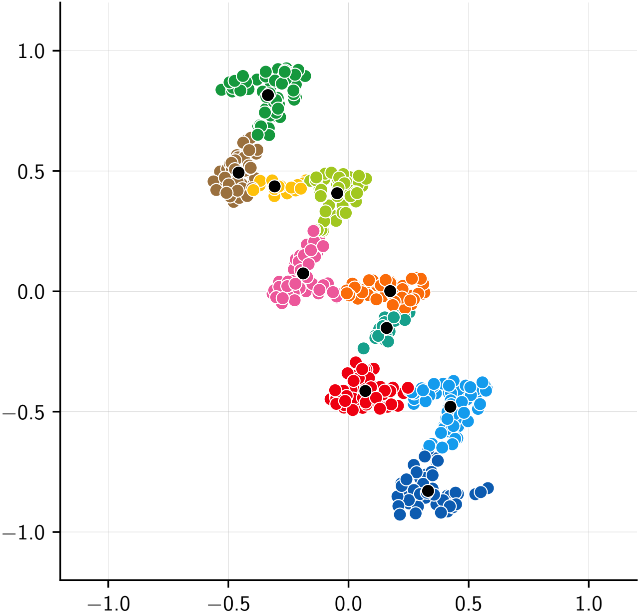
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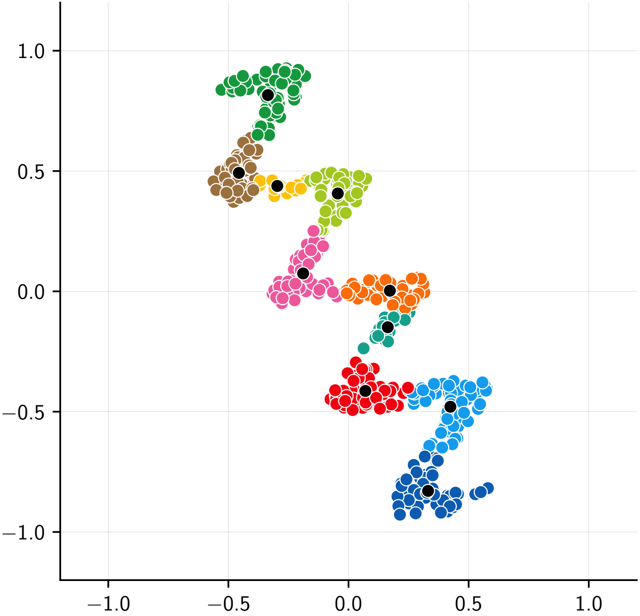

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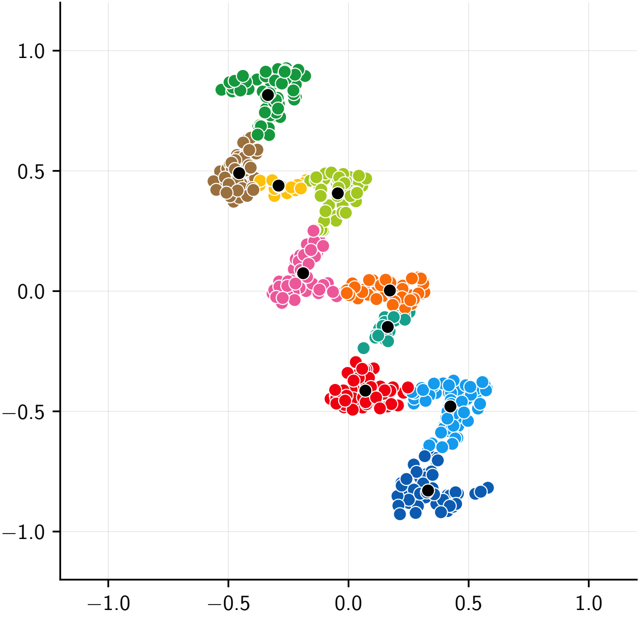
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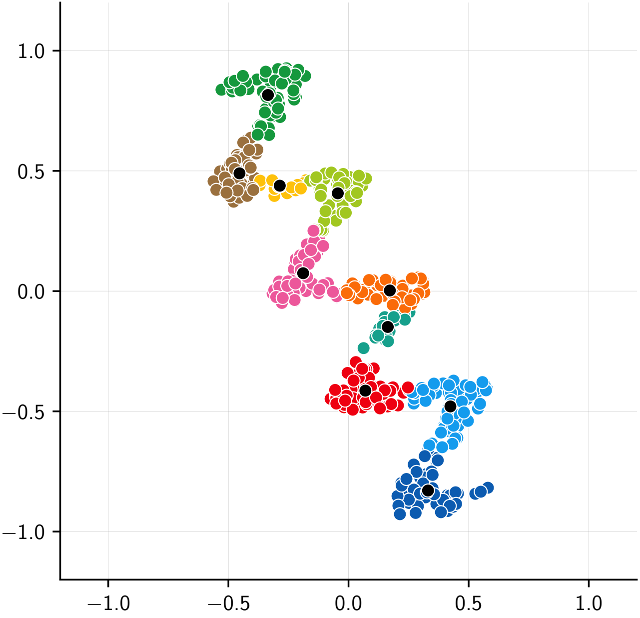
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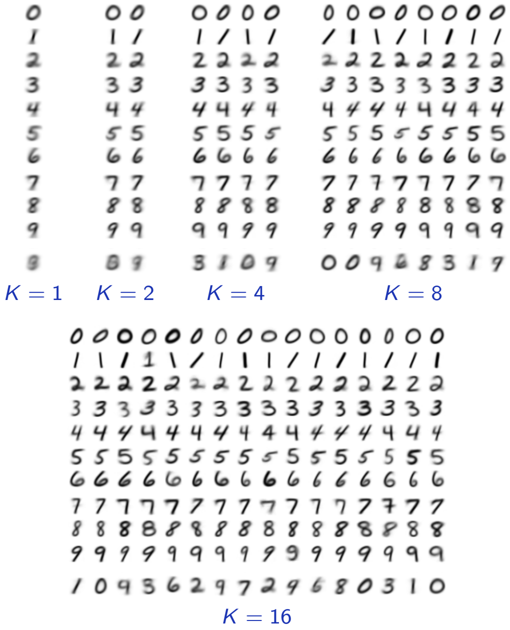
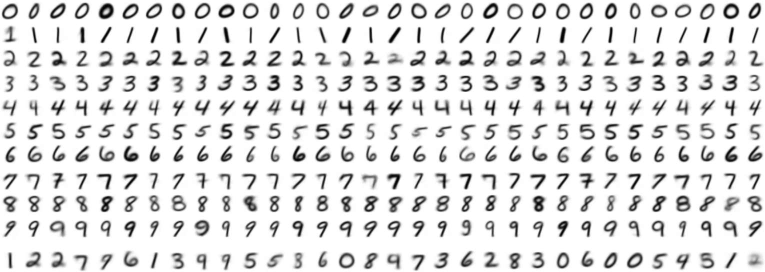
We can apply that algorithm to images from MNIST ($1 \times 28 \times 28$) or CIFAR10 ($3 \times 32 \times 32$) by considering them as vectors from $\mathbb{R}^{784}$ and $\mathbb{R}^{3072}$ respectively.

Centroids can similarly be visualized as images, and clustering can be done per-class, or for all the classes mixed.


$K = 1$
$K = 2$
$K = 4$
$K = 8$
$K = 16$



$K = 32$

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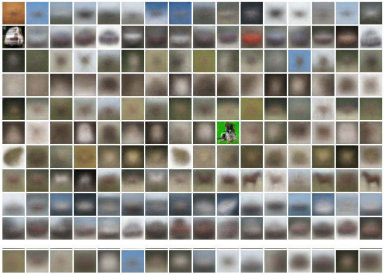

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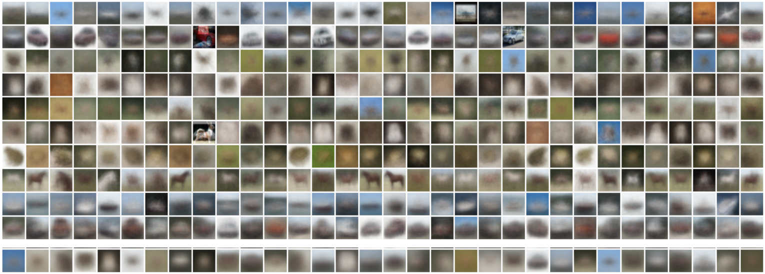

$K = 32$

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

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

(A) compute the average and center the data

$$\begin{aligned} \bar{x} &= \frac{1}{N} \sum_n x_n \\ \forall n, \; x_n^{(0)} &= x_n - \bar{x} \end{aligned}$$

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

(B) pick the direction and project the data

$$\begin{aligned} v_t &= \underset{\|v\|=1}{\operatorname{argmax}} \sum_n \left(v \cdot x_n^{(t-1)} \right)^2 \\ \forall n, \; x_n^{(t)} &= x_n^{(t-1)} - \left(v_t \cdot x_n^{(t-1)} \right) v_t . \end{aligned}$$

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

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

the centered data points, we have

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

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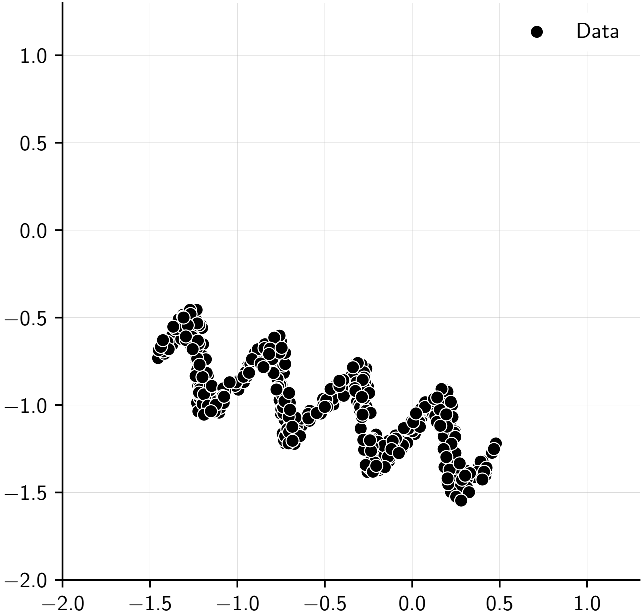
From this we can derive that $v_1, v_2, \dots, v_D$ are the eigenvectors of $X^\top X$ ranked according to [the absolute values of] their eigenvalues.


Data
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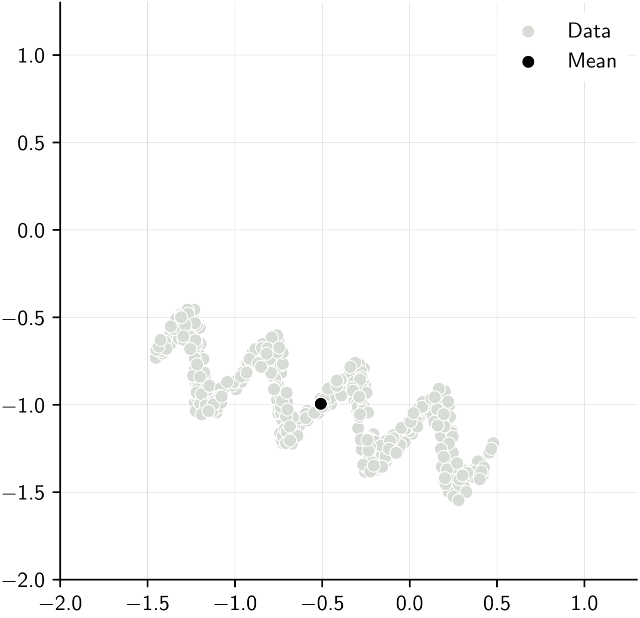
Data
Mean
1.0
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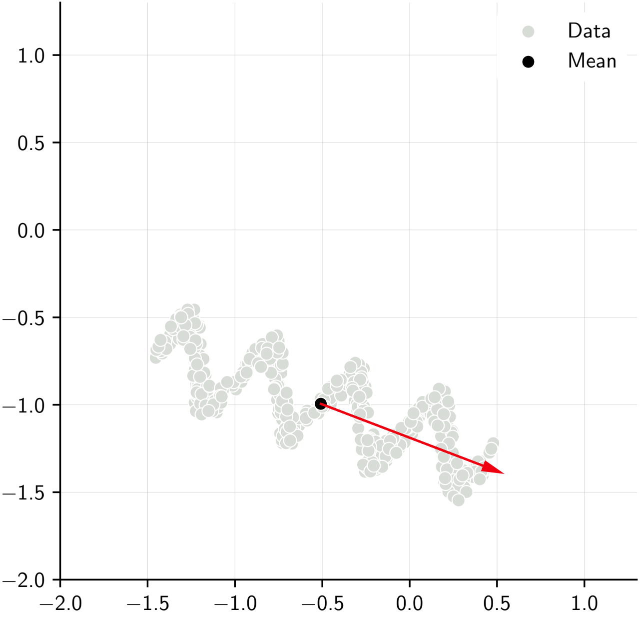

Data
Mean
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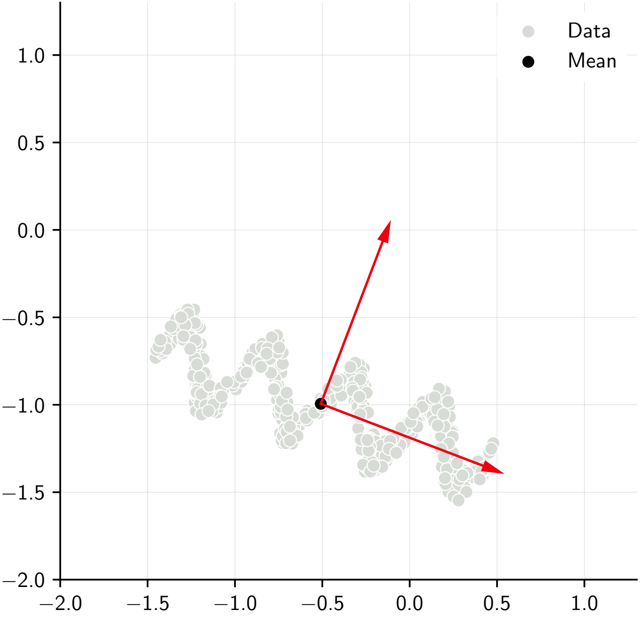
Data
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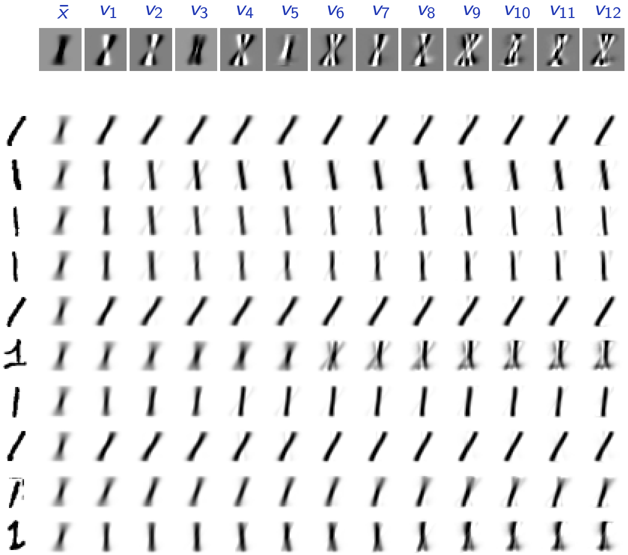
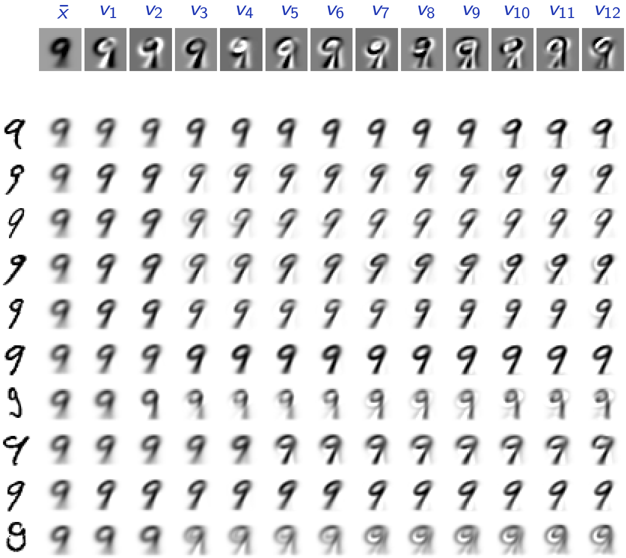
As for K-means, we can apply that algorithm to images from MNIST or CIFAR10 by considering them as vectors.

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

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



$\bar{x}$ v_1 v_2 v_3 v_4 v_5 v_6 v_7 v_8 v_9 v_{10} v_{11} v_{12}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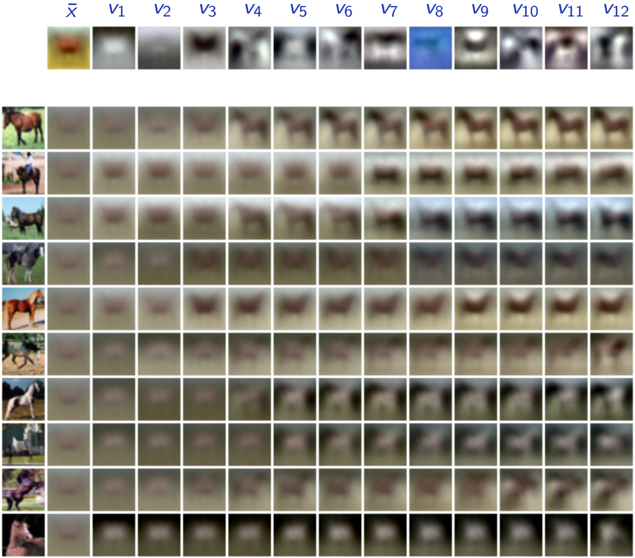
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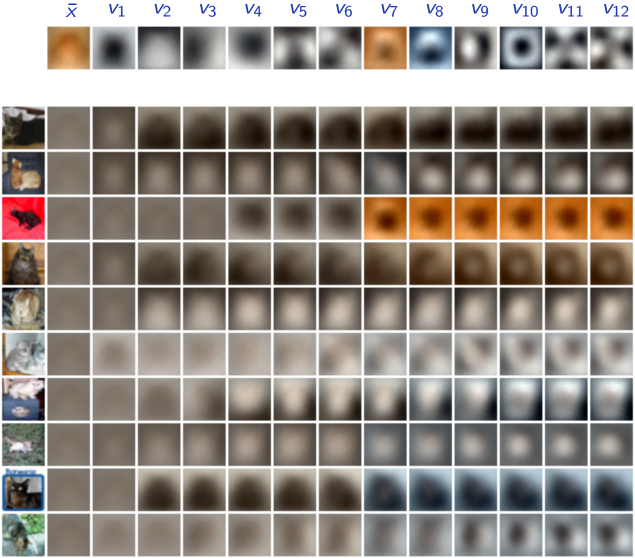
$\bar{x}$ v_1 v_2 v_3 v_4 v_5 v_6 v_7 v_8 v_9 v_{10} v_{11} v_{12}

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, and "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.