EE-559 – Deep learning

2.5. Basic clustering and embeddings

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

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- K-means, and
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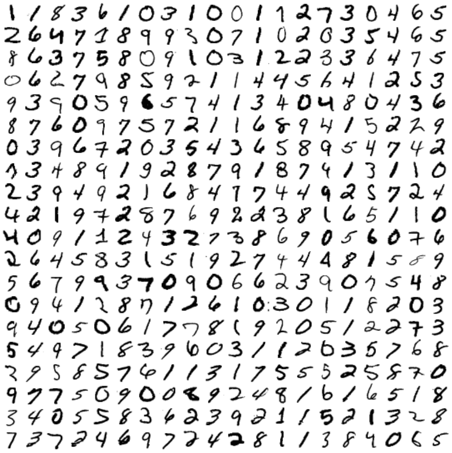
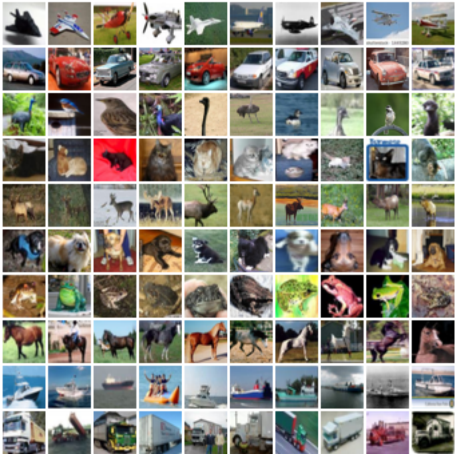
We will illustrate these methods on our two favorite data-sets.

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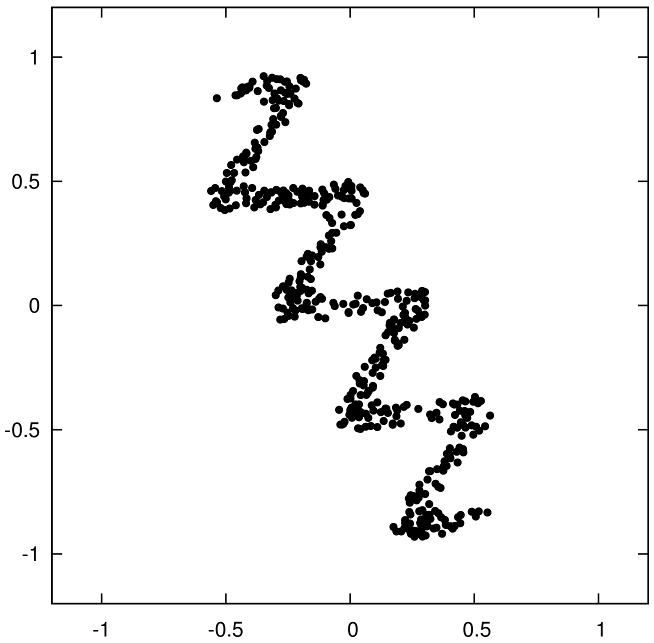
$$\underset{c_1,\dots,c_K \in \mathbb{R}^D}{\operatorname{argmin}} \sum_n \min_k \|x_n - c_k\|^2.$$

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

$$\begin{aligned} \forall n, k_n^t &= \underset{k}{\operatorname{argmin}} \|x_n - c_k^t\| & (1) \\ \forall k, c_k^{t+1} &= \frac{1}{|n : k_n^t = k|} \sum_{n : k_n^t = k} x_n & (2) \end{aligned}$$

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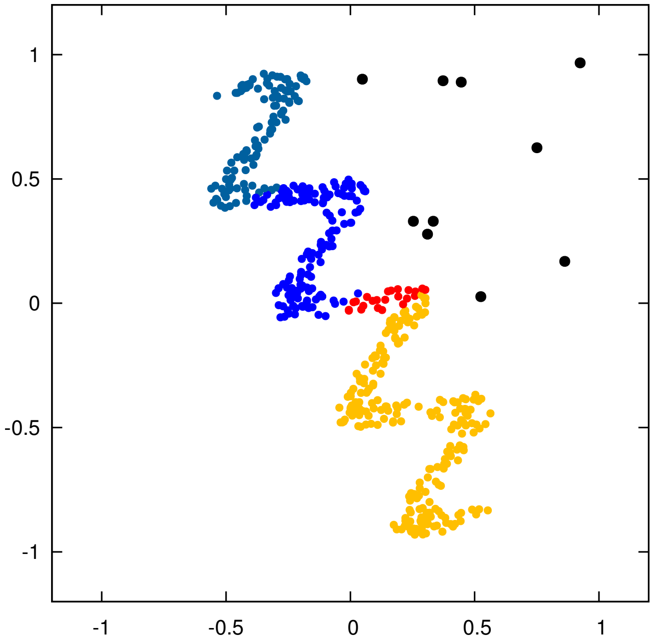
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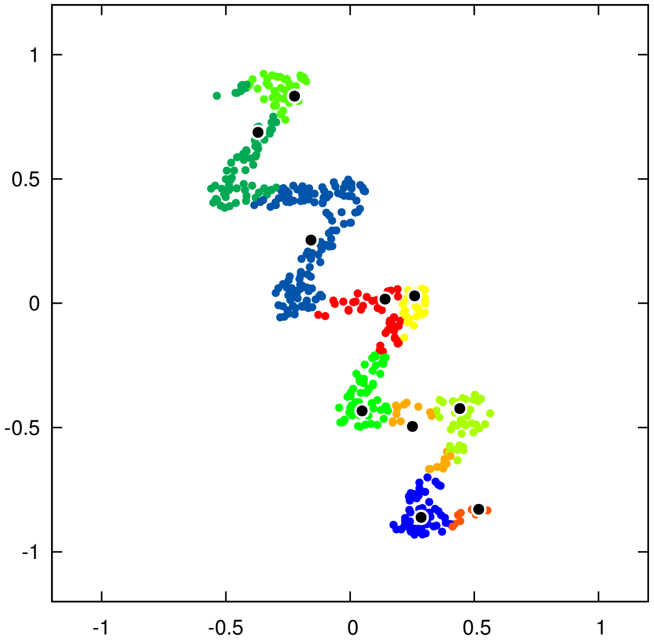
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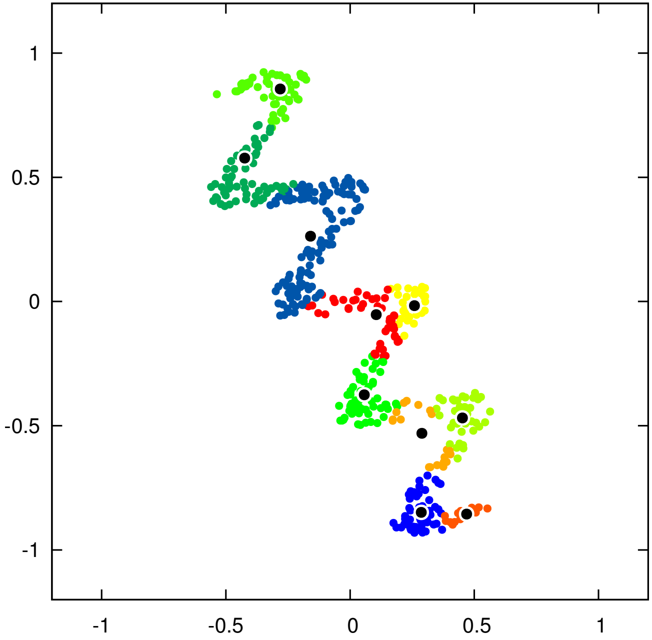
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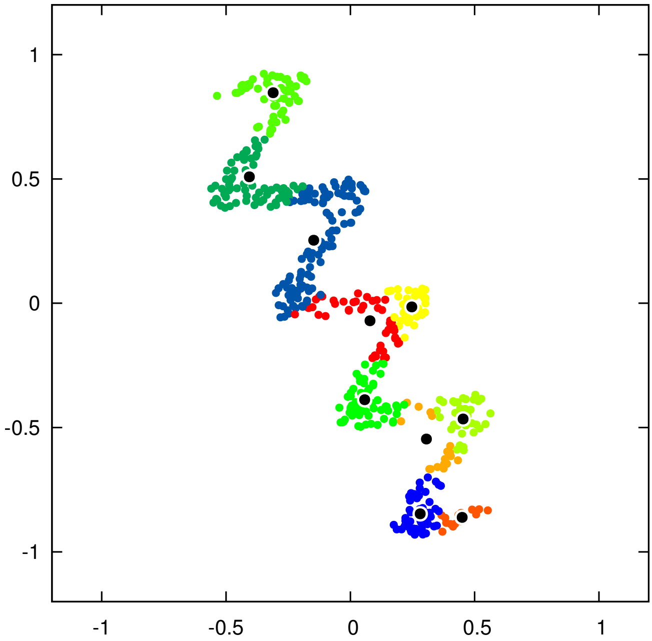
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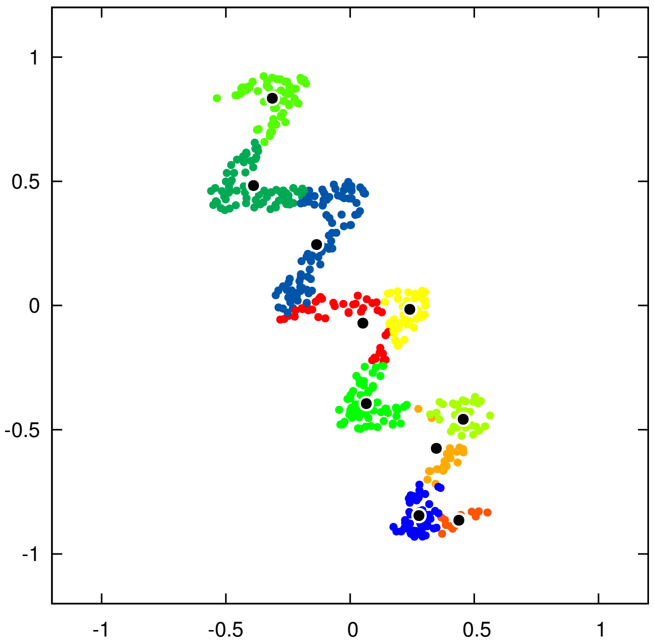
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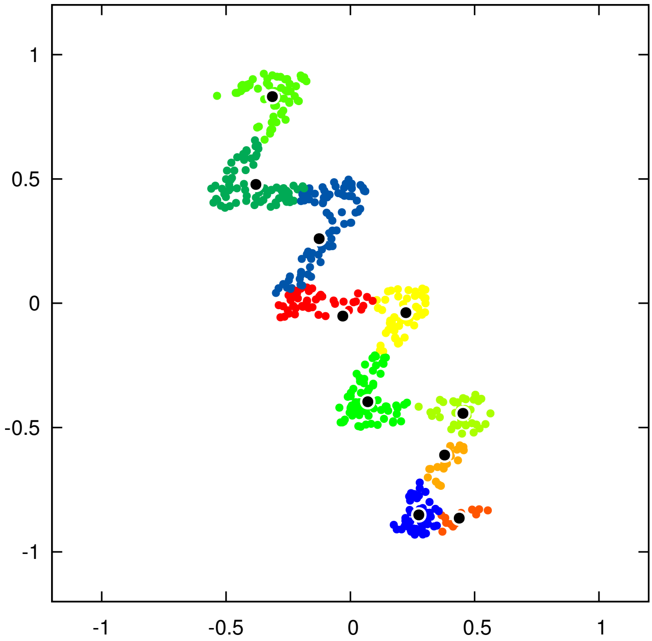
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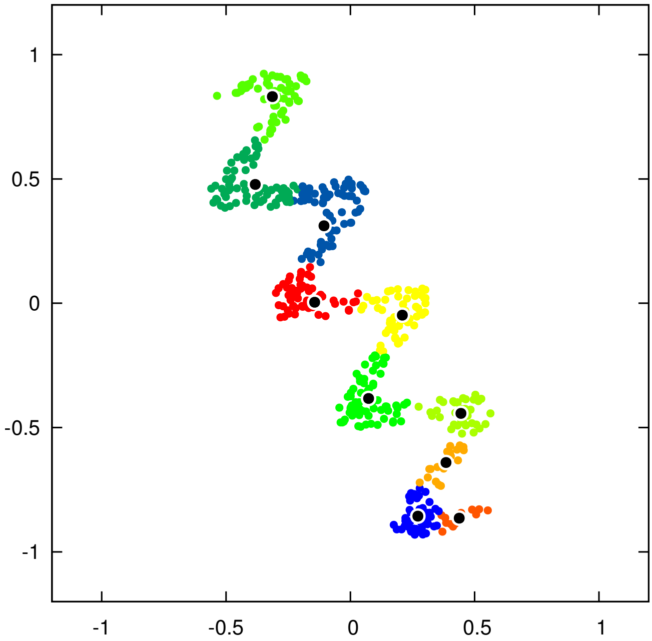
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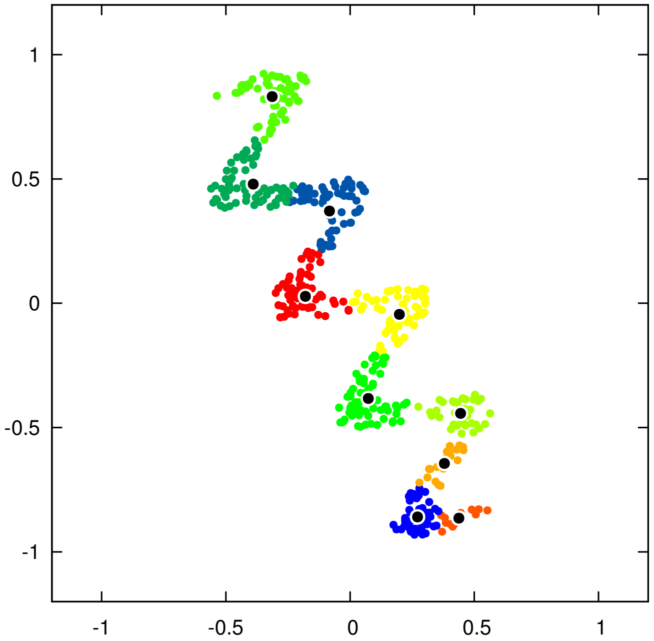
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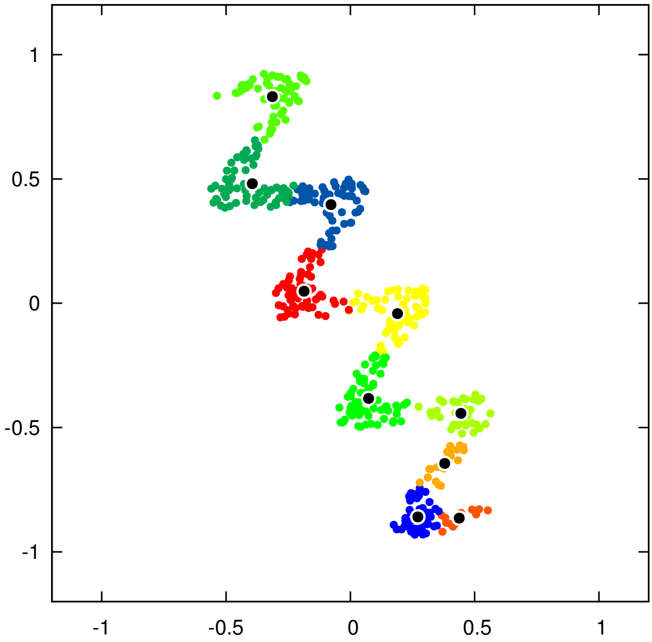
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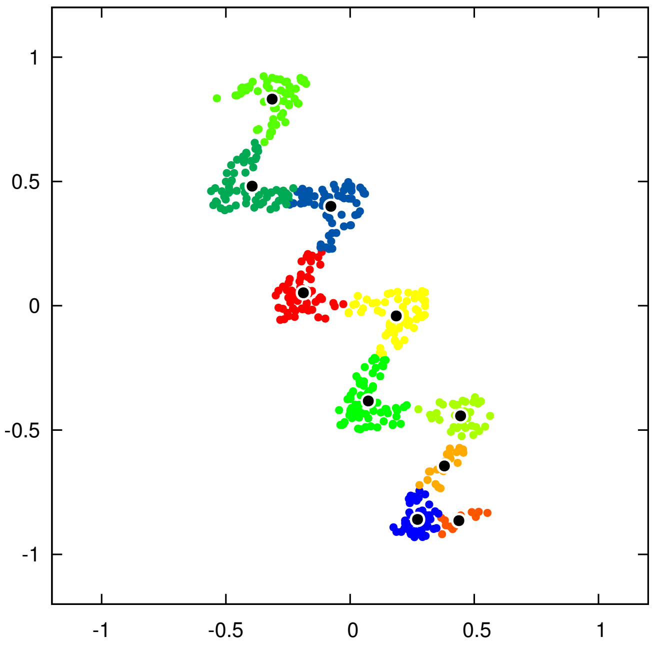
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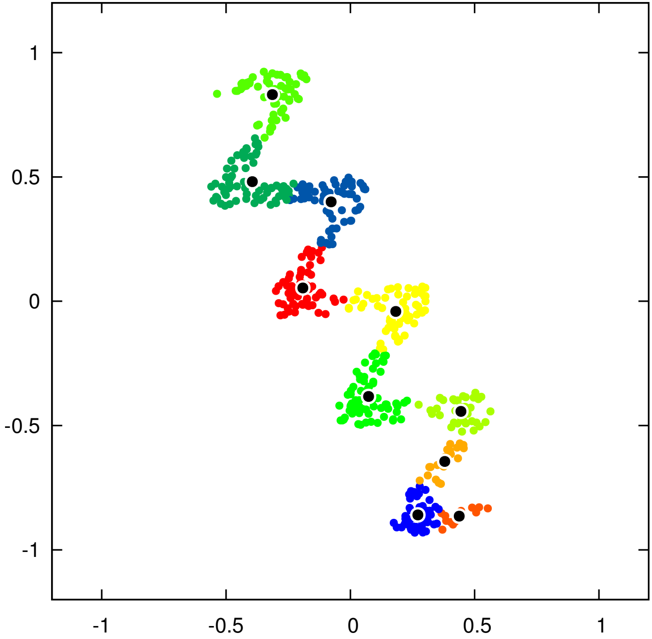
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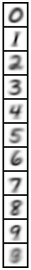
We can apply that algorithm to images from MNIST ($28 \times 28 \times 1$) or CIFAR ($32 \times 32 \times 3$) by considering them as vectors from $\mathbb{R}^{784}$ and $\mathbb{R}^{3072}$ respectively.

Centroids can similarly be visualized as images.

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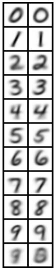
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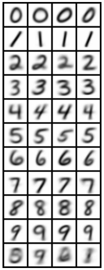
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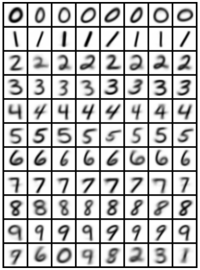
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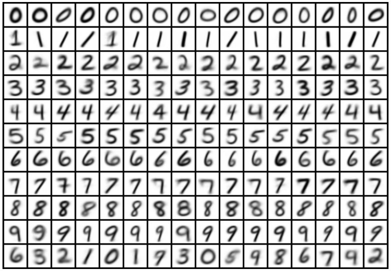
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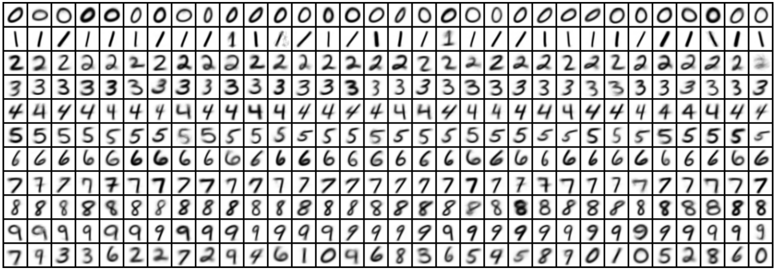
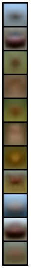
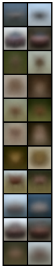


$K = 32$


$K = 1$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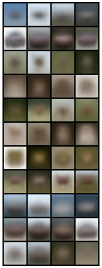
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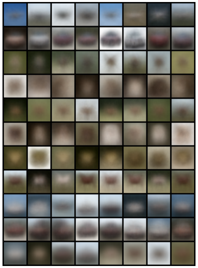
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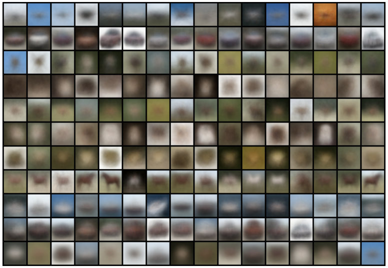
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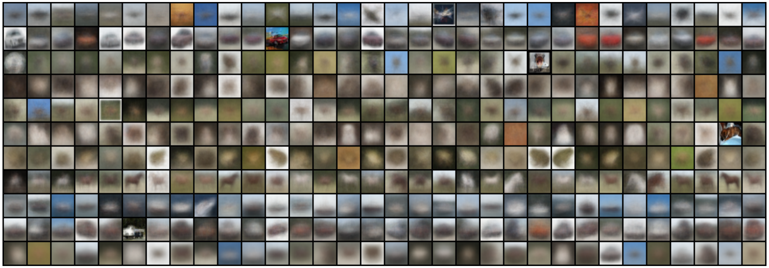

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The Principal Component Analysis (PCA) aims also at extracting an information in a L^2 sense. Instead of clusters, it looks for an "affine subspace", *i.e.* a point and a basis, that spans the data.

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 eigendecomposition. With

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

we have

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$$\begin{aligned}
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&= \left\| v X^T \right\|_2^2 \\
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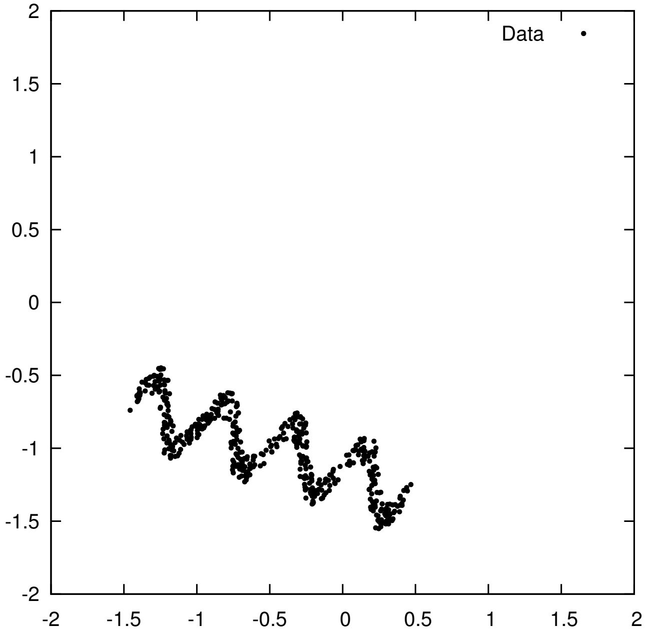
From this we can derive that $v_1, v_2, \dots, v_D$ are the eigenvectors of $X^T X$ ranked according to [the absolute values of] their eigenvalues.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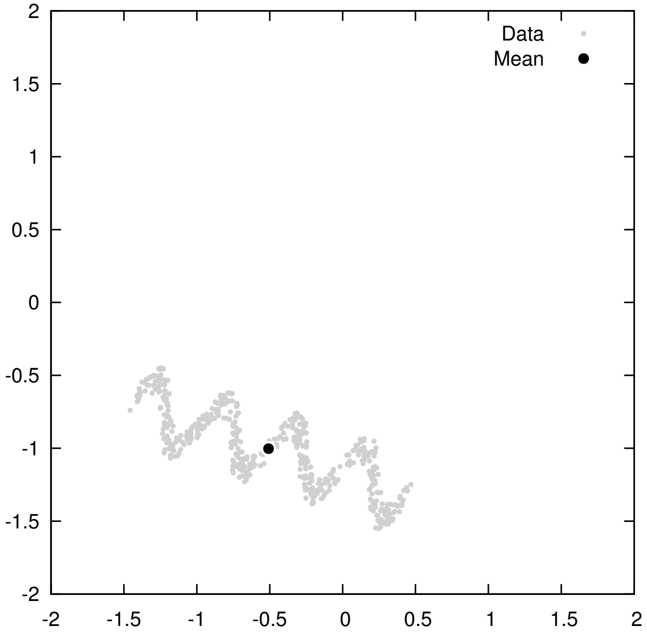
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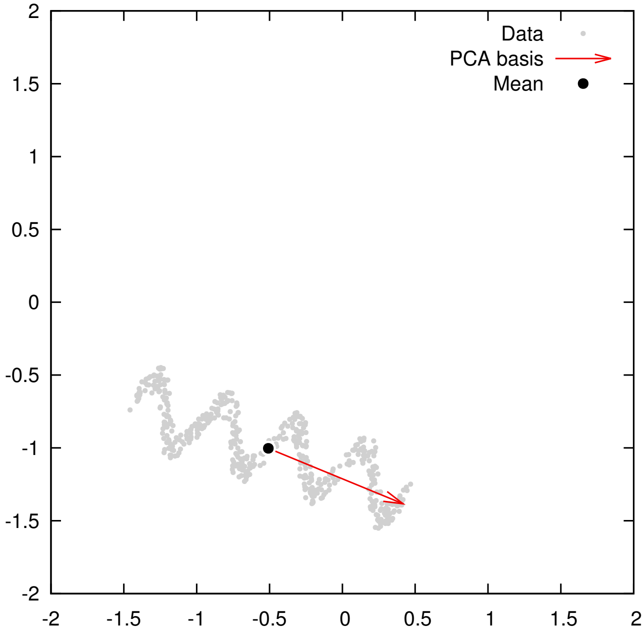
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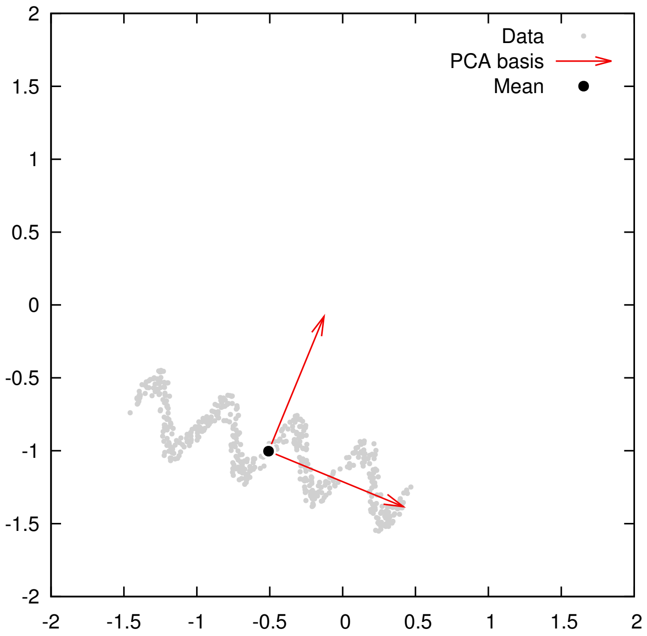
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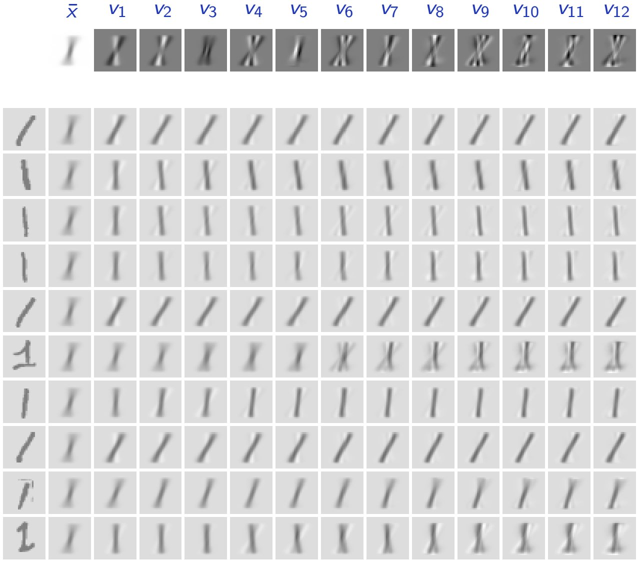
As for K-means, we can apply that algorithm to images from MNIST or CIFAR by considering them as vectors.

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

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


$\bar{x}$
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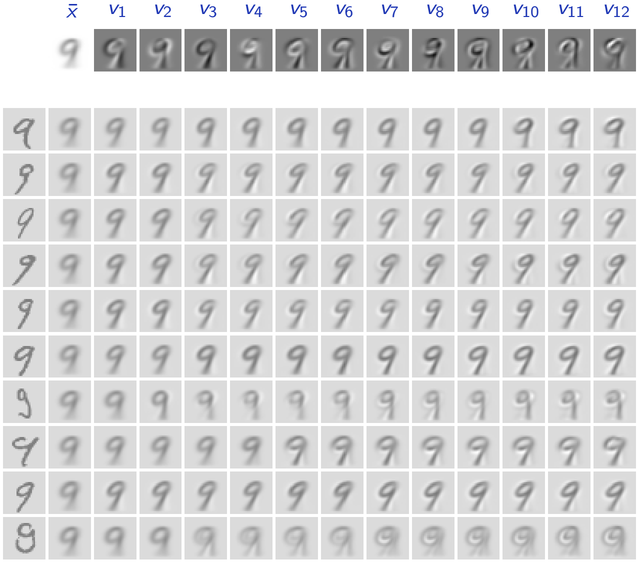
v_{10}
v_{11}
v_{12}


$\bar{x}$
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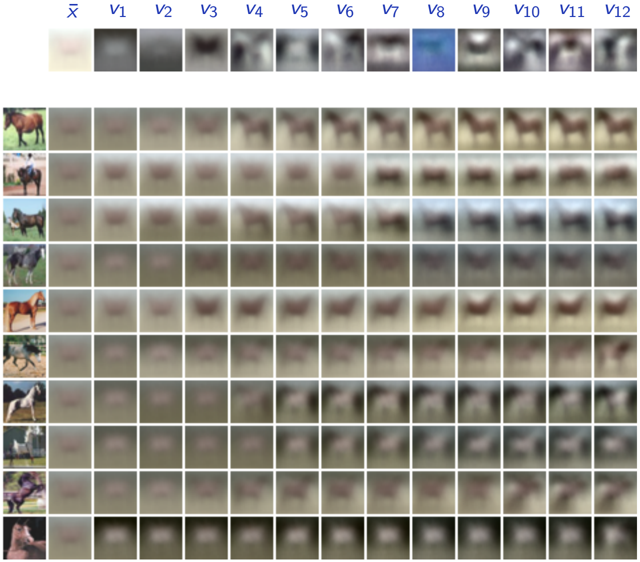
$\bar{x}$
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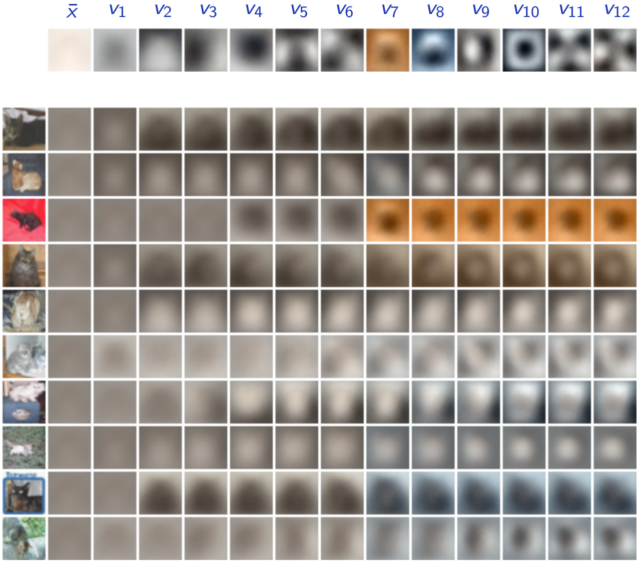
v_{12}


$\bar{x}$
v_1
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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. “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.