Manifold Learning

HIGH-DIMENSIONAL DATA

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Master Informatique Parcours Data Mining





Olivetti faces: 400 total images, 64x64 size



Grayscale faces 8b, a few images of several different people

From objets to vectors (or points)

- Oray images of size $N = m \times n$ are seen as N-dimensional vectors (by row/col concatenation)
- Call $\mathfrak{X} = \{X_1, \dots, X_k\} \subset \mathbb{R}^n$ the vector set of images
- \bigcirc Geometrically, $\mathfrak X$ is shown as a point cloud in a Euclidean space.

- O Goals: sorting, recognition
- \bigcirc Key element: reduce N to a very low quantity (e.g. 2 or 3)

Curse of Dimensionality

In general, the sample size required to estimate a function of several variables to a given degree of accuracy grows exponentially with the increasing number of variables

EXAMPLE

We want to cover the unit cube $[0,1]^D$ with a 1/10 grid. We need 10^D points which grows exponentially with D!!!

A related fact: the empty space phenomenon

High-dimensional spaces are inherently sparse

Hypervolume of Cubes and Spheres in \mathbb{R}^D

Volume of the sphere with radius r and cube of size 2r

$$V_{sph}^{D}(r) = \frac{\pi^{D/2} r^{D}}{\Gamma(D/2+1)}$$
 $V_{cube}^{D}(r) = (2r)^{D}$

Astonishingly, we get

$$\lim_{D \to \infty} \frac{V_{sph}^{D}(r)}{V_{cube}^{D}(r)} = 0$$

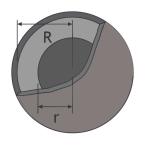
In high-dimensional spaces, the volume of the cube concentrates in its corners.

Hypervolume of a Thin Spherical Shell

Consider 2 concentric spheres with radii r and R, r < R.

(Relative) Hypervolume of the Thin

$$\frac{V_{sph}^D(R) - V_{sph}^D(r)}{V_{sph}^D(R)} = 1 - \left(\frac{r}{R}\right)^D$$



Which tends to 1 when $D \mapsto \infty$

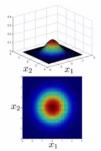
All the content of a D-dimensional sphere concentrates on its surface (which is only a (D-1) dimensional manifold)

Tail probability of isotropic Gaussian distributions

Consider an isotropic Gaussian distribution in \mathbb{R}^D which zero-mean and unit variance

Probability mass function

$$f(\mathbf{y}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{r^2}{2}\right), \quad r = \|\mathbf{y}\|$$



D	1	2	5	10	20
$Pr(r \ge 2)$	0.04550	0.13534	0.54942	0.94734	0.99995

(Semi) Diagonals of Cube

- Consider the $[-1,1]^D \subset \mathbb{R}^D$ hypercube.
- O Call **v** a (semi) diagonal from the center to a corner, so $\mathbf{v} = (\pm 1, \dots, \pm 1)^T$

Angle between any v and a coordinate axis e_i

$$\cos \theta = \left\langle \frac{\mathbf{v}}{\|\mathbf{v}\|}, \mathbf{e}_{\mathbf{i}} \right\rangle = \frac{\pm 1}{\sqrt{D}}$$

The diagonals are nearly orthogonal to all coordinate axes (for large D): visualization of high dimensional data by pairwise scatter plots may be misleading

Concentration of distances

Let $\mathbf{y} \in \mathbb{R}^D$ be a r.v. whose components are iid (and $E||y||^8 < \infty$)

Mean and Variance of the Euclidean Norm of y

$$\mu_{\parallel \mathbf{y} \parallel} \approx \sqrt{aD - b}$$
 $\sigma_{\parallel \mathbf{y} \parallel}^2 \approx b$,

where a and b are known constants and the approximation terms are controlled (for large values of D).

Consequences

- O Successive drawings of y yield almost the same norm
- Distance between any two vectors is approximately constant