Autoencoders

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General framework

The general framework of autoencoders is:

$$\mathcal{X} \ni x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \xrightarrow{B} \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_p \end{bmatrix} \xrightarrow{A} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = y \in \mathcal{Y}$$

Where $B \in \mathcal{B}$ which is a set of functions from $\mathbb{F}^n$ to $\mathbb{G}^p$ while $A \in \mathcal{A}$ which is a set of functions from $\mathbb{G}^p$ to $\mathbb{F}^n$.

General framework

The goal is to find a pair of functions A, B such that the generic dissimilarity function Δ is minimized:

$$\min E(A, B) = \min_{A,B} \sum_{1}^{m} E(x_t, y_t) = \min_{A,B} \sum_{1}^{m} \Delta(A \circ B(x_t), y_t)$$

In the auto-associative case the right side of the autoencoder is again x_t. **The focus is not on the reconstruction of the input but rather on how well we can compress the input data in the hidden layer without losing information.**

Linear autoencoders

In the case of **linear autoencoders** we have:

- $\mathbb{F}, \mathbb{G}$ are fields
- $\mathcal{A}, \mathcal{B}$ are the classes of linear transformations: A, B are respectively matrices of shape $p \times n$ and $n \times p$
- Δ is the squared Euclidean distance (L_2^2 norm)

Linear autoencoders

In general the problem of finding the matrices A, B that minimize the error function E is a non-convex optimization problem.

However, fixing one of the two matrices, the problem becomes convex so **we can find the optimal value by alternating the optimization of the two matrices.** Fixing A the optimal B is:

$$B = \hat{B}(A) = (A^\intercal A)^{-1} A^\intercal$$

While fixing B the optimal A is:

$$A = \hat{A}(B) = \Sigma_{XX} B^\intercal (B \Sigma_{XX} B^\intercal)^{-1}$$

Where Σ_{XX} is the covariance matrix of the input data.

Linear autoencoders

- Since we are applying only linear transformations, the best compression we can achieve is the one that projects the input data on the subspace spanned by the eigenvectors of the covariance matrix of the input data.
- This corresponds to the **Principal Component Analysis (PCA)** when the input is normalized as follows:

$$\hat{x}_{i,j} = \frac{1}{\sqrt{m}} \left(x_{ij} - \frac{1}{m} \sum_{k=1}^{m} x_{kj} \right)$$

Boolean autoencoders

In the case of **Boolean autoencoders** we have:

- $\mathbb{F}, \mathbb{G}$ are the Boolean fields, i.e $\{0, 1\}$, the Galois field $\mathbb{F}_2$
- $\mathcal{A}, \mathcal{B}$ are the classes of Boolean transformations: A, B are respectively matrices of shape $p \times n$ and $n \times p$ with entries in $\{0, 1\}$
- Δ is the Hamming distance

Boolean autoencoders

We start defining the following lemma:

Lemma

The vector Majority(p) is a vector in $\mathbb{H}^n$ closest to the center of gravity of the vectors $p_1, \ldots, p_k$ and it minimizes the function $E(q) = \sum_{i=1}^{k} \Delta(p_i, q)$.

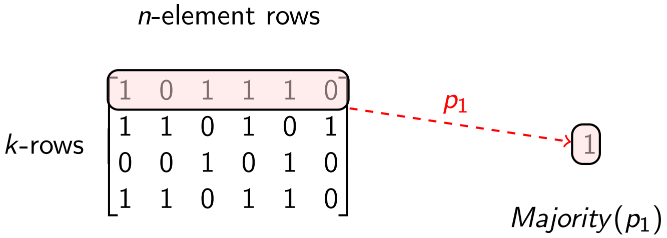
Where the center of gravity is the vector c in $\mathbb{R}^n$ with coordinates

$$c_j = \frac{\left(\sum_{i=1}^{k} p_{ji} \right)}{k}$$

So, each c_j is the average of the j-th components of the vectors $p_1, \ldots, p_k$. For any j, $(p)_j$ is the closest binary value to c_j.

Boolean autoencoders

This means that for each row, we check the majority of the values and we set the value of the row to the majority value.



$$\begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}$$

Boolean autoencoders

A **Voronoi partition** of $\mathbb{H}^n$ generated by the vectors $p_1, \dots, p_k$ is a partition of $\mathbb{H}^n$ into k regions $\mathcal{C}^{Vor}(p_1), \dots, \mathcal{C}^{Vor}(p_k)$ such that for each x in $\mathbb{H}^n$:

$$x \in \mathcal{C}^{Vor}(p_i) \iff \Delta(x, p_i) \leq \Delta(x, p_j) \text{ for all } j \neq i$$

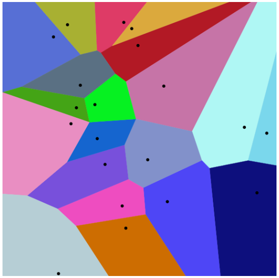


Figure: Euclidean distance

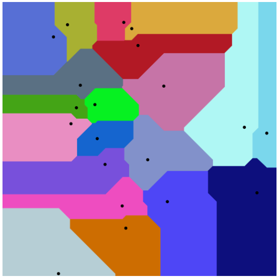


Figure: Manhattan distance

Boolean autoencoders

Considering the two steps mapping:

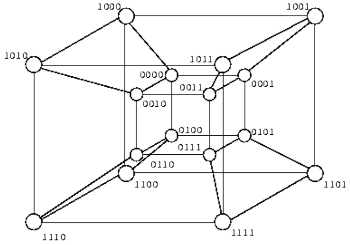
$$x \xrightarrow{B} h \xrightarrow{A} y$$

Theorem

Fixed layer solution: *if the A mapping is fixed , then the optimal mapping B^* is given by $B^*(x) = h_i$ for any x in $\mathcal{C}_i = \mathcal{C}^{\mathsf{Vor}}(A(h_i))$. Conversely, if B is fixed, then the optimal mapping A^* is given by $A^*(h_i) = Majority\left[\mathcal{X} \cap B^{-1}(h_i)\right]$*

Boolean autoencoders

If we consider the input-output layers to have a cardinality of 4 and the hidden layer to have a cardinality of 2, then this would mean that there would be $2^2 = 4$ centroids given by the A mapping in the space $\mathbb{H}^4$ showed in figure:



So, the Voronoi partition would be the partition of the hypercube into 4 regions using as metric the Hamming distance, i.e. the number of edges that need to be crossed to go from one point to each centroid.

Complexity recap

The basic classes for complexity are:

- $\mathcal{P}$ is the class of problems that can be *solved* in polynomial time by a deterministic TM
- $\mathcal{NP}$ is the class of problems for which a solution can be *verified* in polynomial time by a deterministic TM. The class $\mathcal{NP}$ is the class of problems that can be solved non-deterministically in polynomial time
  - $\mathcal{NP}$-**complete** if it is in $\mathcal{NP}$ and every problem in $\mathcal{NP}$ can be reduced to it in polynomial time
  - $\mathcal{NP}$-**hard** if there is a $\mathcal{NP}$-complete problem that can be reduced to it in polynomial time

Complexity recap

Theorem

Consider the following hypercube clustering problem:

- **Input:** *m binary vectors $x_1, \ldots, x_m$ of length n and an integer k*
- **Output:** *k binary vectors $c_1, \ldots, c_k$ of length n (the centroids) and a function f from $\{x_1, \ldots, x_m\}$ to $\{c_1, \ldots, c_k\}$ that minimizes the distortion*

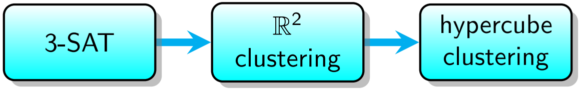
  $$E = \sum_{t=1}^{m} \Delta(x_t, f(x_t))$$

  Where Δ is Hamming distance.

The hypercube clustering decision problem $\mathcal{NP}$-hard when $k \sim m^{\epsilon}$ $(\epsilon > 0)$

Clustering complexity

To prove the hypercube clustering problem is $\mathcal{NP}$-hard we need to reduce prove that an $\mathcal{NP}$-complete problem can be reduced to it in polynomial time. The following reductions are used:


3-SAT
$\mathbb{R}^2$ clustering
hypercube clustering