# Lecture FYS5429, March 19, 2024

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# Autoencoders

input $x$

encoder part $h = f(W, x)$

linear approx $h = W \cdot x$

decoder part $\tilde{x} = g(V, h)$

linear approx $\tilde{x} = V \cdot h$

$= V \cdot W \cdot x$

## Reconstruction error

$$J(x) = \frac{1}{n} \|(x - \tilde{x})\|_2^2$$

$$= \frac{1}{n} \|(x - VW \cdot x)\|_2^2$$

$$X^{OLS} = \begin{bmatrix} | & | & & | \\ x_0 & x_1 & \cdots & x_{p-1} \\ | & | & & | \end{bmatrix}$$

covariance mtx

$$\Sigma_x = \frac{1}{n} X^T X = \mathbb{E}[X X^T]$$

$$X \in \mathbb{R}^{n \times p}$$

SVD of $X = U D V^T$

$U \in \mathbb{R}^{n \times n}$, $D \in \mathbb{R}^{n \times p}$

$$V \in \mathbb{R}^{p \times p}$$

$$VV^T = V^T V = \mathbb{1}_{p \times p} \quad \wedge \quad UU^T = U^T U = \mathbb{1}_{n \times n}$$

$$D = \begin{bmatrix} \sigma_0 & & & 0 \\ & \sigma_1 & & \\ & 0 & \ddots & \\ & & & \sigma_{p-1} \\ & & & 0 \end{bmatrix}$$

$$\sigma_0 > \sigma_1 > \dots > \sigma_{p-1} > 0$$

$$\Sigma_x = \mathrm{cov}[x]$$

$$S^T \Sigma_x S = \Sigma_y =$$

$$= \begin{bmatrix} \mathrm{var}[y_0] & & 0 \\ & \ddots & \\ 0 & & \mathrm{var}[y_{p-1}] \end{bmatrix}$$

$$\mathrm{var}[y_i] = \sigma_i^2/n$$

$$\mathrm{var}[y_0] > \mathrm{var}[y_1] \dots > \mathrm{var}[y_{p-1}]$$

$$\Sigma_x = \frac{1}{n} X^T X = \frac{1}{n} V D^2 V^T$$

$$\Sigma_x V = \frac{1}{n} V D^2 \Rightarrow$$

$$\Sigma_x v_i' = \frac{1}{n} \sigma_i^2 v_i'$$

$$V = \begin{bmatrix} | & & | \\ v_0 & \cdots & v_{p-1} \\ | & & | \end{bmatrix}$$

Define reduced space $d$

$$\sum_{i=0}^{d-1} \mathrm{var}[y_i] \leq \Lambda \qquad d \leq P$$

$\Lambda = 0.95$ of total variance

$$= \sum_{i=0}^{P-1} \mathrm{var}[y_i]$$

$$= \sum_{i=0}^{P-1} \sigma_i^2 / n$$

$d = 1 \qquad v_0 \qquad v_0^T v_0 = \delta_{00}$

Reconstruction error

$$J(x) = \frac{1}{n} \| (x - \underbrace{v_0 v_0^T x}_{\tilde{x}}) \|_2^2$$

Autoencoder

linear approx $\quad \frac{1}{n} \| (x - \underbrace{VW}_{v_0 v_0^T} x) \|_2^2$

Statistical approach to PCA

Theorem: assume vector $x$ has its principal component which can be computed from the eigenvector of its covariance matrix

$$\Sigma_x = \mathbb{E}[xx^T]$$

$(XX^T)$

Then the first _d_ principal components

of a zero-mean multivariate random variable $X$ with

$y_i \,, \quad i = 0, \ldots d-1$

$y_i = u_i^T X$

where $u_i \,, i = 0, \ldots d-1$, are orthonormal vectors of

$\Sigma_x = \mathbb{E}[XX^T]$ associated

with the $d$-largest eigen values, $\sigma_i = \mathrm{var}[y_i]$

**Proof**

$$\mathrm{var}[u^T x]$$

$$= \mathbb{E}[(u^T x)^2]$$

$$= \mathbb{E}[u^T x x^T u]$$

$$= u^T \mathbb{E}[x x^T] u$$

$$= u^T \Sigma_x u$$

$$= \Sigma_y = \begin{bmatrix} \mathrm{var}[y_0] & 0 \\ 0 & \ddots \end{bmatrix}$$

optimization

$$\max \quad u_0^T \Sigma_x u_0$$

$$\text{s.t.} \quad u_0^T u_0 = 1$$

$$\mathcal{L} = u_0^T \Sigma_x u_0 + \lambda_0 (1 - u_0^T u_0)$$

derivatives wrt $u_0, \lambda_0$

$$\Sigma_x u_0 = \lambda_0 u_0 \quad \text{and} \quad u_0^T u_0 = 1$$

$$\lambda_0 = \mathrm{var}[y_0]$$

second principal component

$$u_1^T u_0 = 0$$

$$\mathcal{L} = u_1^T \Sigma_X u_1 + \lambda_1 (1 - u_1^T u_1) + \gamma\, u_0^T u_1$$

Derivatives w.r.t. $u_1, \lambda_1, \gamma$

$$\Sigma_X u_1 + \gamma/2\, u_0 = \lambda_1 u_1$$

$$u_1^T u_1 = 0 \quad \wedge \quad u_1^T u_0 = 0$$

multiply with $u_0^T$

$$\underbrace{u_0^T \Sigma_X}_{\lambda_0 u_0^T} u_1 + \gamma/2\, \underbrace{u_0^T u_0}_{=1} = \lambda_1 \underbrace{u_0^T u_1}_{=0}$$

$$\Rightarrow \gamma = 0$$

$$\Rightarrow \quad \Sigma_x u_1 = \lambda_1 u_1$$

$$\Rightarrow \quad \mathrm{var}[y_1] = u_1^T \Sigma_x u_1$$

in general

$$\mathcal{L} = u_i^T \Sigma_x u_i + \lambda_i (1 - u_i^T u_i)$$

$$+ \sum_{j=0}^{i-1} \gamma_j \, u_i^T u_j$$

Generative Methods:-

$$P(x;\theta) = \frac{f(x;\theta)}{Z(\theta)}$$

$$Z(\theta) = \int_{x \in D} dx\, f(x;\theta)$$