c∗GMVÆs—q

Kolb, Yiftach

January 30, 2023

MAX-PLANCK-INSTITUT
FÜR MOLEKULARE GENETIK

c∗GMVÆs—q

a Master Thesis in Bioinformatics

Advisor / Reviewer: Professor Martin Vingron
Reviewer: Professor Tim Conrad

Freie Universität Berlin

Topics to cover

- what was our initial subject of interest
- AEs are non-linear PCA basically
- VAEs
- other animals
- GMVAE and why I derived c$*$GMVÆ
- example use of c$*$GMVÆ on synthetic conditional-categorical data
- examples on MNIST
- examples on scRNAseq

Autoencoders

A "vanilla" autoencoder is a neural networks that "learns" the identity (subject to dimensional restriction).

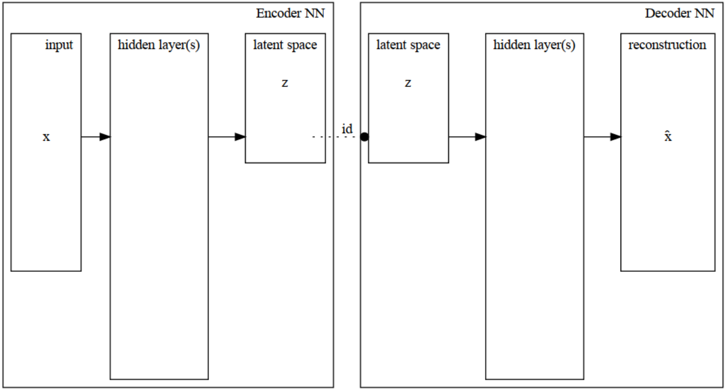

Figure: Autoencoder

Autoencoders and PCA

(On centered data[2])

PCA

$$\tilde{\boldsymbol{V}} = \operatorname{argmin}_{\mathbf{W}}\{\|\mathbf{X} - \mathbf{X}\boldsymbol{W}\boldsymbol{W}^T\|_F^2 \quad : \quad \boldsymbol{W} \in \mathbb{R}^{n\times l}, \boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{I}_l\} \tag{1}$$

Linear AE

$$\operatorname{argmin}_{\boldsymbol{E},\boldsymbol{D}}\{\|\mathbf{X} - \mathbf{X}\boldsymbol{E}\boldsymbol{D}\|_F^2 \quad : \quad \boldsymbol{E}, \boldsymbol{D}^{\boldsymbol{T}} \in \mathbb{R}^{n\times l},\} \tag{2}$$

$$\tilde{\boldsymbol{W}} \in \operatorname{argmin}_{\mathbf{W}}\{\|\mathbf{X} - \mathbf{X}\boldsymbol{W}\boldsymbol{W}^\dagger\|_F^2 \quad : \quad \boldsymbol{W} \in \mathbb{R}^{n\times l},\} \tag{3}$$

$$\operatorname{span}\{\tilde{\boldsymbol{W}}\} = \operatorname{span}\{\tilde{\boldsymbol{V}}\}$$

VAEs

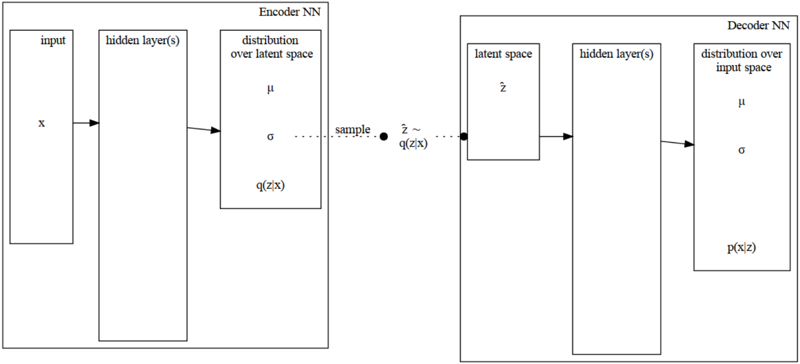

Figure: VAE

$$
\begin{aligned}
\frac{1}{N}\log p(\boldsymbol{X}) &= \frac{1}{N}\log\int p(\boldsymbol{X},\boldsymbol{Z})d\boldsymbol{Z} && \text{taking marginal} \\
&= \frac{1}{N}\log\int \frac{p(\boldsymbol{X},\boldsymbol{Z})}{q(\boldsymbol{Z})}q(\boldsymbol{Z})d\boldsymbol{Z} && \text{multiplying by 1 inside} \\
&= \frac{1}{N}\log\int \frac{p(\boldsymbol{X},\boldsymbol{Z})}{q(\boldsymbol{Z})}dq(\boldsymbol{Z}) && \text{definition of } dq(\mathbf{Z}) \\
&\geq \frac{1}{N}\int \log\frac{p(\boldsymbol{X},\boldsymbol{Z})}{q(\boldsymbol{Z})}dq(\boldsymbol{Z}) && \text{Jensen inequality} \\
&= \frac{1}{N}\int\sum_{1}^{N}\log\frac{p(\mathbf{x}_i,\mathbf{z}_i)}{q(\mathbf{z}_i)}dq(\mathbf{z}_i) && \text{using the iid property} \\
&= \frac{1}{N}\sum_{1}^{N}-\mathcal{L}(q,p,\mathbf{x}_i) && \text{definition of } \mathcal{L}(q,p,\mathbf{x}_i) \\
&= -\mathcal{L}(q,p,X) \triangleq -\mathcal{L}(q,p) && \text{again definition of } \mathcal{L}(p,q) \quad \square
\end{aligned}
\tag{4}
$$

normal text tiny text normal text And now to something [1] completely different ...

[1] Xifeng Guo et al. “Improved deep embedded clustering with local structure preservation.”. In: *Ijcai*. 2017, pp. 1753–1759.

[2] Elad Plaut. “From principal subspaces to principal components with linear autoencoders”. In: *arXiv preprint arXiv:1804.10253* (2018).