# c∗GM∆VÆs—q

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# c∗GMΔVÆs—q

a Master Thesis in Bioinformatics

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# 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$*$GM$\Delta$VÆ
- example use of c$*$GM$\Delta$VÆ 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).

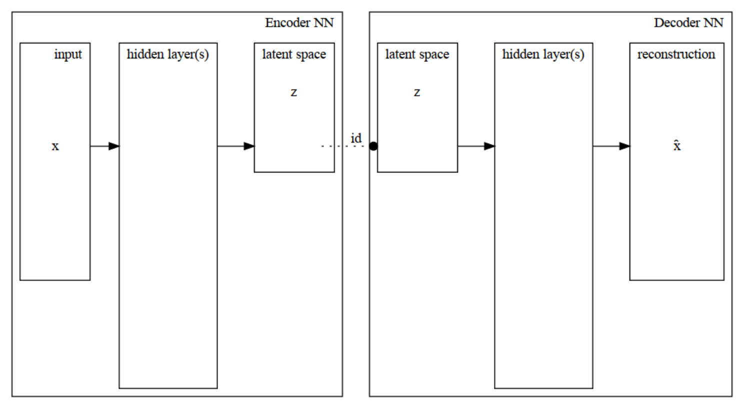



Figure: Autoencoder

# Autoencoders and PCA

(On centered data[8])

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

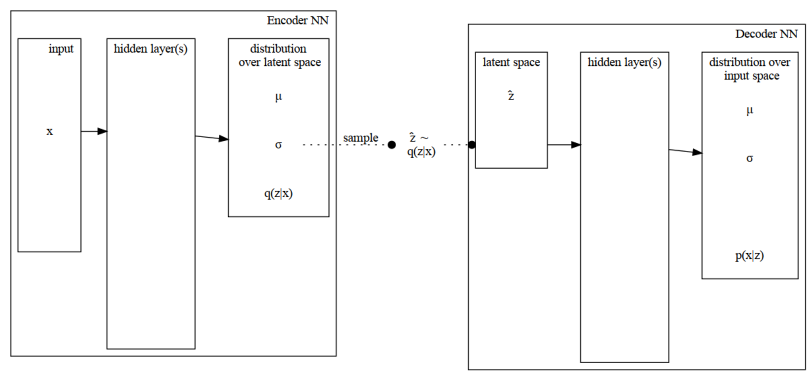



Figure: VAE

# VAE: encoding

Instead of deterministic mapping, define distribution.

Define distribution on the laten space ($\mathbf{z}$) by mapping $x$ into the distribution parameters e.g. $\mu(\mathbf{x}), \Sigma(\mathbf{x})$ when we use Gaussian $q(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}|\mu, \Sigma)$.

# VAE: decoding

sample from the latent space $\mathbf{z} \sim \mathcal{N}(\cdot|\mu, \Sigma)$

map $\mathbf{z}$ to a distribution on the input space $p(\mathbf{x}|\mathbf{z})$

# VAE: loss function

The *evidence lower bound (ELBO)* with respect to $p, q$ is:

$$-\mathcal{L}(q, p, \mathbf{x}) \triangleq \int \log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})} dq(\boldsymbol{z}) \tag{4}$$

$$-\mathcal{L}(q, p) \triangleq -\mathcal{L}(q, p, \mathbf{X}) = \frac{1}{N} \sum_{1}^{N} (-\mathcal{L}(q, p, \mathbf{x}_i) \tag{5}$$

$$\approx \mathbf{E}_{\mathbf{x}}[-\mathcal{L}(q, p, \mathbf{x})] \tag{6}$$

We minimize the minus ELBO function:

# VAE: log evidence

It can be shown that maximizing the ELBO is equivalent to maximinizing the "log evidence" $\log p(\mathbf{X})$

$$
\begin{aligned}
\frac{1}{N}\log p(\boldsymbol{X}) &= \frac{1}{N}\log\int p(\boldsymbol{X},\boldsymbol{Z})d\boldsymbol{Z} && \text{taking marginal}\\
&= \frac{1}{N}\log\int \frac{p(\boldsymbol{X},\boldsymbol{Z})}{q(\boldsymbol{Z})}q(\boldsymbol{Z})d\boldsymbol{Z} && \text{multiplying by 1 inside}\\
&= \frac{1}{N}\log\int \frac{p(\boldsymbol{X},\boldsymbol{Z})}{q(\boldsymbol{Z})}dq(\boldsymbol{Z}) && \text{definition of } dq(\mathbf{Z})\\
&\geq \frac{1}{N}\int \log\frac{p(\boldsymbol{X},\boldsymbol{Z})}{q(\boldsymbol{Z})}dq(\boldsymbol{Z}) && \text{Jensen inequality}\\
&= \frac{1}{N}\int\sum_{1}^{N}\log\frac{p(\mathbf{x}_i,\mathbf{z}_i)}{q(\mathbf{z}_i)}dq(\mathbf{z}_i) && \text{using the iid property}\\
&= \frac{1}{N}\sum_{1}^{N}-\mathcal{L}(q,p,\mathbf{x}_i) && \text{definition of } \mathcal{L}(q,p,\mathbf{x}_i)\\
&= -\mathcal{L}(q,p,X)\triangleq -\mathcal{L}(q,p) && \text{again definition of } \mathcal{L}(p,q) \quad \square
\end{aligned}
\tag{7}
$$

# VAE: compounding the latent distribution

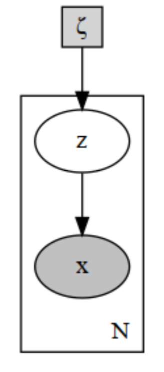
More complicated distributions such as mixture distribution can be modelled by "unpacking" the latent $\mathbf{z}$ and the observed $\mathbf{x}$

1. Define the set of observed random vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_k$, and the set of latent random vectors and stochastic parameters $\mathbf{z}_1, \ldots \mathbf{z}_l$.
2. Specify how to factor the generative model $p(\mathbf{x}_1, \ldots, \mathbf{x}_k | \mathbf{z}_1 \ldots, \mathbf{z}_l)$
3. Specify how to factor the inference model $q(\mathbf{z}_1 \ldots \mathbf{z}_l | \mathbf{x}1, \ldots \mathbf{x}_k)$
4. Choose appropriate priors $p(\mathbf{z}_i)$ and
5. Choose appropriate distribution families for the $\mathbf{x}_i$ and $\mathbf{z}_i$, and choose priors $p(\mathbf{z}_i)$.

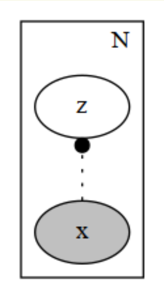
# VAE: Graphical representation

Evry distribution can be represented by a DAG. Nodes represent random variables (and also priors), and directed arrows represent conditional dependency.

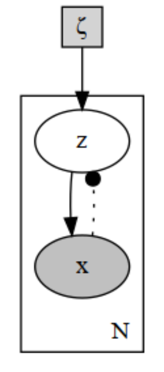
# VAE: base case




(a) generative model $p(x, z)$



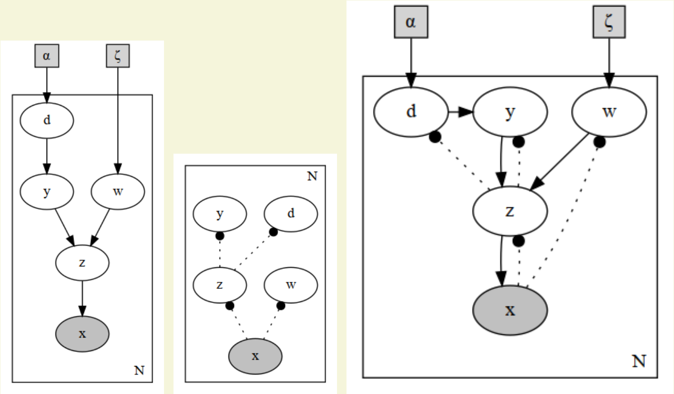

(b) inference model $q(z|x)$




(c) the combined graphical model

Figure: VAE graphical model

# VAE: patholocigacl case



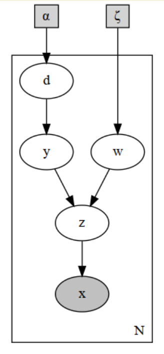

(a) generative model $p(x, z)$

(b) inference model $q(z|x)$

(c) the combined graphical model

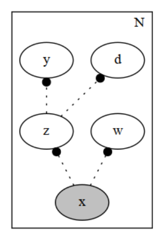
Figure: c∗GMΔVÆ graphical model

# c∗GMΔVÆ generative model




$$
\begin{aligned}
p(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w}, \mathbf{d}) &= p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{w}, \mathbf{y})p(\mathbf{y}|\mathbf{d})p(\mathbf{d})p(\mathbf{w}) \\
p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{1}) \\
p(\mathbf{d}) &= \mathrm{Dir}(\mathbf{d}|\alpha) \\
p(\mathbf{y}|\mathbf{d}) &= \mathrm{Cat}(\mathbf{y}|\mathbf{d}) \\
p(\mathbf{z}|\mathbf{w}, \mathbf{y}) &= \mathcal{N}(\mathbf{z}|\mu(\mathbf{w})_{\mathbf{y}}, \sigma(\mathbf{w})_{\mathbf{y}})) \\
p(\mathbf{x}|\mathbf{z}) &= \mathcal{N}(\mathbf{x}|\mu(\mathbf{z}), \sigma(\mathbf{z}))
\end{aligned}
\tag{8}
$$

# c∗GMΔVÆ inference model




$$\begin{aligned}
q(\mathbf{y}, \mathbf{z}, \mathbf{w}, \mathbf{d}|\mathbf{x}) &= q(\mathbf{z}|\mathbf{x})q(\mathbf{w}|\mathbf{x})q(\mathbf{y}|\mathbf{z})q(\mathbf{d}|\mathbf{z}) \\
q(\mathbf{z}|\mathbf{x}) &= \mathcal{N}(\mathbf{z}|\mu_z(\mathbf{x}), \sigma_z(\mathbf{x})) \\
q(\mathbf{w}|\mathbf{x}) &= \mathcal{N}(\mathbf{w}|\mu_w(\mathbf{x}), \sigma_w(\mathbf{x})) \\
q(\mathbf{y}|\mathbf{z}) &= \mathrm{Cat}(\mathbf{y}|f(\mathbf{z})) \\
q(\mathbf{d}|\mathbf{z}) &= \mathrm{Dir}(\mathbf{d}|g(\mathbf{z}))
\end{aligned} \tag{9}$$

# c∗GMΔVÆ loss function

The loss function remains the -ELBO and we can break it into different terms:

$$
\begin{aligned}
\mathcal{L}(p, q, \mathbf{x}) &= \int -\log \frac{p(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w}, \mathbf{d})}{q(\mathbf{z}, \mathbf{y}, \mathbf{w}, \mathbf{d}|\mathbf{x})} dq(\mathbf{z}, \mathbf{y}, \mathbf{w}, \mathbf{d}|\mathbf{x}) && (10) \\
&= \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{w}, \mathbf{y})p(\mathbf{y}|\mathbf{d})p(\mathbf{w})p(\mathbf{d})}{q(\mathbf{z}|\mathbf{x})q(\mathbf{w}|\mathbf{x})q(\mathbf{y}|\mathbf{z})q(\mathbf{d}|\mathbf{z})} dq && (11) \\
&= \int -\log p(\mathbf{x}|\mathbf{z}) dq && (12) \\
&+ \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{w}, \mathbf{y})} dq && (13) \\
&+ \int \log \frac{q(\mathbf{w}|\mathbf{x})}{p(\mathbf{w})} dq && (14) \\
&+ \int \log \frac{q(\mathbf{y}|\mathbf{z})}{p(\mathbf{y}|\mathbf{d})} dq && (15) \\
&+ \int \log \frac{q(\mathbf{d}|\mathbf{z})}{p(\mathbf{d})} dq && (16)
\end{aligned}
$$

# Monte Carlo integration

As you can see we the loss function requires us to compute an integral, which usually cannot be done analytically.

Instead the integral is approximated by Monte Carlo integration.

$$\begin{aligned} &\text{sample } \mathbf{z}_i \sim q(\mathbf{z}|\mathbf{x}) \text{ then :} \\ \mathcal{L}(p, q, \mathbf{x}) &= \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} dq(\mathbf{z}|\mathbf{x}) \\ = \int -\log p(\mathbf{x}|\mathbf{z}) dq(\mathbf{z}|\mathbf{x}) &+ \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})} dq(\mathbf{z}|\mathbf{x}) \\ &\approx \frac{1}{k} \sum_{i=1}^{k} [-\log p(\mathbf{x}|\mathbf{z}_i) + \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i)}] \end{aligned} \tag{17}$$

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