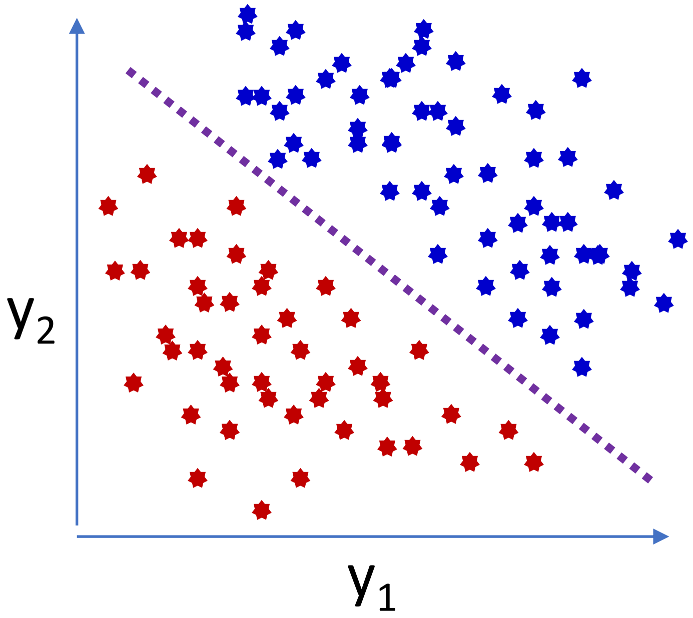
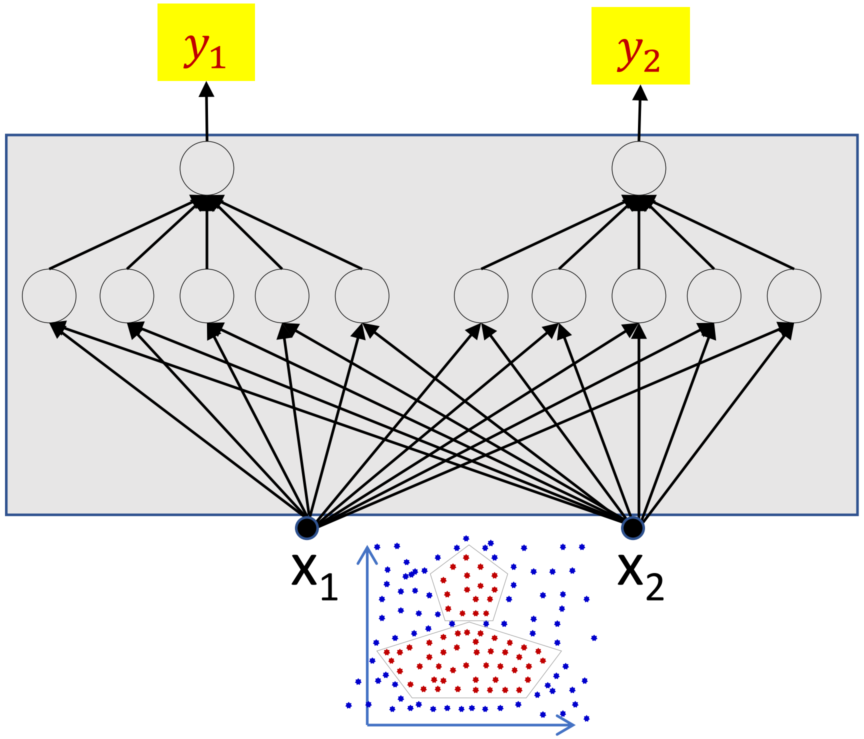
Variational Autoencoders

Recap: Story so far

- A classification MLP actually comprises two components
    - A “feature extraction network” that converts the inputs into linearly separable features
        - Or *nearly* linearly separable features
    - A final linear classifier that operates on the linearly separable features
- Neural networks can be used to perform linear or non-linear PCA
    - “Autoencoders”
    - Can also be used to compose constructive dictionaries for data
        - Which, in turn can be used to model data distributions

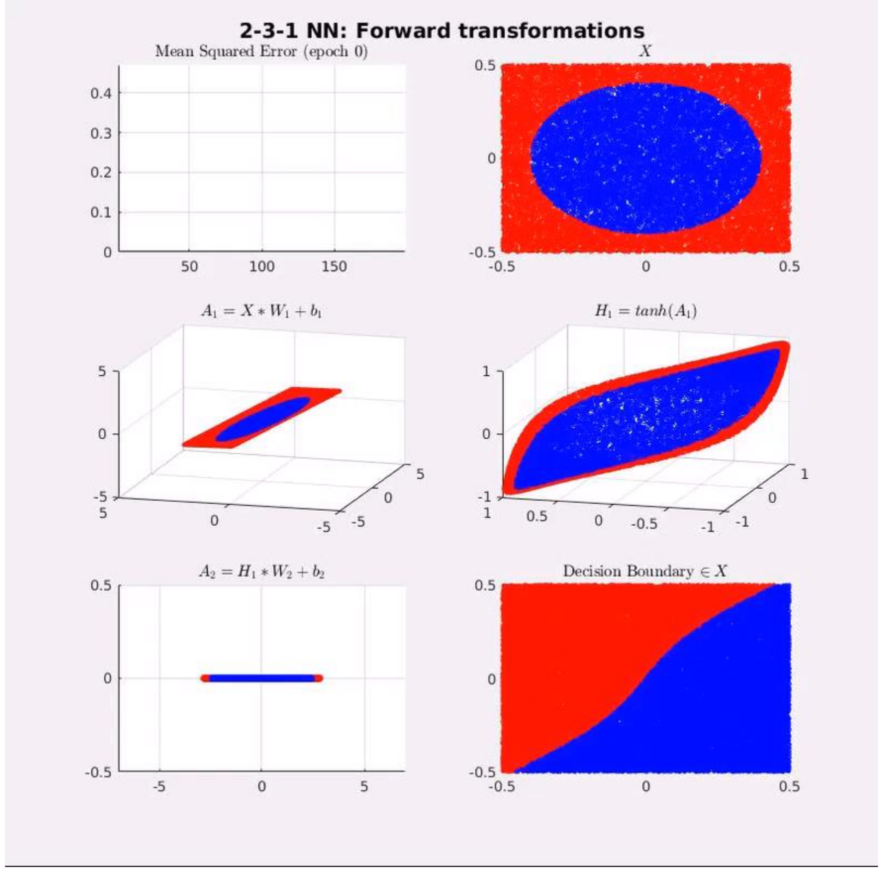
Recap: The penultimate layer





- The network up to the output layer may be viewed as a transformation that transforms data from non-linear classes to linearly separable features

Recap: The behavior of the layers



2-3-1 NN: Forward transformations

Mean Squared Error (epoch 0)

X

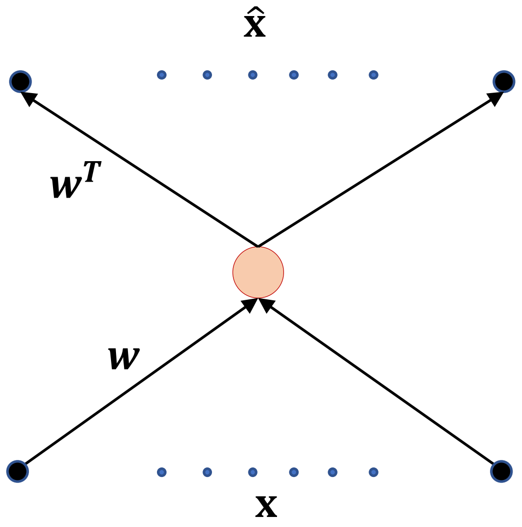
$A_1 = X * W_1 + b_1$

$H_1 = tanh(A_1)$

$A_2 = H_1 * W_2 + b_2$

Decision Boundary $\in X$

Recap: Auto-encoders and PCA



Training: Learning W by minimizing L2 divergence

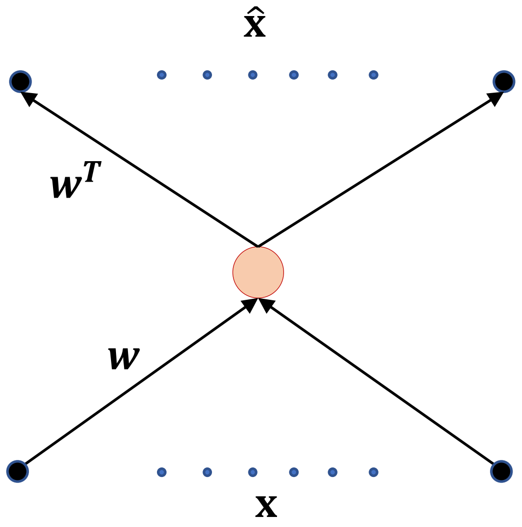
$$\hat{\mathrm{x}} = w^T w\mathrm{x}$$

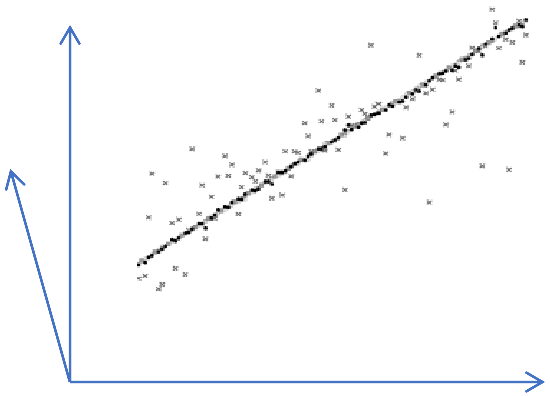
$$div(\hat{\mathrm{x}}, \mathrm{x}) = \|\mathrm{x} - \hat{\mathrm{x}}\|^2 = \|\mathrm{x} - \mathrm{w}^T w\mathrm{x}\|^2$$

$$\widehat{W} = \underset{W}{\operatorname{argmin}} E[div(\hat{\mathrm{x}}, \mathrm{x})]$$

$$\widehat{W} = \underset{W}{\operatorname{argmin}} E[\|\mathrm{x} - \mathrm{w}^T w\mathrm{x}\|^2]$$

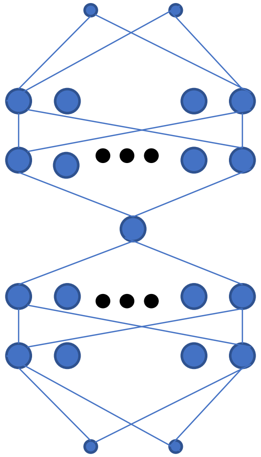
Recap: Auto-encoders and PCA

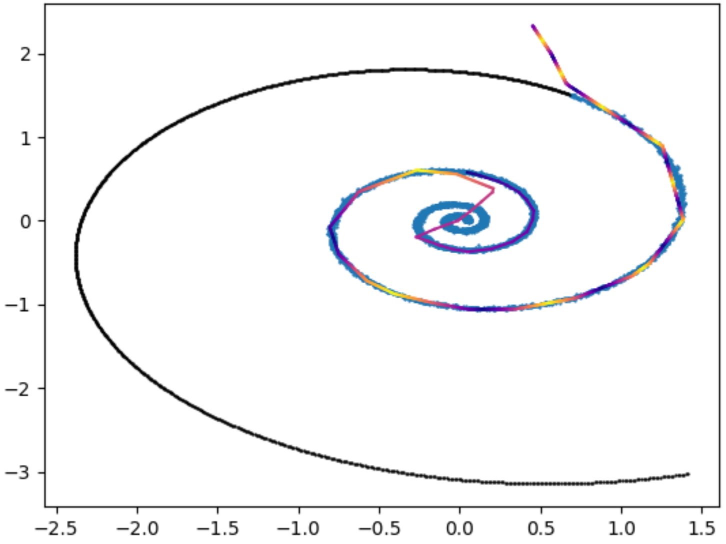


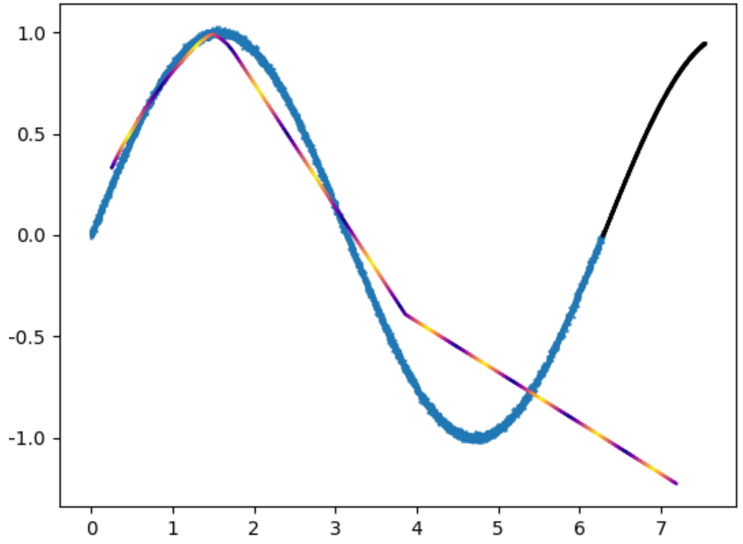


- The autoencoder finds the direction of maximum energy
  - Variance if the input is a zero-mean RV
- All input vectors are mapped onto a point on the principal axis

Recap: Auto-encoders and PCA



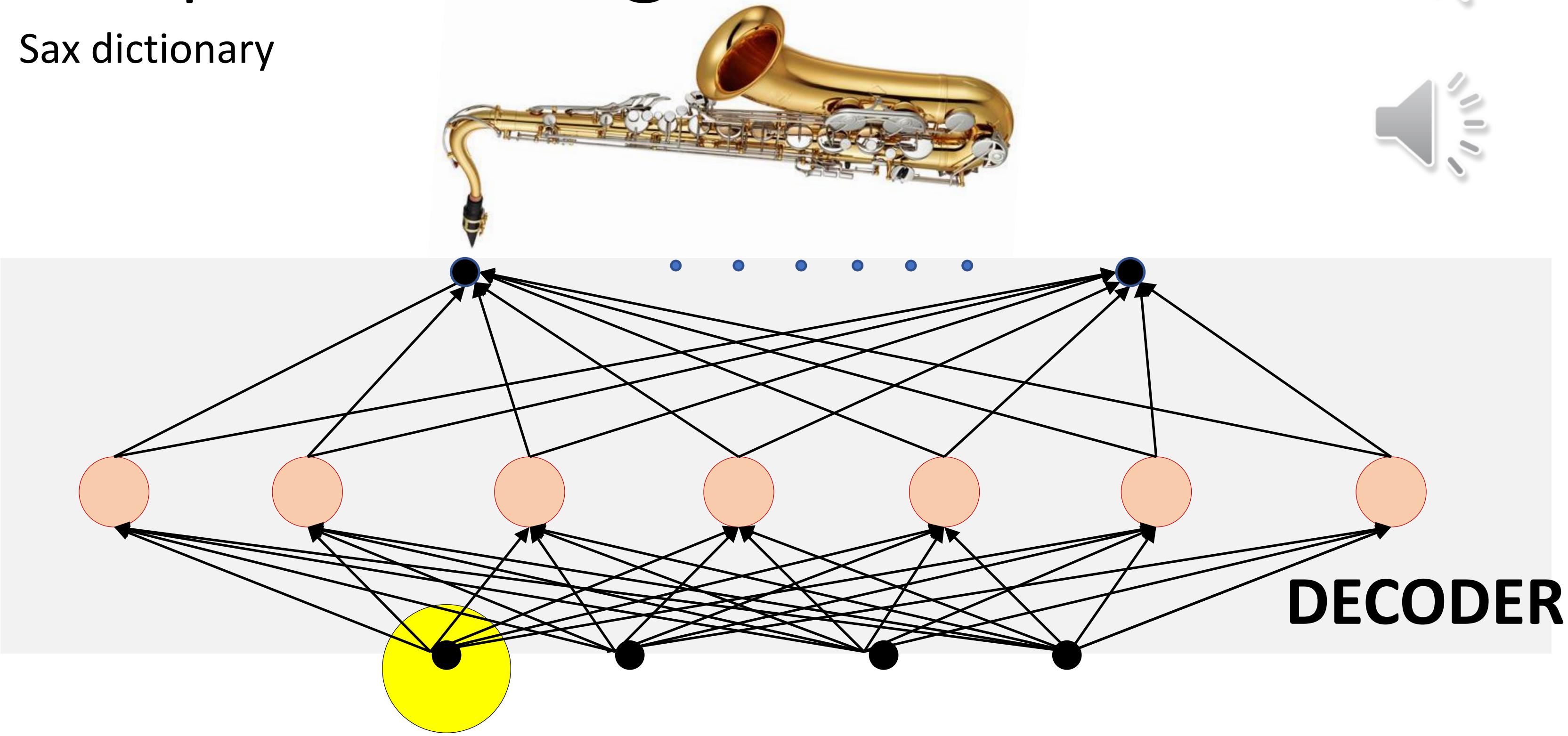




- Varying the hidden layer value only generates data along the learned manifold
  - May be poorly learned
  - *Any input* will result in an output along the learned manifold

Recap: Learning a data-manifold

Sax dictionary



- The decoder represents a source-specific generative *dictionary*
- Exciting it will produce typical data from the source!

Overview

- Just as autoencoders can be viewed as performing a non-linear PCA, variational autoencoders can be viewed as performing a non-linear Factor Analysis (FA)
- Variational autoencoders (VAEs) get their name from variational inference, a technique that can be used for parameter estimation
- We will introduce Factor Analysis, variational inference and expectation maximization, and finally VAEs

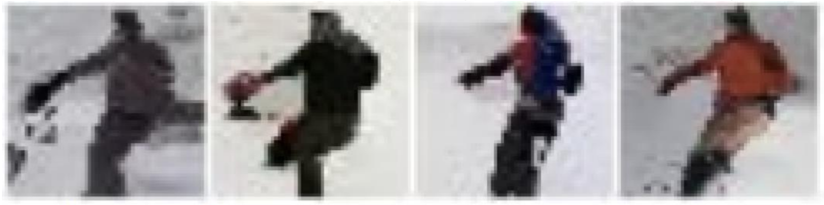
Why Generative Models? Training data

- Unsupervised/Semi-supervised learning: More training data available
- E.g. all of the videos on YouTube

Why generative models? Many right answers

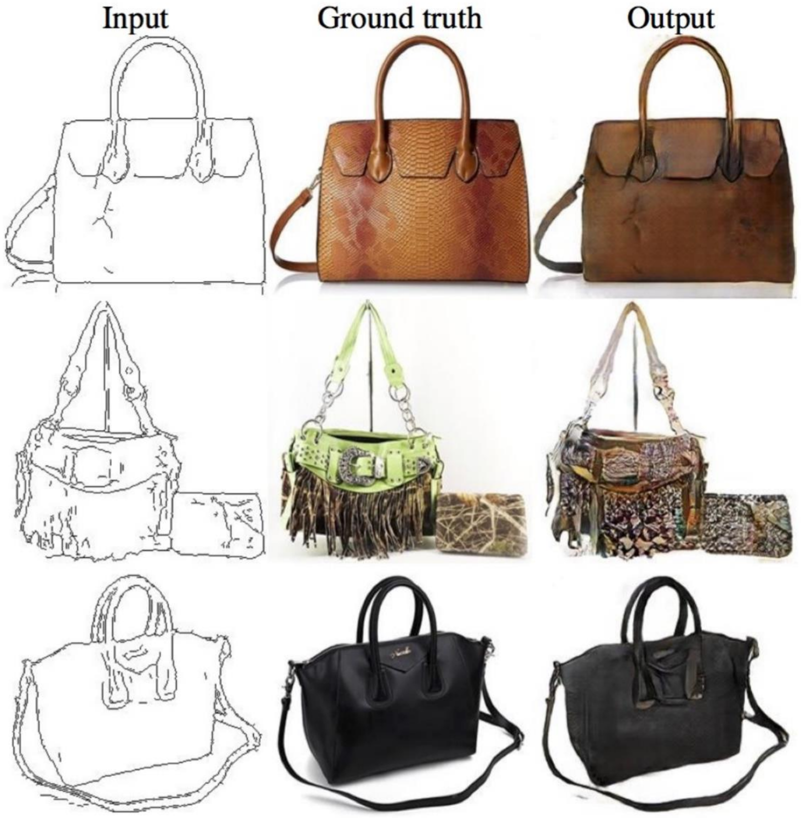
- Caption -> Image

https://openreview.net/pdf?id=Hyvw0L9el



A man in an orange jacket with sunglasses and a hat skis down a hill

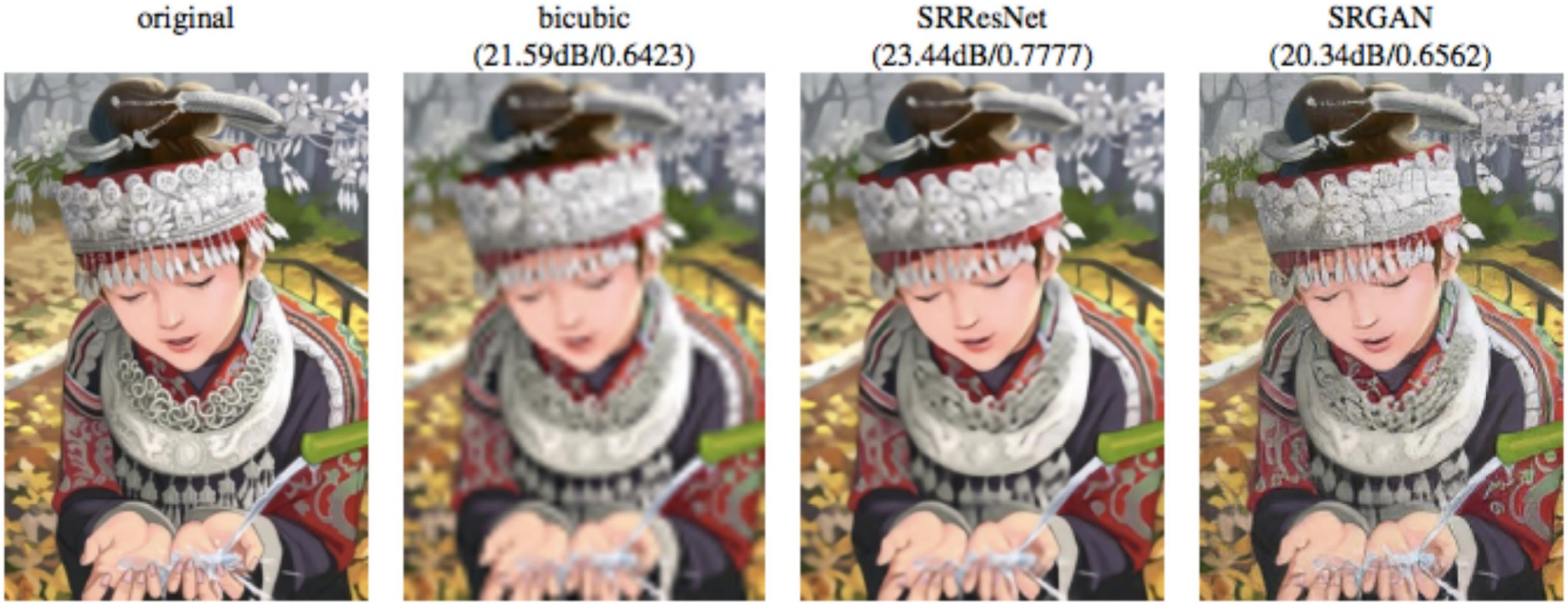
- Outline -> Image



https://arxiv.org/abs/1611.07004

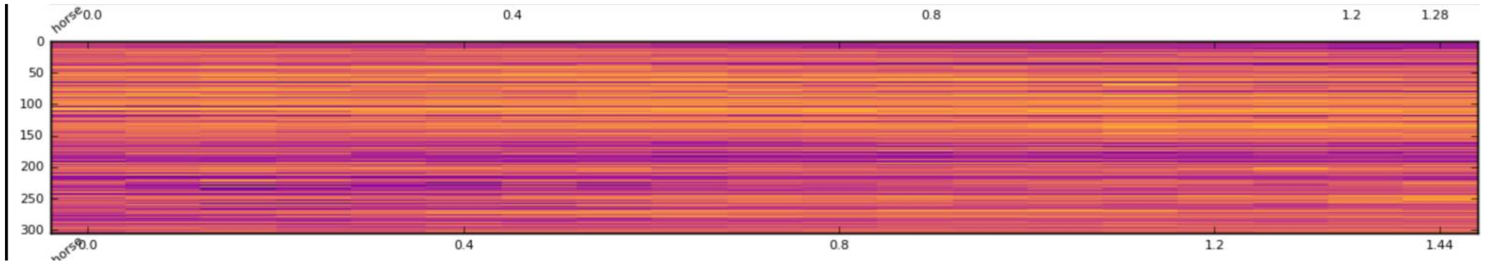
Why generative models? Intrinsic to task

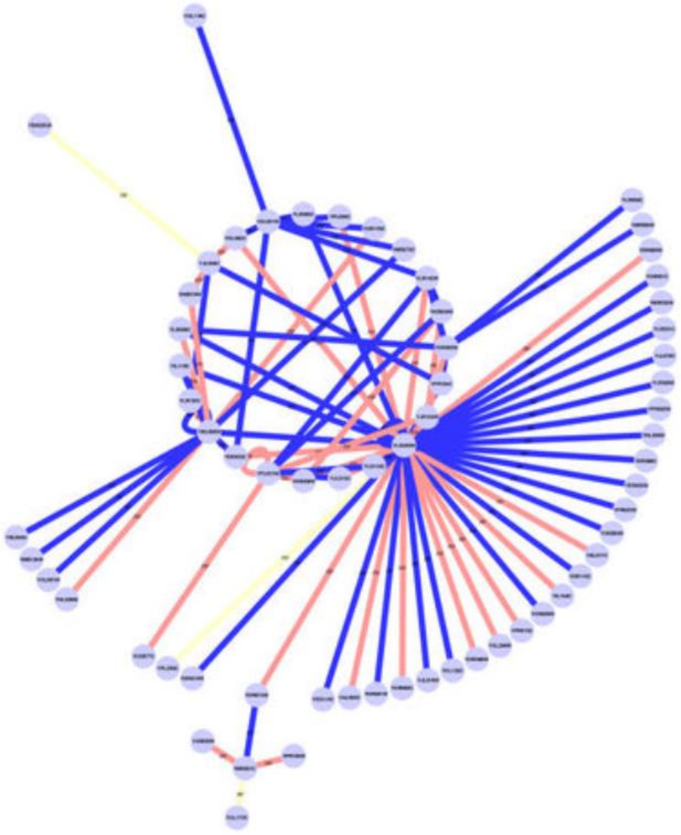
Example: Super resolution



https://arxiv.org/abs/1609.04802

Why generative models? Insight



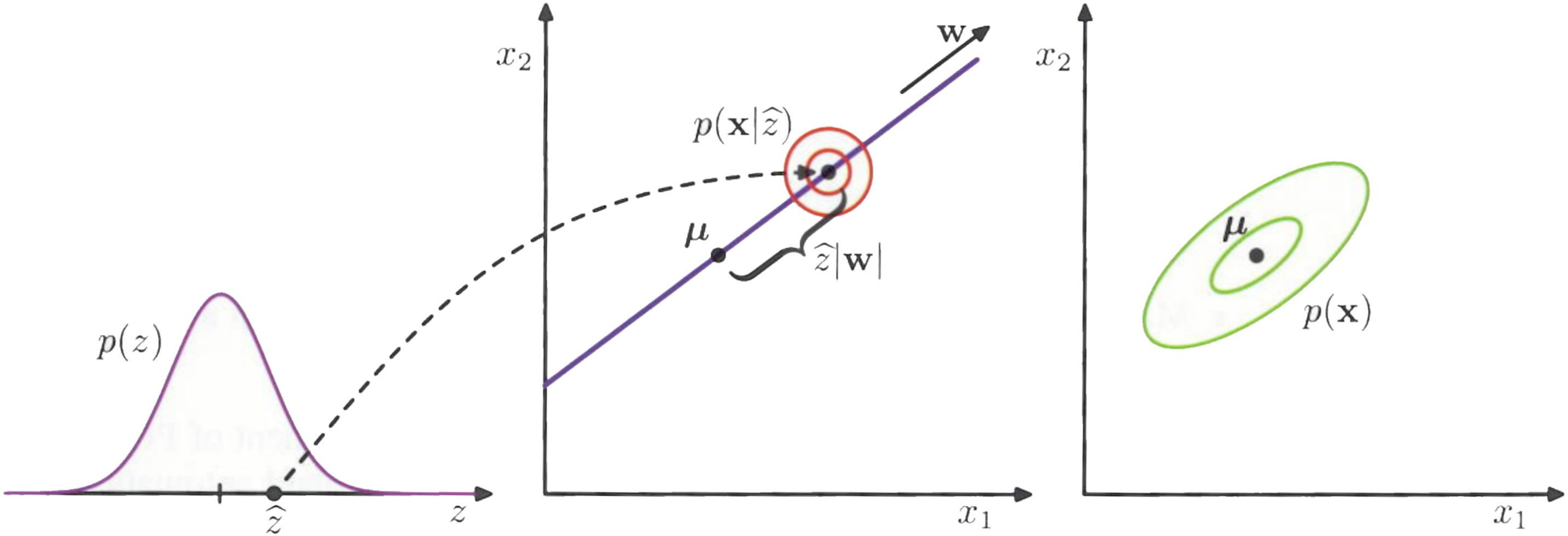


https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-12-327

- What kind of structure can we find in complex observations (MEG recording of brain activity above, gene-expression network to the left)?
- Is there a low dimensional manifold underlying these complex observations?
- What can we learn about the brain, cellular function, etc. if we know more about these manifolds?

Factor Analysis

- Generative model: Assumes that data are generated from real valued latent variables



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Factor Analysis model

Factor analysis assumes a generative model

- where the ith observation, $\boldsymbol{x_i} \in \mathbb{R}^D$ is conditioned on
- a vector of real valued latent variables $\boldsymbol{z_i} \in \mathbb{R}^L$.

Here we assume the prior distribution is Gaussian:

$$p(\boldsymbol{z_i}) = \mathcal{N}(\boldsymbol{z_i}|\boldsymbol{\mu_0}, \boldsymbol{\Sigma_0})$$

We also will use a Gaussian for the data likelihood:

$$p(\boldsymbol{x_i}|\boldsymbol{z_i}, \boldsymbol{W}, \boldsymbol{\mu}, \boldsymbol{\Psi}) = \mathcal{N}(\boldsymbol{W}\boldsymbol{z_i} + \boldsymbol{\mu}, \boldsymbol{\Psi})$$

Where $\boldsymbol{W} \in \mathbb{R}^{D\times L}, \boldsymbol{\Psi} \in \mathbb{R}^{D\times D}, \boldsymbol{\Psi}$ is diagonal

Marginal distribution of observed $\boldsymbol{x_i}$

$$p(\boldsymbol{x_i}|\boldsymbol{W},\boldsymbol{\mu},\boldsymbol{\Psi}) = \int \mathcal{N}(\boldsymbol{W}\boldsymbol{z_i}+\boldsymbol{\mu},\boldsymbol{\Psi})\,\mathcal{N}(\boldsymbol{z_i}|\boldsymbol{\mu_0},\boldsymbol{\Sigma_0})\mathbf{d}\boldsymbol{z_i}$$

$$= \mathcal{N}(\boldsymbol{x_i}|\boldsymbol{W}\boldsymbol{\mu_0}+\boldsymbol{\mu},\boldsymbol{\Psi}+\boldsymbol{W}\,\boldsymbol{\Sigma_0}\boldsymbol{W}^T)$$

Note that we can rewrite this as:

$$p\left(\boldsymbol{x_i}\middle|\widehat{\boldsymbol{W}},\widehat{\boldsymbol{\mu}},\boldsymbol{\Psi}\right) = \mathcal{N}\left(\boldsymbol{x_i}\middle|\widehat{\boldsymbol{\mu}},\boldsymbol{\Psi}+\widehat{\boldsymbol{W}}\widehat{\boldsymbol{W}}^T\right)$$

Where $\widehat{\boldsymbol{\mu}} = \boldsymbol{W}\boldsymbol{\mu_0}+\boldsymbol{\mu}$ and $\widehat{\boldsymbol{W}} = \boldsymbol{W}\boldsymbol{\Sigma_0}^{-\frac{1}{2}}$.

Thus without loss of generality (since $\boldsymbol{\mu_0},\boldsymbol{\Sigma_0}$ are absorbed into learnable parameters) we let:

$$p(\boldsymbol{z_i}) = \mathcal{N}(\boldsymbol{z_i}|\boldsymbol{0},\boldsymbol{I})$$

And find:

$$p(\boldsymbol{x_i}|\boldsymbol{W},\boldsymbol{\mu},\boldsymbol{\Psi}) = \mathcal{N}(\boldsymbol{x_i}|\boldsymbol{\mu},\boldsymbol{\Psi}+\boldsymbol{W}\boldsymbol{W}^T)$$

Marginal distribution interpretation

- We can see from $p(\boldsymbol{x}_i|\boldsymbol{W},\boldsymbol{\mu},\boldsymbol{\Psi}) = \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu},\boldsymbol{\Psi}+\boldsymbol{W}\boldsymbol{W}^T)$ that the covariance matrix of the data distribution is broken into 2 terms
- A diagonal part $\boldsymbol{\Psi}$: **variance not shared between variables**
- A low rank matrix $\boldsymbol{W}\boldsymbol{W}^T$: **shared variance due to latent factors**

Special Case: Probabilistic PCA (PPCA)

- Probabilistic PCA is a special case of Factor Analysis
- We further restrict $\mathbf{\Psi} = \sigma^2 \boldsymbol{I}$ (assume isotropic independent variance)
- Possible to show that when the data are centered ($\boldsymbol{\mu}$ = $\mathbf{0}$), the limiting case where $\sigma \to 0$ gives back the same solution for $\boldsymbol{W}$ as PCA
- Factor analysis is a generalization of PCA that models non-shared variance (can think of this as noise in some situations, or individual variation in others)

Inference in FA

- To find the parameters of the FA model, we use the Expectation Maximization (EM) algorithm
- EM is very similar to variational inference
- We’ll derive EM by first finding a lower bound on the log-likelihood we want to maximize, and then maximizing this lower bound

Evidence Lower Bound decomposition

- For any distributions $q(z), p(z)$ we have:

$$\mathrm{KL}\big(q(z) \,||\, p(z)\big) \triangleq \int q(z) \log \frac{q(z)}{p(z)} \,\mathbf{d}z$$

- Consider the KL divergence of an **arbitrary** weighting distribution $q(z)$ from a conditional distribution $p(z|x,\theta)$:

$$\mathrm{KL}\big(q(z) \,||\, p(z|x,\theta)\big) \triangleq \int q(z) \log \frac{q(z)}{p(z|x,\theta)} \,\mathbf{d}z$$

$$= \int q(z)[\log q(z) - \log p(z|x,\theta)] \,\mathbf{d}z$$

Applying Bayes

$$\log p(z|x,\theta) = \log\left[\frac{p(x|z,\theta)p(z|\theta)}{p(x|\theta)}\right]$$

$$= \log p(x|z,\theta) + \log p(z|\theta) - \log p(x|\theta)$$

Then:

$$\mathrm{KL}\big(q(z)\,||\,p(z|x,\theta)\big) = \int q(z)[\log q(z) - \log p(z|x,\theta)]\,\mathbf{d}z$$

$$= \int q(z)[\log q(z) - \log p(x|z,\theta) - \log p(z|\theta) + \log p(x|\theta)]\mathbf{d}z$$

Rewriting the divergence

- Since the last term does not depend on z, and we know $\int q(z)\mathrm{d}z = 1$, we can pull it out of the integration:

$$\int q(z)[\log q(z) - \log p(x|z,\theta) - \log p(z|\theta) + \log p(x|\theta)]\mathbf{d}z$$

$$= \int q(z)[\log q(z) - \log p(x|z,\theta) - \log p(z|\theta)]\mathbf{d}z + \log p(x|\theta)$$

$$= \int q(z)\log\left[\frac{q(z)}{p(x|z,\theta)p(z,\theta)}\right]\mathbf{d}z + \log p(x|\theta)$$

$$= \int q(z)\log\left[\frac{q(z)}{p(x,z\,|\theta)}\right]\mathbf{d}z + \log p(x|\theta)$$

Then we have:

$$\mathrm{KL}\big(q(z)\;||\;p(z|x,\theta)\big) = \mathrm{KL}\big(q(z)\;||\;p(x,z\,|\theta)\big) + \;\log p(x|\theta)$$

Evidence Lower Bound

- From basic probability we have:

$$\mathrm{KL}\big(q(z)\;||\;p(z|x,\theta)\big) = \mathrm{KL}\big(q(z)\;||\;p(x,z\;|\theta)\big) + \;\log p(x|\theta)$$

- We can rearrange the terms to get the following decomposition:

$$\log p(x|\theta) = \mathrm{KL}\big(q(z)\;||\;p(z|x,\theta)\big) - \mathrm{KL}\big(q(z)\;||\;p(x,z\;|\theta)\big)$$

- We define the *evidence lower bound* (ELBO) as:

$$\mathcal{L}(q,\theta) \triangleq -\mathrm{KL}\big(q(z)\;||\;p(x,z\;|\theta)\big)$$

Then:

$$\log p(x|\theta) = \mathrm{KL}\big(q(z)||p(z|x,\theta)\big) + \mathcal{L}(q,\theta)$$

Why the name evidence lower bound?

- Rearranging the decomposition

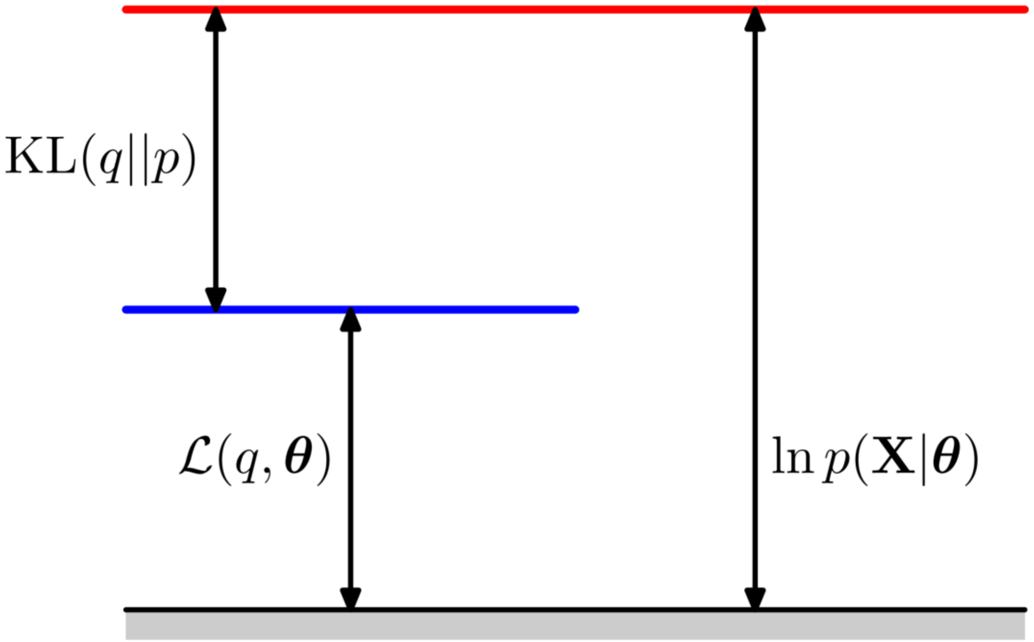
$$\log p(x|\theta) = \mathrm{KL}\big(q(z)||p(z|x,\theta)\big) + \mathcal{L}(q,\theta)$$

- we have

$$\mathcal{L}(q,\theta) = \log p(x|\theta) - \mathrm{KL}\big(q(z) \,||\, p(z|x,\theta)\big)$$

- Since $\mathrm{KL}\big(q(z)||p(z|x,\theta)\big) \geq 0$, $\mathcal{L}(q,\theta)$ is a lower bound on the log-likelihood we want to maximize
- $p(x|\theta)$ is sometimes called the evidence
- When is this **bound tight**? When $q(z) = p(z|x,\theta)$
- The ELBO is also sometimes called the variational bound

Visualizing ELBO decomposition


$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$

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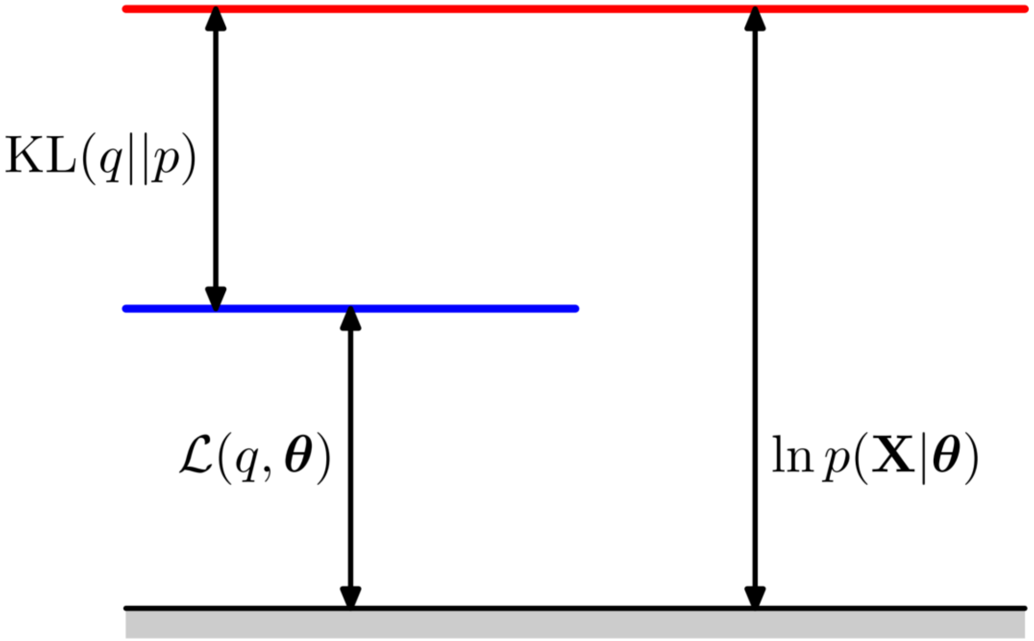
- Note: all we have done so far is decompose the log probability of the data, we still have exact equality
- This holds for any distribution q

Expectation Maximization

- Expectation Maximization alternately optimizes the ELBO, $\mathcal{L}(q, \theta)$, with respect to q (the E step) and θ (the M step)

- Initialize $\theta^{(0)}$
- At each iteration $t = 1, \ldots$
  - **E step:** Hold $\theta^{(t-1)}$ fixed, find $q^{(t)}$ which maximizes $\mathcal{L}\left(q, \theta^{(t-1)}\right)$
  - **M step:** Hold $q^{(t)}$ fixed, find $\theta^{(t)}$ which maximizes $\mathcal{L}\left(q^{(t)}, \theta\right)$

The E step


$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$

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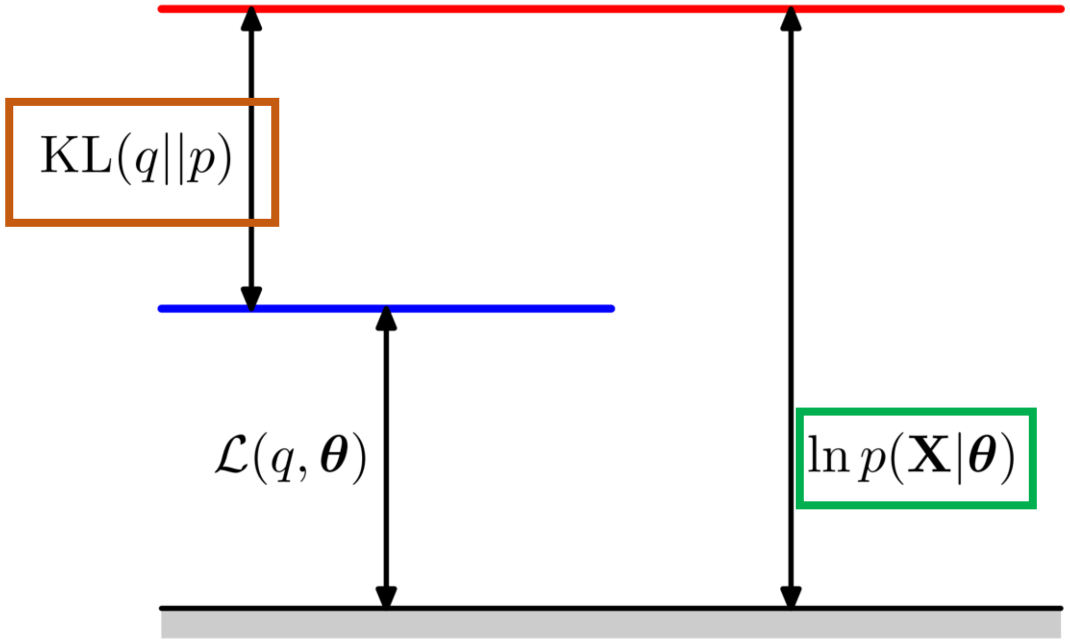
- Suppose we are at iteration t of our algorithm. How do we maximize $\mathcal{L}\left(q, \theta^{(t-1)}\right)$ with respect to q? We know that:

$$\mathrm{argmax}_q\, \mathcal{L}\left(q, \theta^{(t-1)}\right) = \mathrm{argmax}_q \log p\left(x|\theta^{(t-1)}\right) - \mathrm{KL}\left(q(z) \,||\, p\left(z|x, \theta^{(t-1)}\right)\right)$$

The E step


$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$

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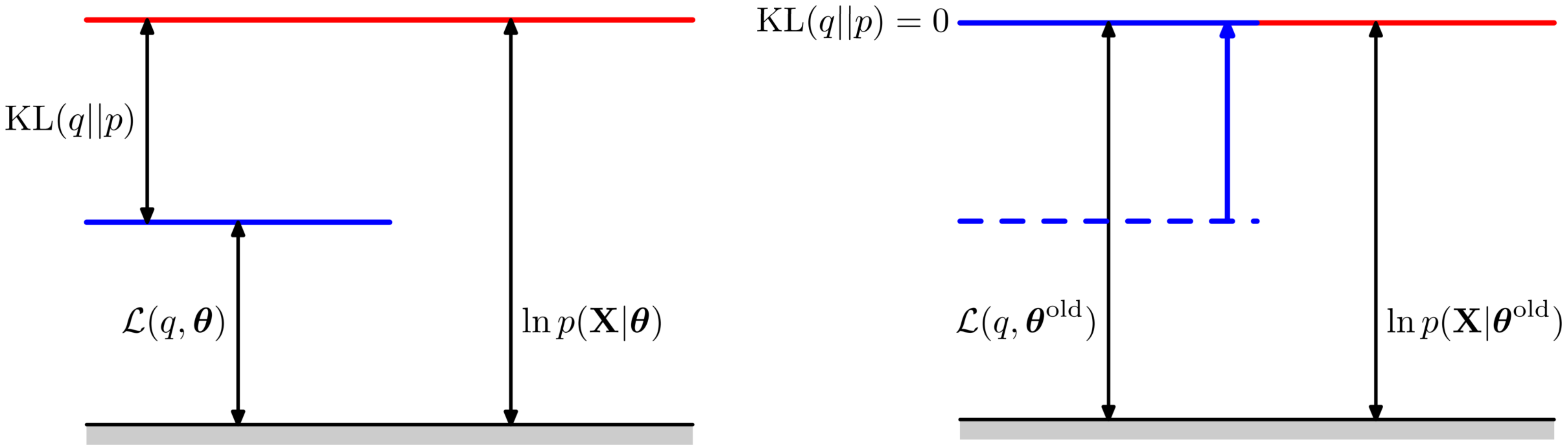
- The first term does not involve q, and we know the KL divergence must be non-negative
- The best we can do is to make the KL divergence 0
- Thus the solution is to set $\boldsymbol{q}^{(t)}(\boldsymbol{z}) \leftarrow \boldsymbol{p}\left(\boldsymbol{z}\middle|\boldsymbol{x}, \boldsymbol{\theta}^{(t-1)}\right)$

- Suppose we are at iteration t of our algorithm. How do we maximize $\mathcal{L}\left(q, \theta^{(t-1)}\right)$ with respect to q? We know that:

$$\operatorname{argmax}_q \mathcal{L}\left(q, \theta^{(t-1)}\right) = \operatorname{argmax}_q \log p\left(x|\theta^{(t-1)}\right) - \mathrm{KL}\left(q(z) \,||\, p\left(z|x, \theta^{(t-1)}\right)\right)$$

The E step


$\mathrm{KL}(q||p)$
$\mathcal{L}(q,\boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$
$\mathrm{KL}(q||p)=0$
$\mathcal{L}(q,\boldsymbol{\theta}^{\mathrm{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{old}})$

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- Suppose we are at iteration t of our algorithm. How do we maximize $\mathcal{L}\left(q,\theta^{(t-1)}\right)$ with respect to q? $\boldsymbol{q}^{(t)}(\boldsymbol{z}) \leftarrow \boldsymbol{p}\left(\boldsymbol{z}\middle|\boldsymbol{x},\boldsymbol{\theta}^{(t-1)}\right)$

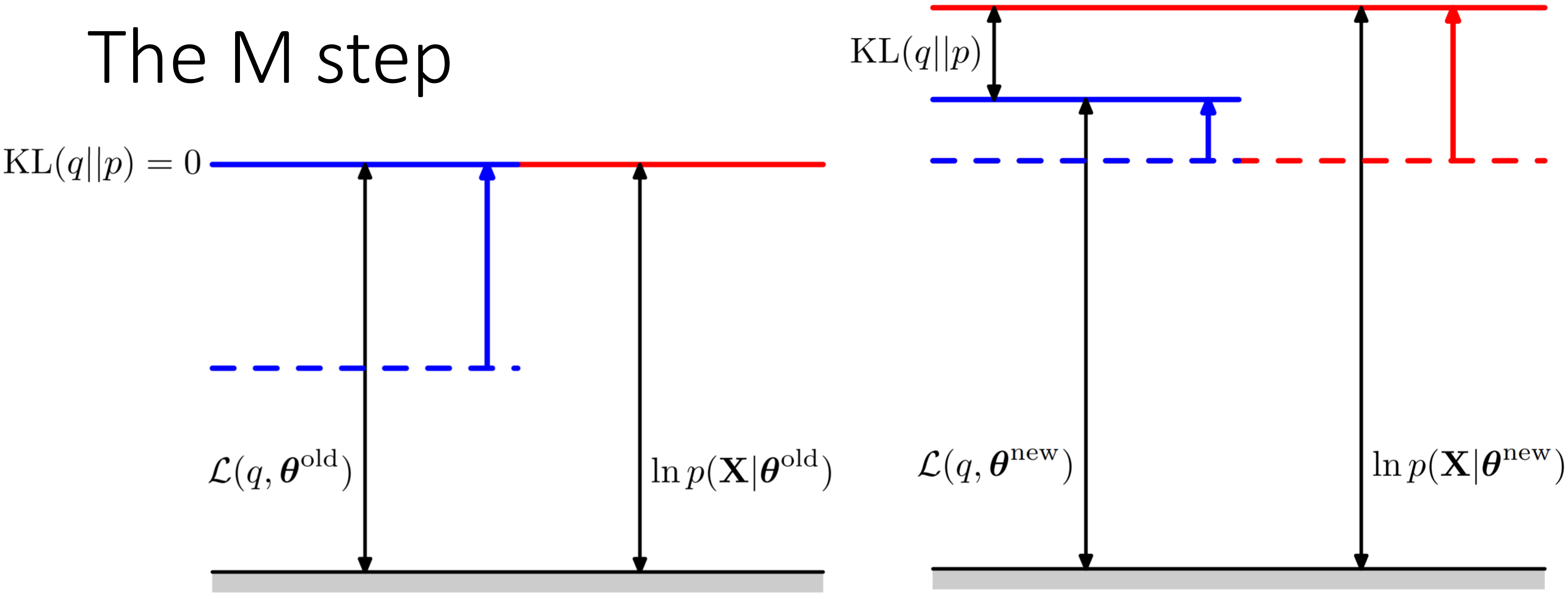
The M step

- Fixing $q^{(t)}(z)$ we now solve:

$$
\begin{aligned}
\operatorname{argmax}_\theta \mathcal{L}\left(q^{(t)}, \theta\right) &= \operatorname{argmax}_\theta -\mathrm{KL}\left(q^{(t)}(z) \,||\, p(x, z|\theta)\right) \\
&= \operatorname{argmax}_\theta - \int q^{(t)}(z) \log\left[\frac{q^{(t)}(z)}{p(x, z|\theta)}\right] \mathbf{d}z \\
&= \operatorname{argmax}_\theta \int q^{(t)}(z) [\log p(x, z\,|\theta) - \log q^{(t)}(z)] \mathbf{d}z \\
&= \operatorname{argmax}_\theta \int q^{(t)}(z) \log p(x, z\,|\theta) \boxed{- q^{(t)}(z) \log q^{(t)}(z)\, \mathbf{d}z} \\
&= \operatorname{argmax}_\theta \int q^{(t)}(z) \log p(x, z\,|\theta)\, \mathbf{d}z \\
&= \operatorname{argmax}_\theta \mathbb{E}_{q^{(t)}(z)}[\log p(x, z\,|\theta)]
\end{aligned}
$$

Constant w.r.t. θ

The M step



$\mathrm{KL}(q||p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\mathrm{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{old}})$
$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta}^{\mathrm{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{new}})$

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- After applying the E step, we increase the likelihood of the data by finding better parameters according to: $\theta^{(t)} \leftarrow \mathbf{argmax}_{\boldsymbol{\theta}}\, \mathbb{E}_{\boldsymbol{q}^{(t)}(\boldsymbol{z})}[\mathbf{log}\, \boldsymbol{p}(\boldsymbol{x}, \boldsymbol{z}\, |\boldsymbol{\theta})]$

EM algorithm

- Initialize $\theta^{(0)}$
- At each iteration $t = 1, \dots$
    - **E step:** Update $q^{(t)}(z) \leftarrow p\left(z \middle| x, \theta^{(t-1)}\right)$
    - **M step:** Update $\theta^{(t)} \leftarrow \mathrm{argmax}_\theta \, \mathbb{E}_{q^{(t)}(z)}[\log p(x, z \,|\theta)]$

Why does EM work?

- EM does coordinate ascent on the ELBO, $\mathcal{L}(q, \theta)$
- Each iteration increases the log-likelihood until $q^{(t)}$ converges (i.e. we reach a local maximum)!
- Simple to prove

Notice after the E step:

$$\begin{aligned} &\mathcal{L}\left(q^{(t)}, \theta^{(t-1)}\right) \\ &= \log p(x|\theta^{(t-1)}) - \mathrm{KL}\left(p\left(z|x, \theta^{(t-1)}\right) \,||\, p\left(z|x, \theta^{(t-1)}\right)\right) \\ &= \log p(x|\theta^{(t-1)}) \end{aligned}$$

The ELBO is tight!

By definition of argmax in the M step:

$$\mathcal{L}\left(q^{(t)}, \theta^{(t)}\right) \geq \mathcal{L}\left(q^{(t)}, \theta^{(t-1)}\right)$$

By simple substitution:

$$\mathcal{L}\left(q^{(t)}, \theta^{(t)}\right) \geq \log p\left(x \middle| \theta^{(t-1)}\right)$$

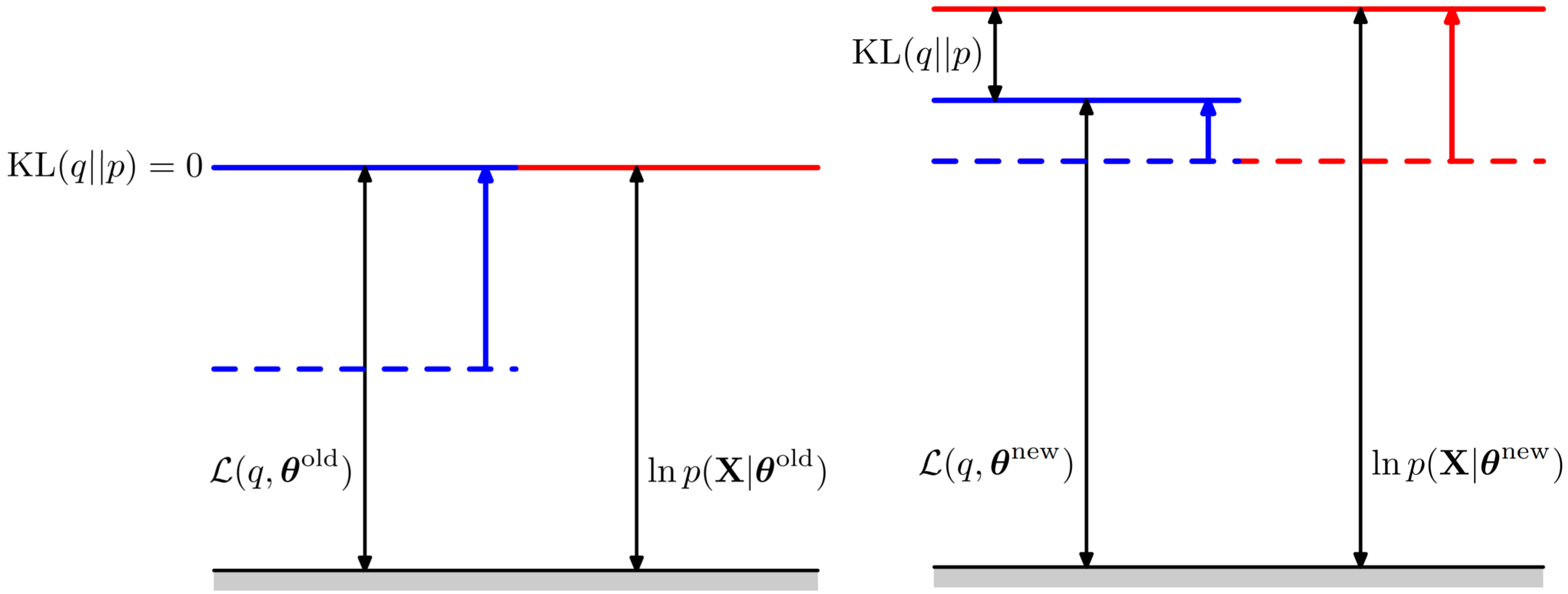
Rewriting the left hand side:

$$\begin{aligned} &\log p(x|\theta^{(t)}) - \mathrm{KL}\left(p\left(z|x, \theta^{(t-1)}\right) \,||\, p\left(z|x, \theta^{(t)}\right)\right) \\ &\geq \log p\left(x \middle| \theta^{(t-1)}\right) \end{aligned}$$

Noting that KL is non-negative:

$$\boldsymbol{\log p\left(x \middle| \theta^{(t)}\right) \geq \log p\left(x \middle| \theta^{(t-1)}\right)}$$

Why does EM work?


$\mathrm{KL}(q||p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$
$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{new}})$

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- This proof is saying the same thing we saw in pictures. Make the KL 0, then improve our parameter estimates to get a better likelihood

A different perspective

- Consider the log-likelihood of a marginal distribution of the data x in a generic latent variable model with latent variable z parameterized by θ:

$$\ell(\theta) \triangleq \sum_{i=1}^{N} \log p(x_i|\theta) = \sum_{i=1}^{N} \log \int p(x_i, z_i|\theta) \mathbf{d} z_i$$

- Estimating θ is difficult because we have a log outside of the integral, so it does not act directly on the probability distribution (frequently in the exponential family)
- If we observed z_i, then our log-likelihood would be:

$$\ell_c(\theta) \triangleq \sum_{i=1}^{N} \log p(x_i, z_i|\theta)$$

This is called the *complete log-likelihood*

Expected Complete Log-Likelihood

- We can take the expectation of this likelihood over a distribution of the latent variable $q(z)$:

$$\mathbb{E}_{q(z)}[\ell_c(\theta)] = \sum_{i=1}^{N} \int q(z_i) \log p(x_i, z_i|\theta) \,\mathrm{d}z_i$$

- This looks similar to marginalizing, but now the log is inside the integral, so it’s easier to deal with
- We can treat the latent variables as observed and solve this more easily than directly solving the log-likelihood
- Finding the q that maximizes this is the E step of EM
- Finding the θ that maximizes this is the M step of EM

Back to Factor Analysis

- For simplicity, assume data is centered. We want:

$$\operatorname{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} \log p(\boldsymbol{X}|\boldsymbol{W},\boldsymbol{\Psi}) = \operatorname{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} \sum_{i=1}^{N} \log p(\boldsymbol{x_i}|\boldsymbol{W},\boldsymbol{\Psi})$$

$$= \operatorname{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} \sum_{i=1}^{N} \log \mathcal{N}(\boldsymbol{x_i}|\boldsymbol{0},\boldsymbol{\Psi}+\boldsymbol{W}\boldsymbol{W}^{T})$$

- No closed form solution in general (PPCA can be solved in closed form)
- $\boldsymbol{\Psi}$, $\boldsymbol{W}$ get coupled together in the derivative and we can’t solve for them analytically

EM for Factor Analysis

$$\text{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}}\, \mathbb{E}_{q^{(t)}(\boldsymbol{z})}[\log p(\boldsymbol{X},\boldsymbol{Z}\,|\boldsymbol{W},\boldsymbol{\Psi})] \; = \text{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} \sum_{i=1}^{N} \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\log p(\boldsymbol{x_i}|\boldsymbol{z_i},\boldsymbol{W},\boldsymbol{\Psi})] + \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\log p(\boldsymbol{z_i})]$$

$$= \text{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} \sum_{i=1}^{N} \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\log p(\boldsymbol{x_i}|\boldsymbol{z_i},\boldsymbol{W},\boldsymbol{\Psi})]$$

$$= \text{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} \sum_{i=1}^{N} \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\log \mathcal{N}(\boldsymbol{W}\boldsymbol{z_i},\boldsymbol{\Psi})]$$

$$= \text{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}}\, \text{const} - \frac{N}{2}\log\det(\boldsymbol{\Psi}) - \sum_{i=1}^{N} \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}\left[\frac{1}{2}(\boldsymbol{x_i}-\boldsymbol{W}\boldsymbol{z_i})^T\boldsymbol{\Psi}^{-1}(\boldsymbol{x_i}-\boldsymbol{W}\boldsymbol{z_i})\right]$$

$$= \text{argmax}_{\boldsymbol{W},\boldsymbol{\Psi}} -\frac{N}{2}\log\det(\boldsymbol{\Psi}) - \sum_{i=1}^{N}\left(\frac{1}{2}\boldsymbol{x}_i^T\boldsymbol{\Psi}^{-1}\boldsymbol{x}_i - \boldsymbol{x_i}^T\boldsymbol{\Psi}^{-1}\boldsymbol{W}\mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z}_i] + \frac{1}{2}\text{tr}\left(\boldsymbol{W}^T\boldsymbol{\Psi}^{-1}\boldsymbol{W}\mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z_i}\boldsymbol{z_i}^T]\right)\right)$$

- **We only need these 2 sufficient statistics to enable the M step.**
- **In practice, sufficient statistics are often what we compute in the E step**

Factor Analysis E step

$$\mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z_i}] = \boldsymbol{G}\boldsymbol{W}^{(\boldsymbol{t-1})^T}\boldsymbol{\Psi}^{(t-1)^{-1}}\boldsymbol{x}_i$$

$$\mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}\left[\boldsymbol{z_i}\boldsymbol{z_i}^T\right] = \boldsymbol{G} + \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z_i}]\mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z_i}]^T$$

Where

$$\boldsymbol{G} = \left(\boldsymbol{I} + \boldsymbol{W}^{(t-1)^T}\boldsymbol{\Psi}^{(t-1)^{-1}}\boldsymbol{W}^{(t-1)}\right)^{-1}$$

This is derived via the Bayes rule for Gaussians

Factor Analysis M step

$$\boldsymbol{W}^{(t)} \leftarrow \left[\sum_{i=1}^{N} \boldsymbol{x}_i \, \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z_i}]^T\right]\left[\sum_{i=1}^{N} \mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}\left[\boldsymbol{z_i}\boldsymbol{z_i}^T\right]\right]^{-1}$$

$$\boldsymbol{\Psi}^{(t)} \leftarrow \operatorname{diag}\left(\frac{1}{N}\sum_{i=1}^{N}\boldsymbol{x_i}\boldsymbol{x_i}^T \; - \boldsymbol{W}^{(t)}\frac{1}{N}\sum_{i=1}^{N}\mathbb{E}_{q^{(t)}(\boldsymbol{z_i})}[\boldsymbol{z_i}]\boldsymbol{x}_i^T\right)$$

From EM to Variational Inference

- In EM we alternately maximize the ELBO with respect to θ and probability distribution (functional) q
- In variational inference, we **drop the distinction between hidden variables and parameters** of a distribution
- I.e. we replace $p(x, z|\theta)$ with $p(x, z)$. Effectively this puts a **probability distribution on the parameters $\boldsymbol{\theta}$**, then absorbs them into z
- Fully Bayesian treatment instead of a point estimate for the parameters

Variational Inference

- Now the ELBO is just a function of our weighting distribution $\mathcal{L}(q)$
- We assume a form for q that we can optimize
- For example *mean field theory* assumes q factorizes:

$$q(Z) = \prod_{i=1}^{M} q_i(Z_i)$$

- Then we optimize $\mathcal{L}(q)$ with respect to one of the terms while holding the others constant, and repeat for all terms
- By assuming a form for q we approximate a (typically) intractable true posterior

Mean Field update derivation

$$\mathcal{L}(q) = \int q(Z)\log\left[\frac{p(X,Z)}{q(Z)}\right] dZ = \int q(Z)\log p(X,Z) \; - q(Z)\log q(Z) \; dZ$$

$$= \int \prod_i q_i(Z_i) \left\{ \log p(X,Z) \; - \sum_k \log q_k(Z_k) \right\} dZ$$

$$= \int q_j(Z_j) \left\{ \int \prod_{i \neq j} q_i(Z_i) \left\{ \log p(X,Z) \; - \sum_k \log q_k(Z_k) \right\} dZ_i \right\} \; dZ_j$$

$$= \int q_j(Z_j) \left\{ \int \log p(X,Z) \prod_{i \neq j} q_i(Z_i) dZ_i - \int \prod_{i \neq j} \sum_k q_i(Z_i) \log q_k(Z_k) \, dZ_i \right\} \; dZ_j$$

$$= \int q_j(Z_j) \left\{ \int \log p(X,Z) \prod_{i \neq j} q_i(Z_i) dZ_i - \log q_j(Z_j) \int \prod_{i \neq j} q_i(Z_i) \; dZ_i \right\} dZ_j + \text{ const}$$

$$= \int q_j(Z_j) \left\{ \int \log p(X,Z) \prod_{i \neq j} q_i(Z_i) dZ_i \right\} \; dZ_j - \; \int q_j\left(Z_j\right) \log q_j\left(Z_j\right) dZ_j + \text{ const}$$

$$= \int q_j\left(Z_j\right) \mathbb{E}_{i \neq j}[\log p(X,Z)] \, dZ_j - \; \int q_j(Z_j) \log q_j\left(Z_j\right) dZ_j + \text{ const}$$

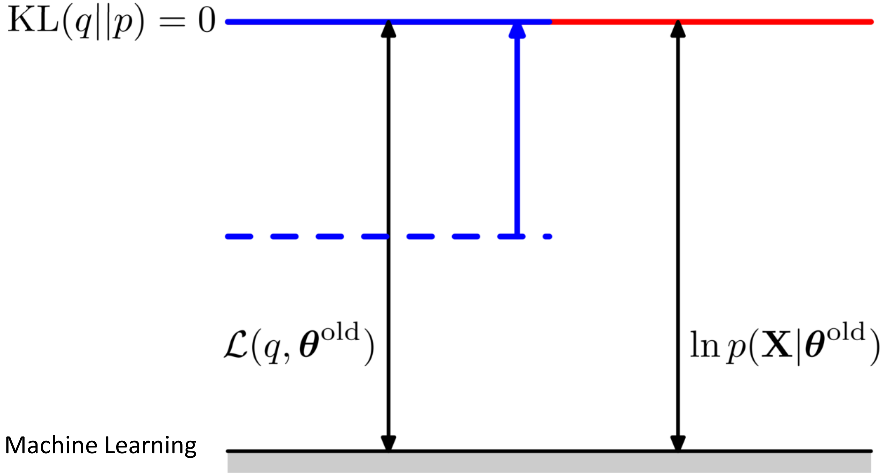
Mean Field update

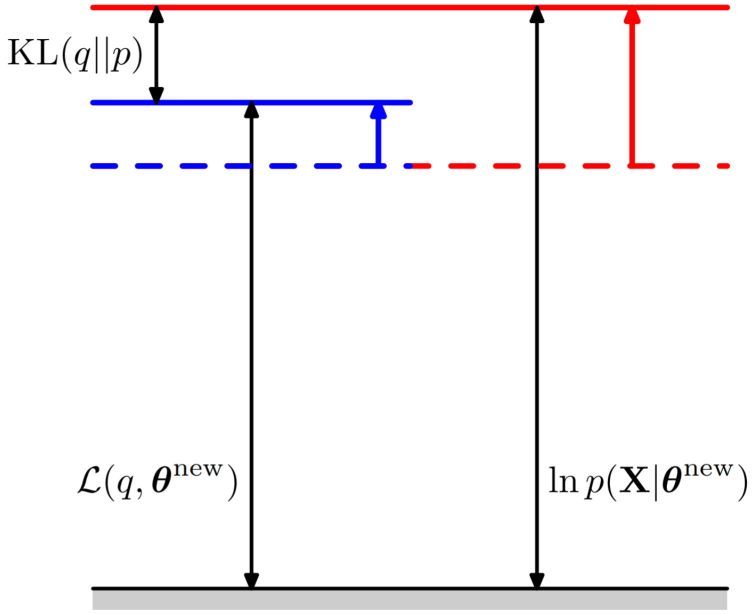
$$q_j(Z_j)^{(t)}$$
$$\leftarrow \ \mathrm{argmax}_{q_j(Z_j)} \int q_j(Z_j)\mathbb{E}_{i\neq j}[\log p(X,Z)]\, dZ_j$$
$$- \int q_j(Z_j) \log q_j(Z_j) dZ_j$$

- The point of this is not the update equations themselves, but the general idea:
  - **freeze some of the variables, compute expectations over those**
  - **update the rest using these expectations**

Why does Variational Inference work?

- The argument is similar to the argument for EM
- When expectations are computed using the current values for the variables not being updated, we implicitly set the KL divergence between the weighting distributions and the posterior distributions to 0
- The update then pushes up the data likelihood


$\mathrm{KL}(q||p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\mathrm{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{old}})$

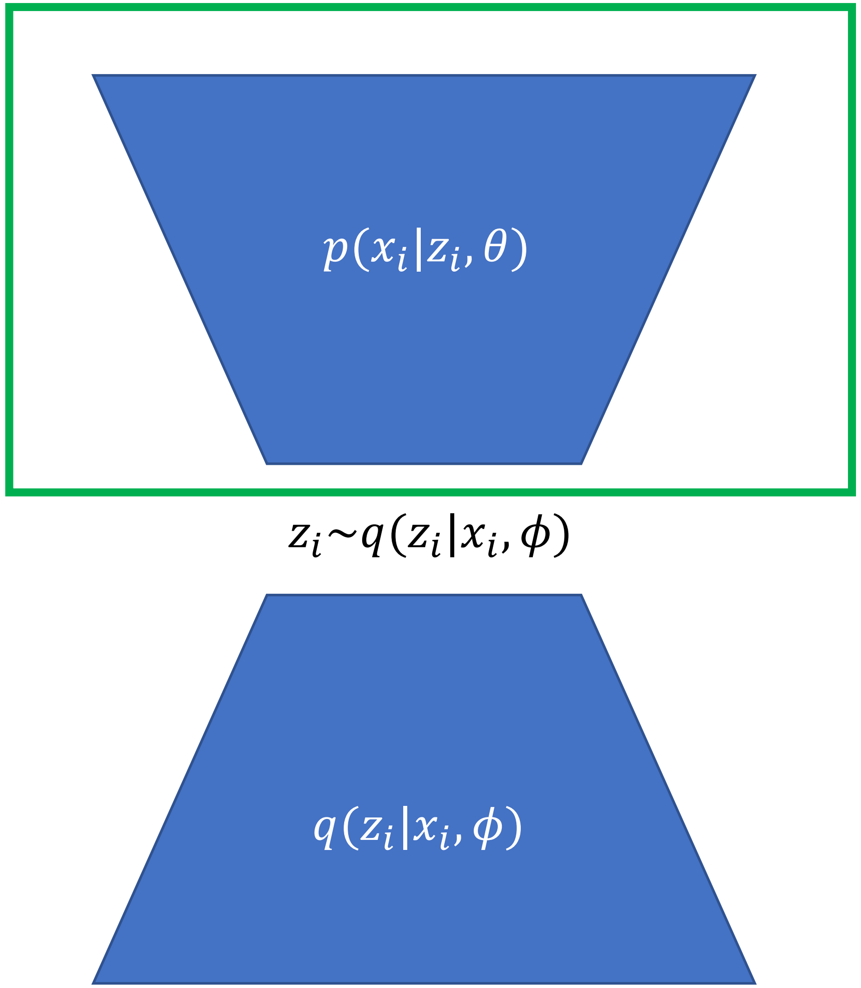

$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta}^{\mathrm{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{new}})$

Bishop – Pattern Recognition and Machine Learning

Variational Autoencoder

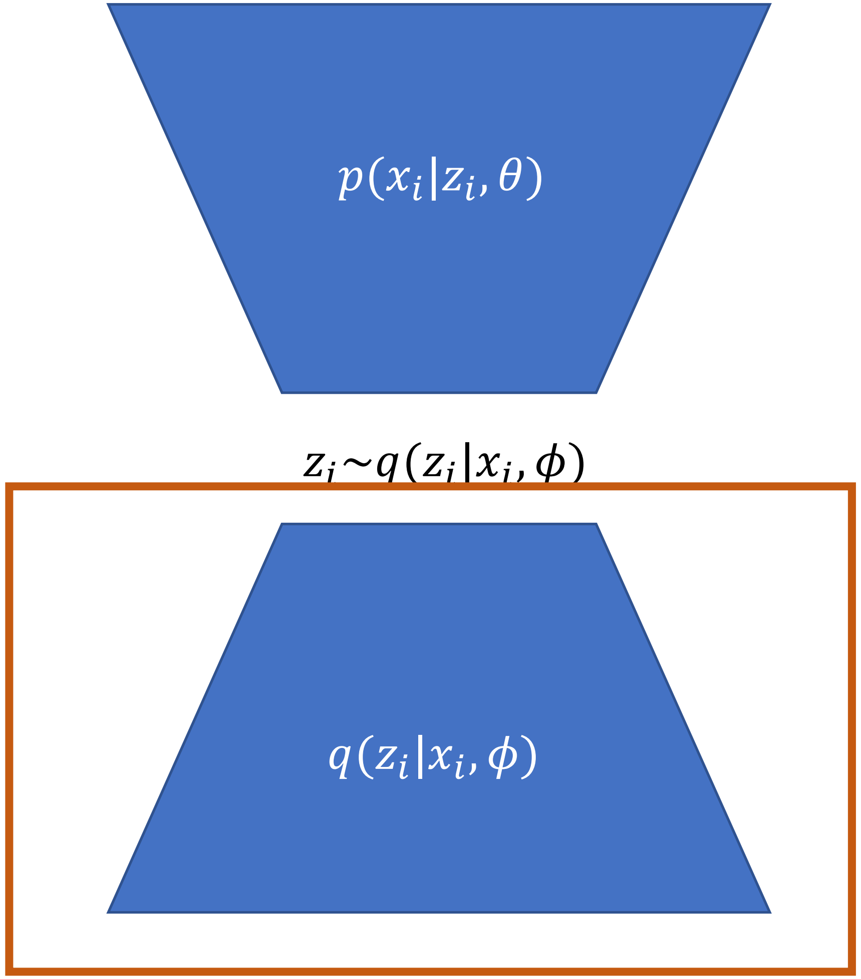
- Kingma & Welling: Auto-Encoding Variational Bayes proposes maximizing the ELBO with a trick to make it differentiable
- Discusses both the variational autoencoder model using parametric distributions and fully Bayesian variational inference, but we will only discuss the variational autoencoder

Problem Setup



- Assume a generative model with a latent variable distributed according to some distribution $p(z_i)$
- The observed variable is distributed according to a conditional distribution $p(x_i|z_i,\theta)$
- Note the similarity to the Factor Analysis (FA) setup so far

Problem Setup

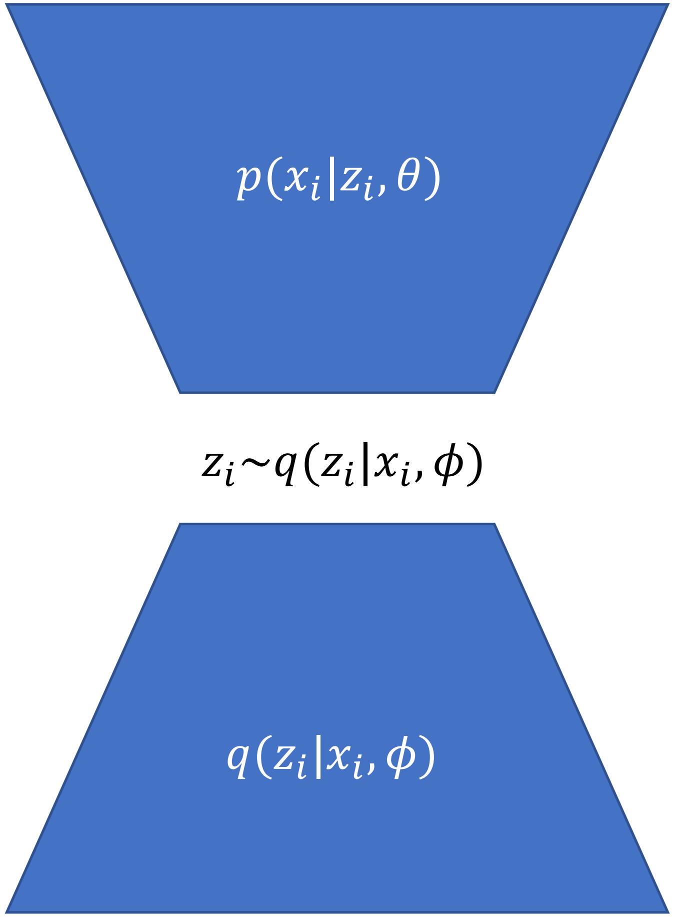


- We also create a weighting distribution $q(z_i|x_i,\phi)$
- This will play the same role as $q(z_i)$ in the EM algorithm, as we will see.
- Note that when we discussed EM, this weighting distribution could be ***arbitrary***: we choose to condition on x_i here. **This is a choice**.
- Why does this make sense?

Using a conditional weighting distribution

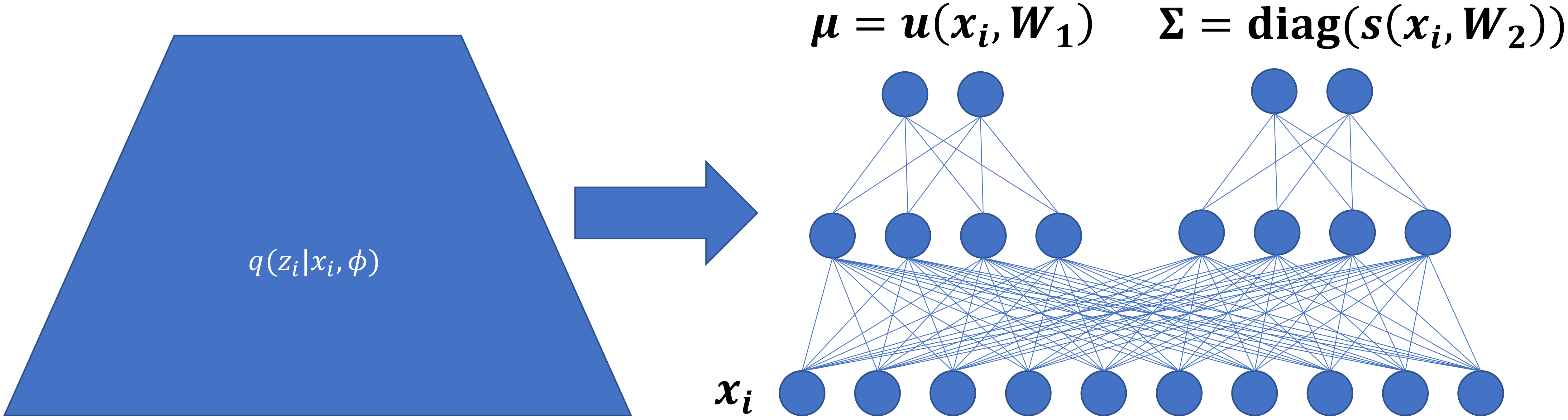
- There are many values of the latent variables that don’t matter in practice – by conditioning on the observed variables, we emphasize the latent variable values we actually care about: the ones most likely given the observations
- We would like to be able to encode our data into the latent variable space. This conditional weighting distribution enables that encoding

Problem setup



- Implement $p(x_i|z_i,\theta)$ as a neural network, this can also be seen as a **probabilistic decoder**
- Implement $q(z_i|x_i,\phi)$ as a neural network, we also can see this as a **probabilistic encoder**
- Sample z_i from $q(z_i|x_i,\phi)$ in the middle

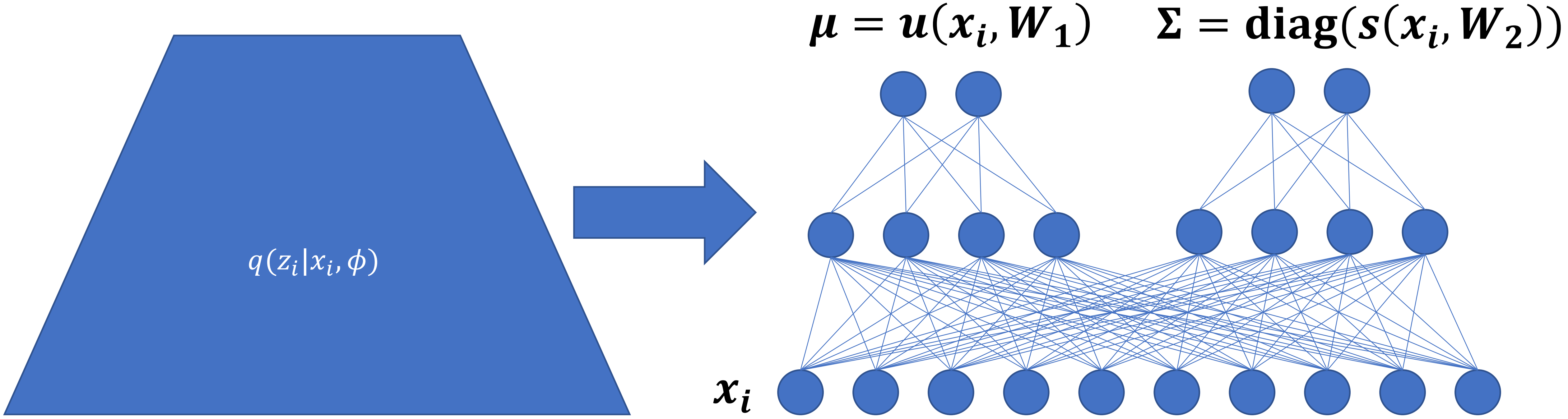
Unpacking the encoder


$q(z_i|x_i,\phi)$
$\boldsymbol{\mu} = \boldsymbol{u}(\boldsymbol{x_i}, \boldsymbol{W_1})$
$\boldsymbol{\Sigma} = \textbf{diag}(\boldsymbol{s}(\boldsymbol{x_i}, \boldsymbol{W_2}))$
$\boldsymbol{x_i}$

- We choose a family of distributions for our conditional distribution q. For example Gaussian with diagonal covariance:

$$q(z_i|x_i,\phi) = \mathcal{N}(z_i|\mu = u(x_i, W_1), \Sigma = \mathrm{diag}(s(x_i, W_2)))$$

Unpacking the encoder



$q(z_i|x_i, \phi)$

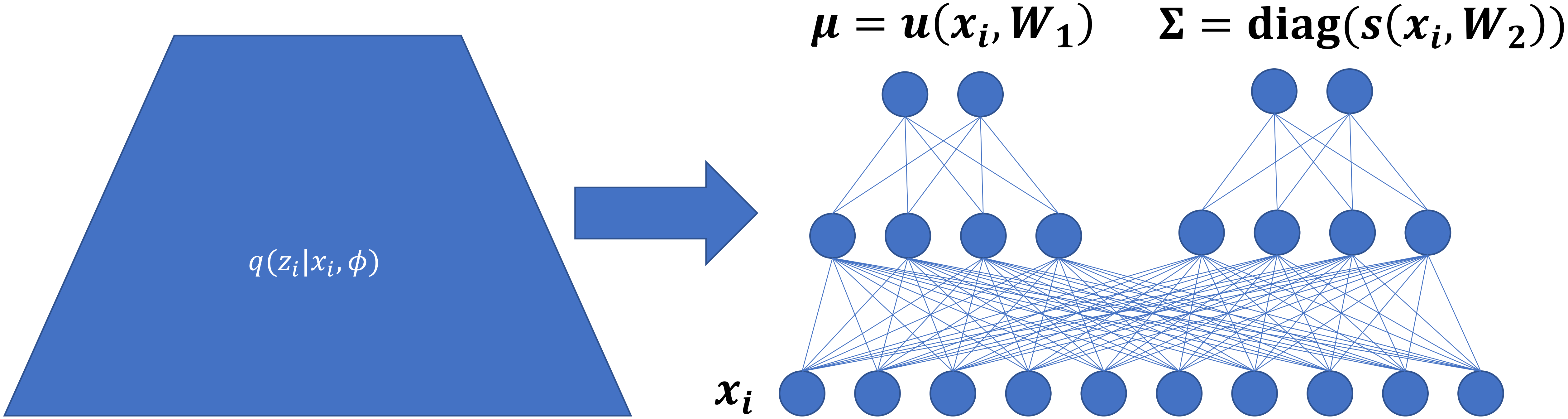
$\boldsymbol{\mu} = \boldsymbol{u}(\boldsymbol{x_i}, \boldsymbol{W_1})$

$\boldsymbol{\Sigma} = \mathbf{diag}(\boldsymbol{s}(\boldsymbol{x_i}, \boldsymbol{W_2}))$

$\boldsymbol{x_i}$

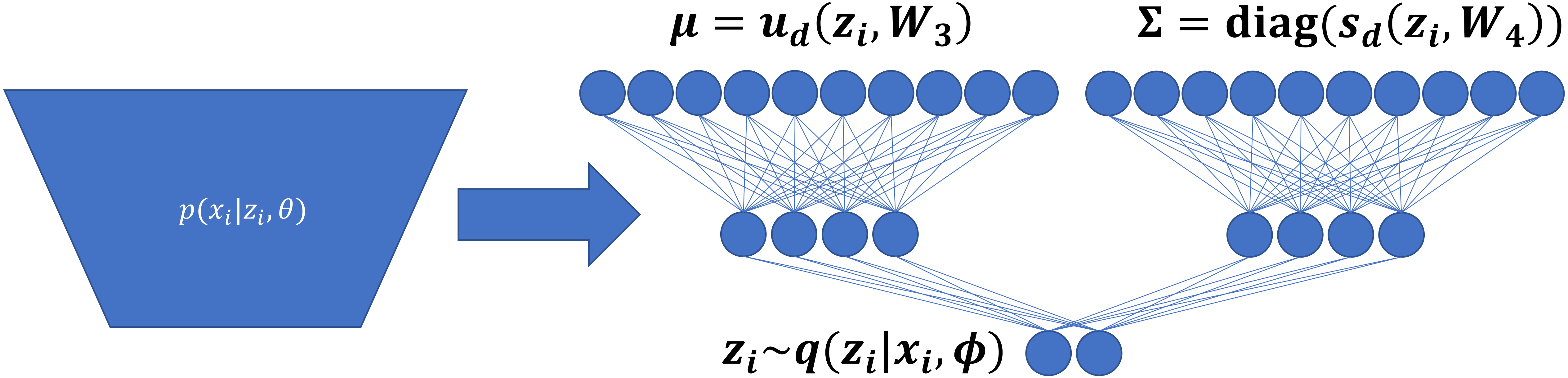
- We create neural networks to predict the parameters of q from our data
- In this case, the outputs of our networks are μ and Σ

Unpacking the encoder


$q(z_i|x_i,\phi)$
$\boldsymbol{\mu} = \boldsymbol{u}(\boldsymbol{x_i}, \boldsymbol{W_1})$
$\boldsymbol{\Sigma} = \mathbf{diag}(\boldsymbol{s}(\boldsymbol{x_i}, \boldsymbol{W_2}))$
$\boldsymbol{x_i}$

- We refer to the parameters of our networks, $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$ collectively as ϕ
- Together, networks $\boldsymbol{u}$ and $\boldsymbol{s}$ parameterize a distribution, $q(z_i|x_i,\phi)$, of the latent variable $\boldsymbol{z_i}$ that depends in a complicated, non-linear way on $\boldsymbol{x_i}$

Unpacking the decoder



$p(x_i|z_i,\theta)$

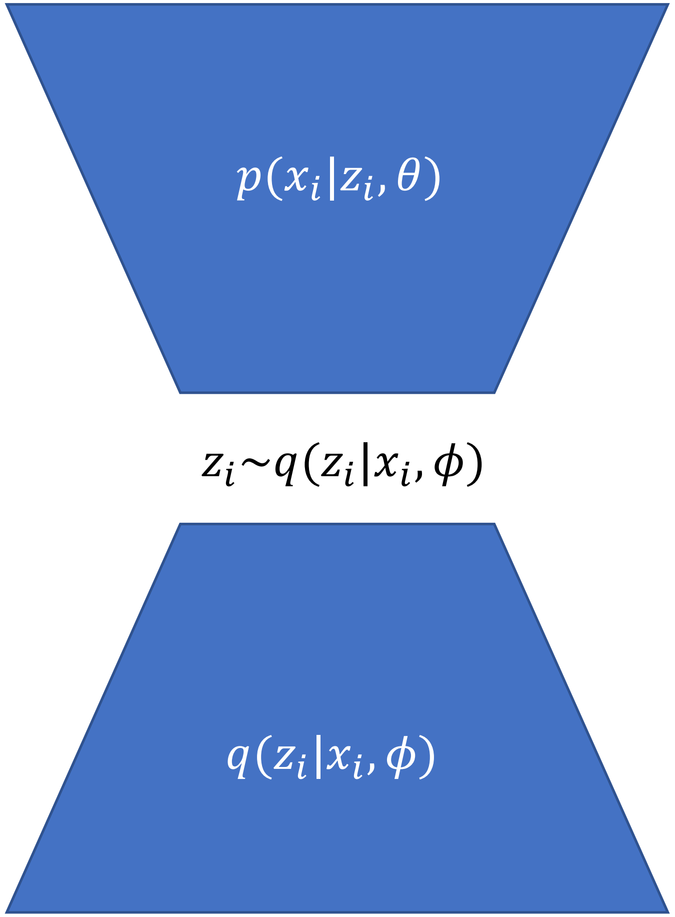
$\boldsymbol{\mu} = \boldsymbol{u_d}(\boldsymbol{z_i}, \boldsymbol{W_3})$

$\boldsymbol{\Sigma} = \mathbf{diag}(\boldsymbol{s_d}(\boldsymbol{z_i}, \boldsymbol{W_4}))$

$\boldsymbol{z_i} \sim \boldsymbol{q}(\boldsymbol{z_i}|\boldsymbol{x_i}, \boldsymbol{\phi})$

- The decoder follows the same logic, just swapping $\boldsymbol{x_i}$ and $\boldsymbol{z_i}$
- We refer to the parameters of our networks, $\boldsymbol{W_3}$ and $\boldsymbol{W_4}$ collectively as θ
- Together, networks $\boldsymbol{u_d}$ and $\boldsymbol{s_d}$ parameterize a distribution, $p(x_i|z_i,\theta)$, of the latent variable $\boldsymbol{x_i}$ that depends in a complicated, non-linear way on $\boldsymbol{z_i}$

Understanding the setup



- Note that p and q do not have to use the same distribution family, this was just an example
- This basically looks like an autoencoder, but the outputs of both the encoder and decoder are parameters of the distributions of the latent and observed variables respectively
- We also have a sampling step in the middle

Using EM for training

- Initialize $\theta^{(0)}$
- At each iteration $t = 1, \ldots, T$
  - **E step:** Hold $\theta^{(t-1)}$ fixed, find $q^{(t)}$ which maximizes $\mathcal{L}\left(q, \theta^{(t-1)}\right)$
  - **M step:** Hold $q^{(t)}$ fixed, find $\theta^{(t)}$ which maximizes $\mathcal{L}\left(q^{(t)}, \theta\right)$

- We will use a modified EM to train the model, but we will transform it so we can use standard back propagation!

Using EM for training

- Initialize $\theta^{(0)}$
- At each iteration $t = 1, \ldots, T$
  - **E step:** Hold $\theta^{(t-1)}$ fixed, find $\phi^{(t)}$ which maximizes $\mathcal{L}\left(\phi, \theta^{(t-1)}, x\right)$
  - **M step:** Hold $\phi^{(t)}$ fixed, find $\theta^{(t)}$ which maximizes $\mathcal{L}\left(\phi^{(t)}, \theta, x\right)$

- First we modify the notation to account for our choice of using a parametric, conditional distribution q

Using EM for training

- Initialize $\theta^{(0)}$
- At each iteration $t = 1, \dots, T$
  - **E step:** Hold $\theta^{(t-1)}$ fixed, find $\frac{\partial \mathcal{L}}{\partial \phi}$ to increase $\mathcal{L}\left(\phi, \theta^{(t-1)}, x\right)$
  - **M step:** Hold $\phi^{(t)}$ fixed, find $\frac{\partial \mathcal{L}}{\partial \theta}$ to increase $\mathcal{L}\left(\phi^{(t)}, \theta, x\right)$

- Instead of fully maximizing at each iteration, we just take a step in the direction that increases $\mathcal{L}$

Computing the loss

- We need to compute the gradient for each mini-batch with B data samples using the ELBO/variational bound $\mathcal{L}(\phi, \theta, x_i)$ as the loss

$$\sum_{i=1}^{B} \mathcal{L}(\phi, \theta, x_i) = \sum_{i=1}^{B} -\mathrm{KL}\big(q(z_i|x_i, \phi) \,||\, p(x_i, z_i|\theta)\big) = \sum_{i=1}^{B} -\mathbb{E}_{q(z_i|x_i,\phi)}\left[\log\left[\frac{q(z_i|x_i, \phi)}{p(x_i, z_i|\theta)}\right]\right]$$

- Notice that this involves an **intractable integral** over all values of z
- We can use Monte Carlo sampling to approximate the expectation using L samples from $q(z_i|x_i, \phi)$:

$$\mathbb{E}_{q(z_i|x_i,\phi)}[f(z_i)] \simeq \frac{1}{L}\sum_{j=1}^{L} f(z_{i,j})$$

$$\mathcal{L}(\phi, \theta, x_i) \simeq \tilde{\mathcal{L}}^{A}(\phi, \theta, x_i) = \frac{1}{L}\sum_{j=1}^{L} \log p\big(x_i, z_{i,j}|\theta\big) - \log q(z_{i,j}|x_i, \phi)$$

A lower variance estimator of the loss

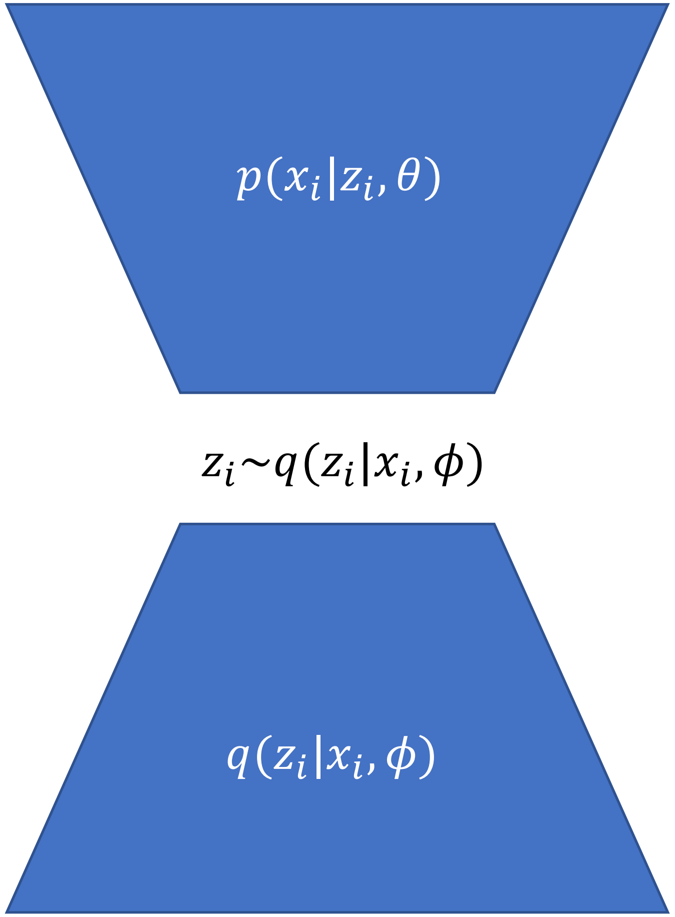
- We can rewrite

$$
\begin{aligned}
\mathcal{L}(\phi,\theta,x) &= -\mathrm{KL}\big(q(z|x,\phi)\ ||\ p(x,z|\theta)\big) \\
&= -\int q(z|x,\phi)\log\left[\frac{q(z|x,\phi)}{p(x|z,\theta)p(z)}\right]\mathbf{d}z \\
&= -\int q(z|x,\phi)\left[\log\left[\frac{q(z|x,\phi)}{p(z)}\right]-\log p(x|z,\theta)\right]\mathbf{d}z = \\
&= -\mathrm{KL}\big(q(z|x,\phi)\ ||\ p(z)\big)+\mathbb{E}_{q(z|x,\phi)}[\log p(x|z,\theta)]
\end{aligned}
$$

- The first term can be computed analytically for some families of distributions (e.g. Gaussian); only the second term must be estimated

$$
\begin{aligned}
&\mathcal{L}(\phi,\theta,x_i) \\
&\simeq \tilde{\mathcal{L}}^B(\phi,\theta,x_i) = -\mathrm{KL}\big(q(z_i|x_i,\phi)\ ||\ p(z_i)\big)+\frac{1}{L}\sum_{j=1}^{L}\log p\big(x_i|z_{i,j},\theta\big)
\end{aligned}
$$

Full EM training procedure (not really used)



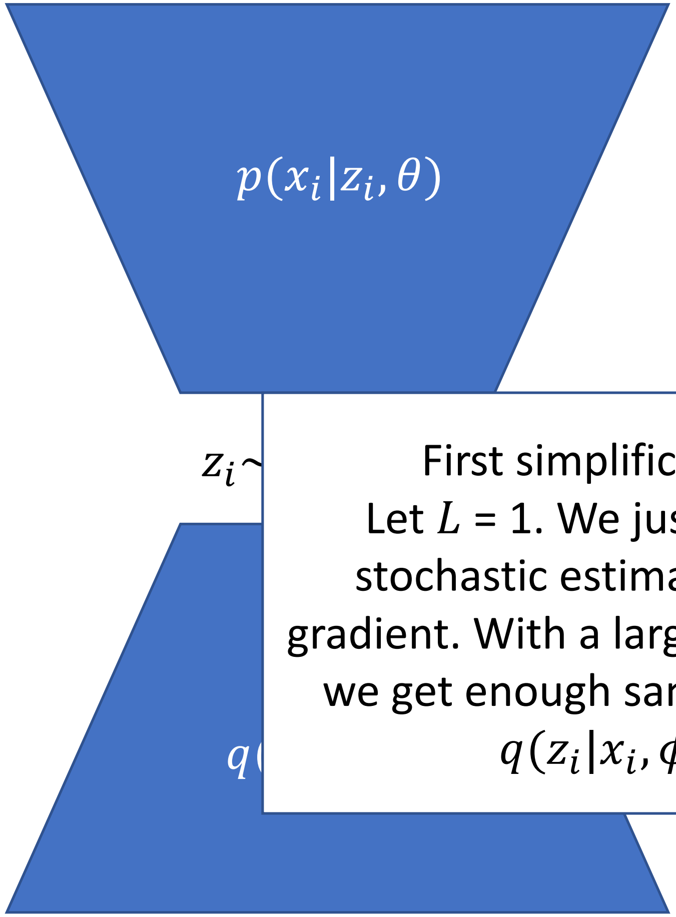
$p(x_i|z_i,\theta)$

$z_i{\sim}q(z_i|x_i,\phi)$

$q(z_i|x_i,\phi)$

- For $t\ =\ 1{:}\,b{:}\,T$
    - Estimate $\frac{\partial\mathcal{L}}{\partial\phi}$ (How do we do this? We'll get to it shortly)
    - Update ϕ
    - Estimate $\frac{\partial\mathcal{L}}{\partial\theta}$:
        - Initialize $\Delta\theta = 0$
        - For $i = t{:}\,t + b - 1$
            - Compute the outputs of the encoder (parameters of q) for x_i
            - For $\ell = 1, \ldots L$
                - Sample $z_i \sim q(z_i|x_i,\phi)$
                - $\Delta\theta_{i,\ell} \leftarrow$ Run forward/backward pass on the decoder (standard back propagation) using either $\tilde{\mathcal{L}}^A$ or $\tilde{\mathcal{L}}^B$ as the loss
                - $\Delta\theta \leftarrow \Delta\theta + \Delta\theta_{i,\ell}$
    - Update θ

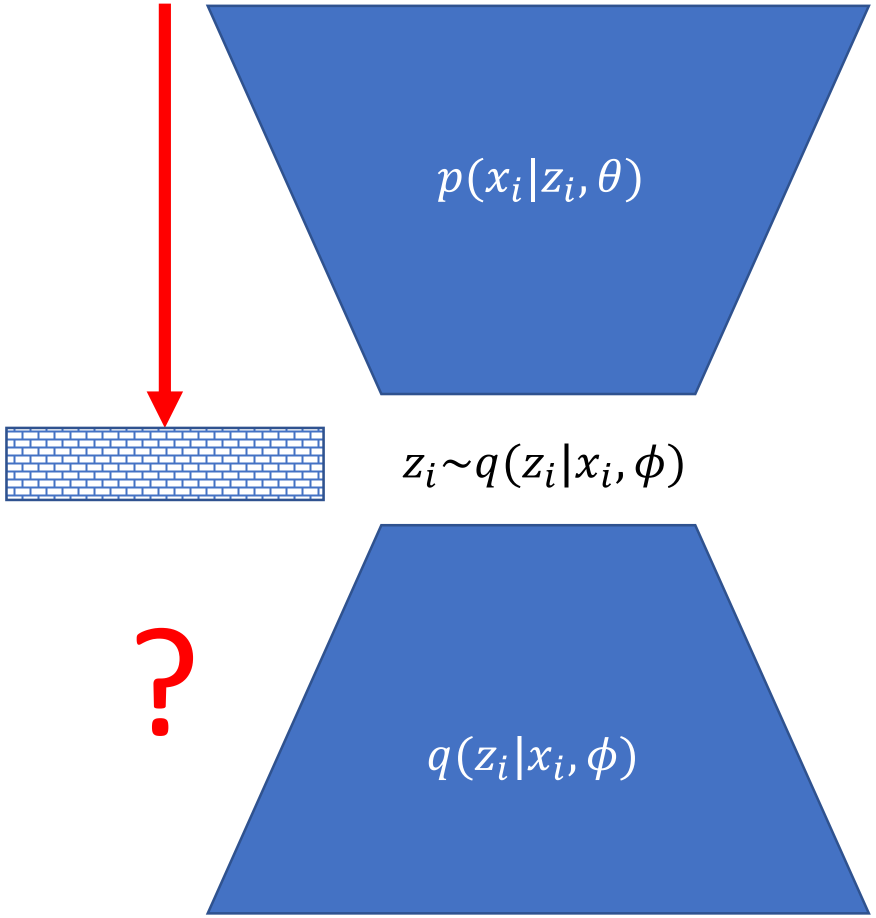
Full EM training procedure (not really used)



First simplification:
Let L = 1. We just want a stochastic estimate of the gradient. With a large enough B, we get enough samples from $q(z_i|x_i,\phi)$

- For $t = 1:b:T$
    - Estimate $\frac{\partial \mathcal{L}}{\partial \phi}$ (How do we do this? We'll get to it shortly)
    - Update ϕ
    - Estimate $\frac{\partial \mathcal{L}}{\partial \theta}$:
        - Initialize $\Delta\theta = 0$
        - For $i = t:t+b-1$
            - Compute the outputs of the encoder (parameters of q) for x_i
            - Sample $z_i \sim q(z_i|x_i,\phi)$
            - $\Delta\theta_i \leftarrow$ Run forward/backward pass on the decoder (standard back propagation) using either $\tilde{\mathcal{L}}^A$ or $\tilde{\mathcal{L}}^B$ as the loss
            - $\Delta\theta \leftarrow \Delta\theta + \Delta\theta_i$
    - Update θ

The E step



- We can use standard back propagation to estimate $\frac{\partial \mathcal{L}}{\partial \theta}$
- How do we estimate $\frac{\partial \mathcal{L}}{\partial \phi}$?
- The sampling step blocks the gradient flow
- Computing the derivatives through q via the chain rule gives a very high variance estimate of the gradient

Reparameterization

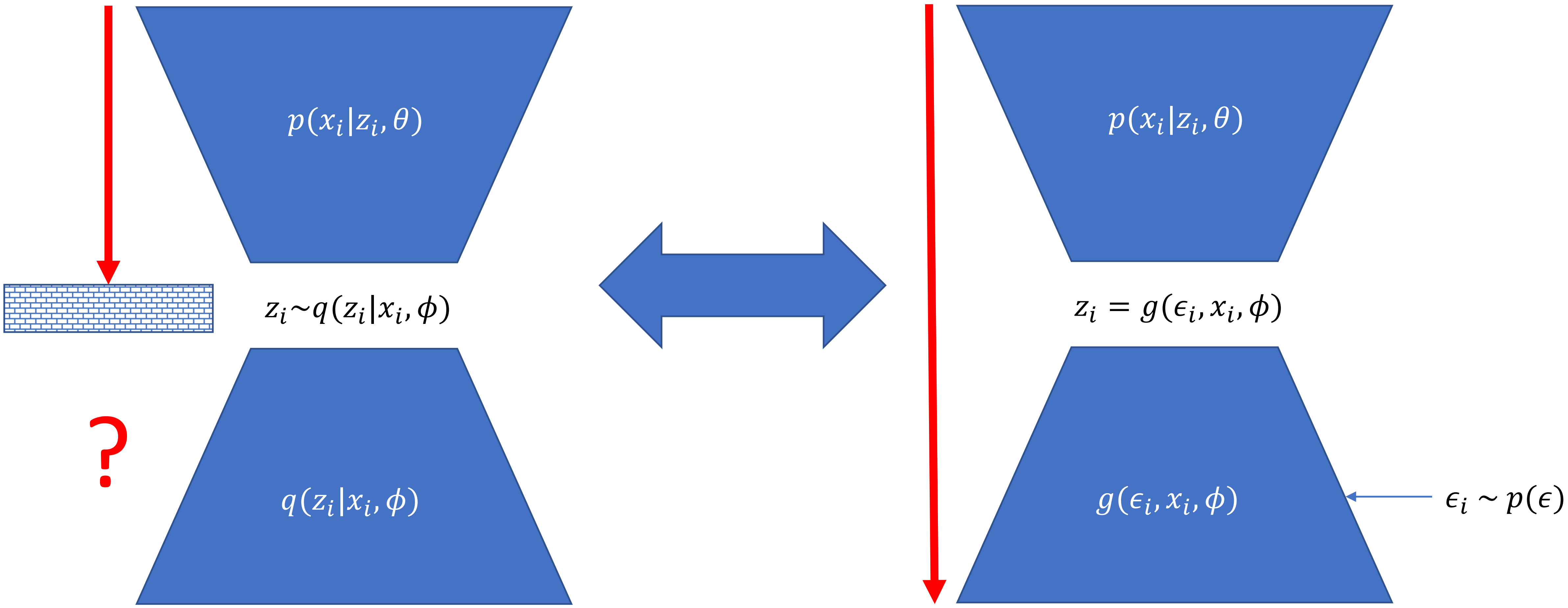
- Instead of drawing $z_i \sim q(z_i|x_i, \phi)$,

  let $z_i = \mathrm{g}(\epsilon_i, x_i, \phi)$, and draw $\epsilon_i \sim p(\epsilon)$
- z_i is still a random variable but depends on ϕ **deterministically**
- Replace $\mathbb{E}_{q(z_i|x_i,\phi)}[f(z_i)]$ with $\mathbb{E}_{p(\epsilon)}[f\big(\mathrm{g}(\epsilon_i, x_i, \phi)\big)]$
- Example – univariate normal:

  $a \sim \mathcal{N}(\mu, \sigma^2)$ is equivalent to

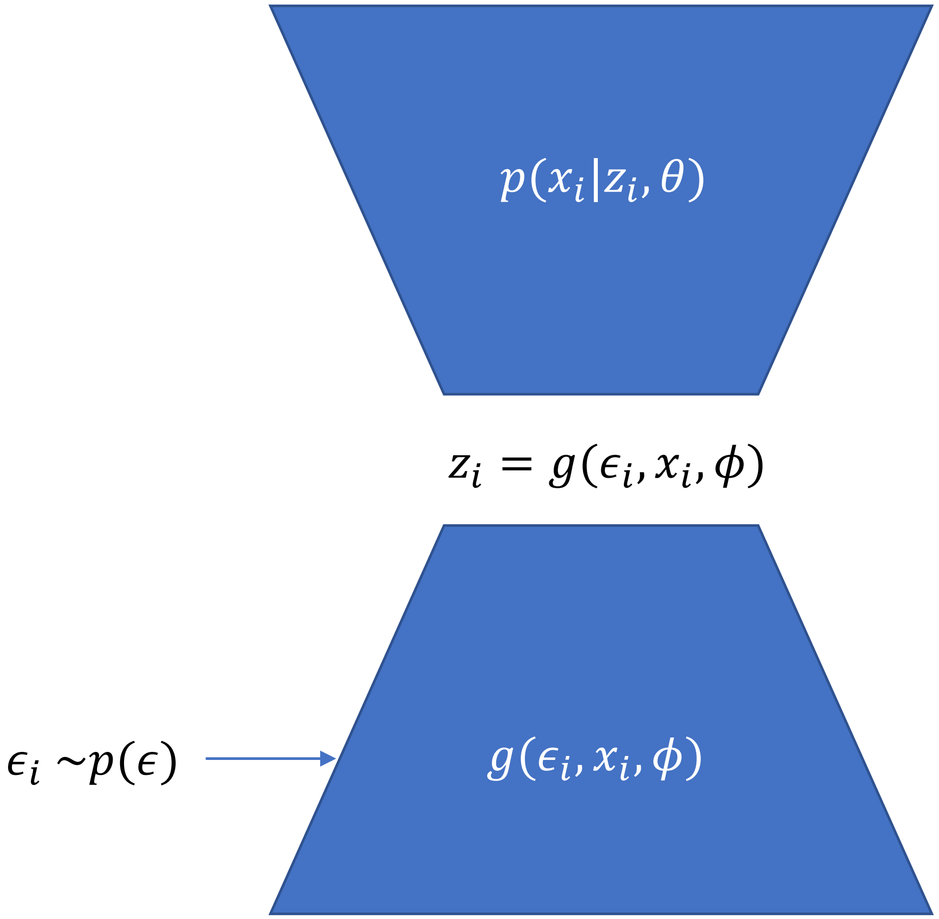
  $a = \mathrm{g}(\epsilon), \epsilon \sim \mathcal{N}(0, 1), \mathrm{g}(b) \triangleq \mu + \sigma b$

Reparameterization



$p(x_i|z_i,\theta)$
$z_i{\sim}q(z_i|x_i,\phi)$
$q(z_i|x_i,\phi)$
?
$p(x_i|z_i,\theta)$
$z_i = g(\epsilon_i,x_i,\phi)$
$g(\epsilon_i,x_i,\phi)$
$\epsilon_i \sim p(\epsilon)$

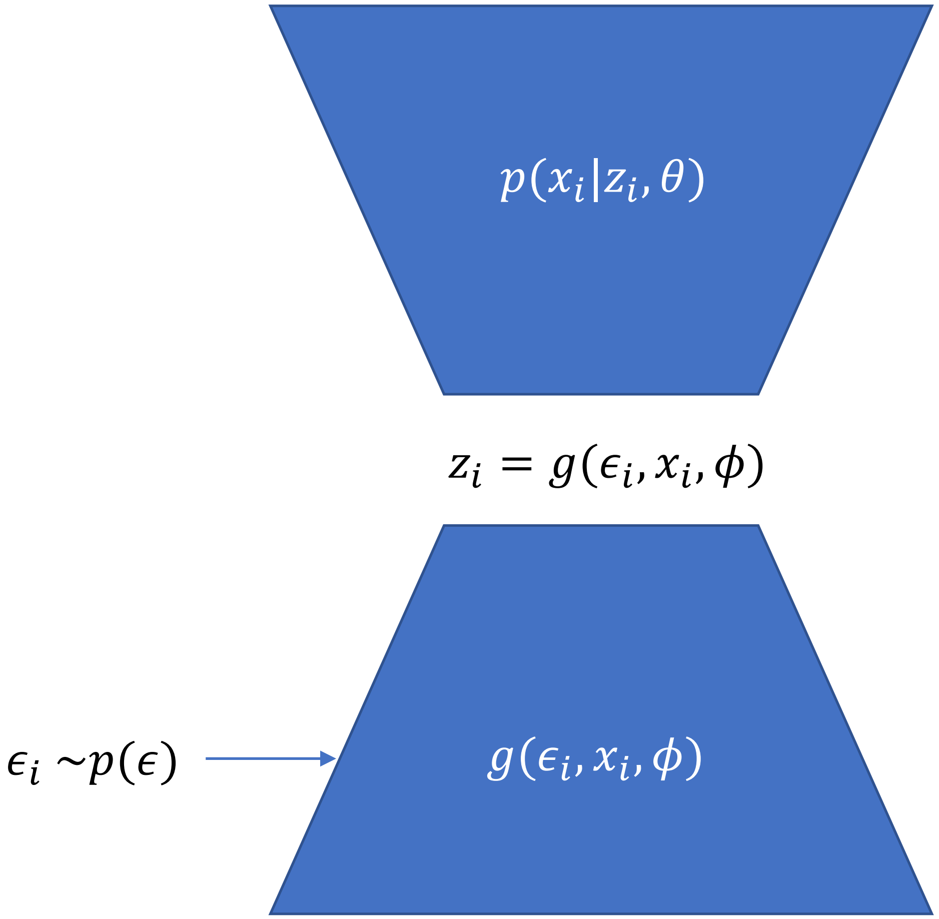
Full EM training procedure (not really used)



$p(x_i|z_i,\theta)$
$z_i = g(\epsilon_i, x_i, \phi)$
$\epsilon_i \sim p(\epsilon)$
$g(\epsilon_i, x_i, \phi)$

- For $t = 1{:}b{:}T$
  - E Step
    - Estimate $\frac{\partial \mathcal{L}}{\partial \phi}$ using standard back propagation with either $\tilde{\mathcal{L}}^A$ or $\tilde{\mathcal{L}}^B$ as the loss
    - Update ϕ
  - M Step
    - Estimate $\frac{\partial \mathcal{L}}{\partial \theta}$ using standard back propagation with either $\tilde{\mathcal{L}}^A$ or $\tilde{\mathcal{L}}^B$ as the loss
    - Update θ

Full training procedure


$p(x_i|z_i,\theta)$
$z_i = g(\epsilon_i, x_i, \phi)$
$\epsilon_i \sim p(\epsilon)$
$g(\epsilon_i, x_i, \phi)$

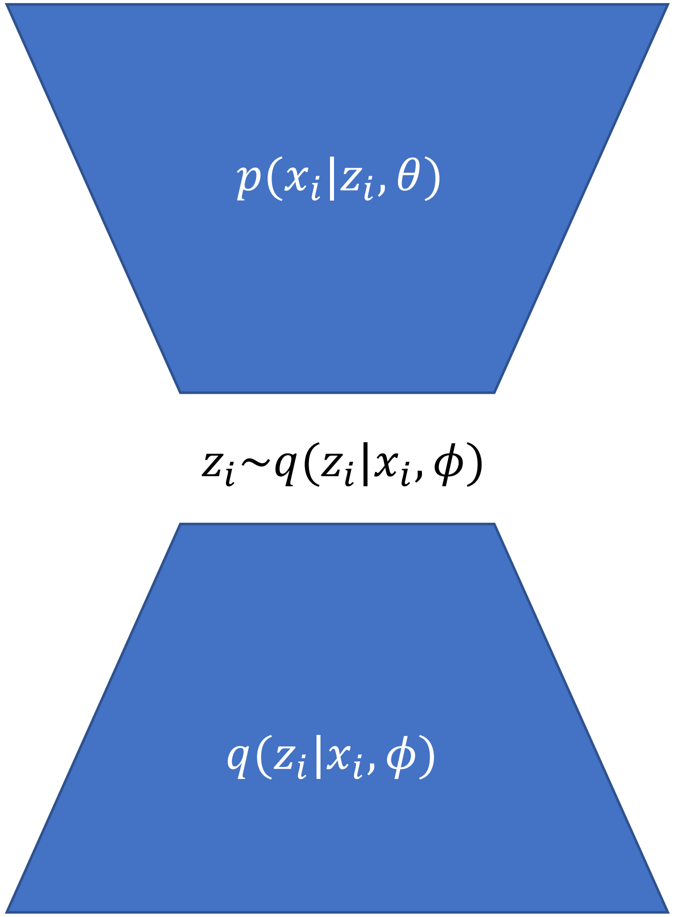
- For $t = 1{:}\,b{:}\,T$
  - Estimate $\frac{\partial \mathcal{L}}{\partial \phi}, \frac{\partial \mathcal{L}}{\partial \theta}$ with either $\tilde{\mathcal{L}}^A$ or $\tilde{\mathcal{L}}^B$ as the loss
  - Update ϕ, θ

- Final simplification: update all of the parameters at the same time instead of using separate E, M steps
- This is standard back propagation. Just use $-\tilde{\mathcal{L}}^A$ or $-\tilde{\mathcal{L}}^B$ as the loss, and run your favorite SGD variant

Running the model on new data

- To get a MAP estimate of the latent variables, just use the mean output by the encoder (for a Gaussian distribution)
- No need to take a sample
- Give the mean to the decoder
- **At test time, this is used just as an auto-encoder**
- You can optionally take multiple samples of the latent variables to estimate the uncertainty

Relationship to Factor Analysis



- VAE performs **probabilistic, non-linear dimensionality reduction**
- It uses a **generative model** with a latent variable distributed according to some prior distribution $p(z_i)$
- The observed variable is distributed according to a conditional distribution $p(x_i|z_i,\theta)$
- Training is approximately running **expectation maximization** to maximize the data likelihood
- This can be seen as a **non-linear version of Factor Analysis**

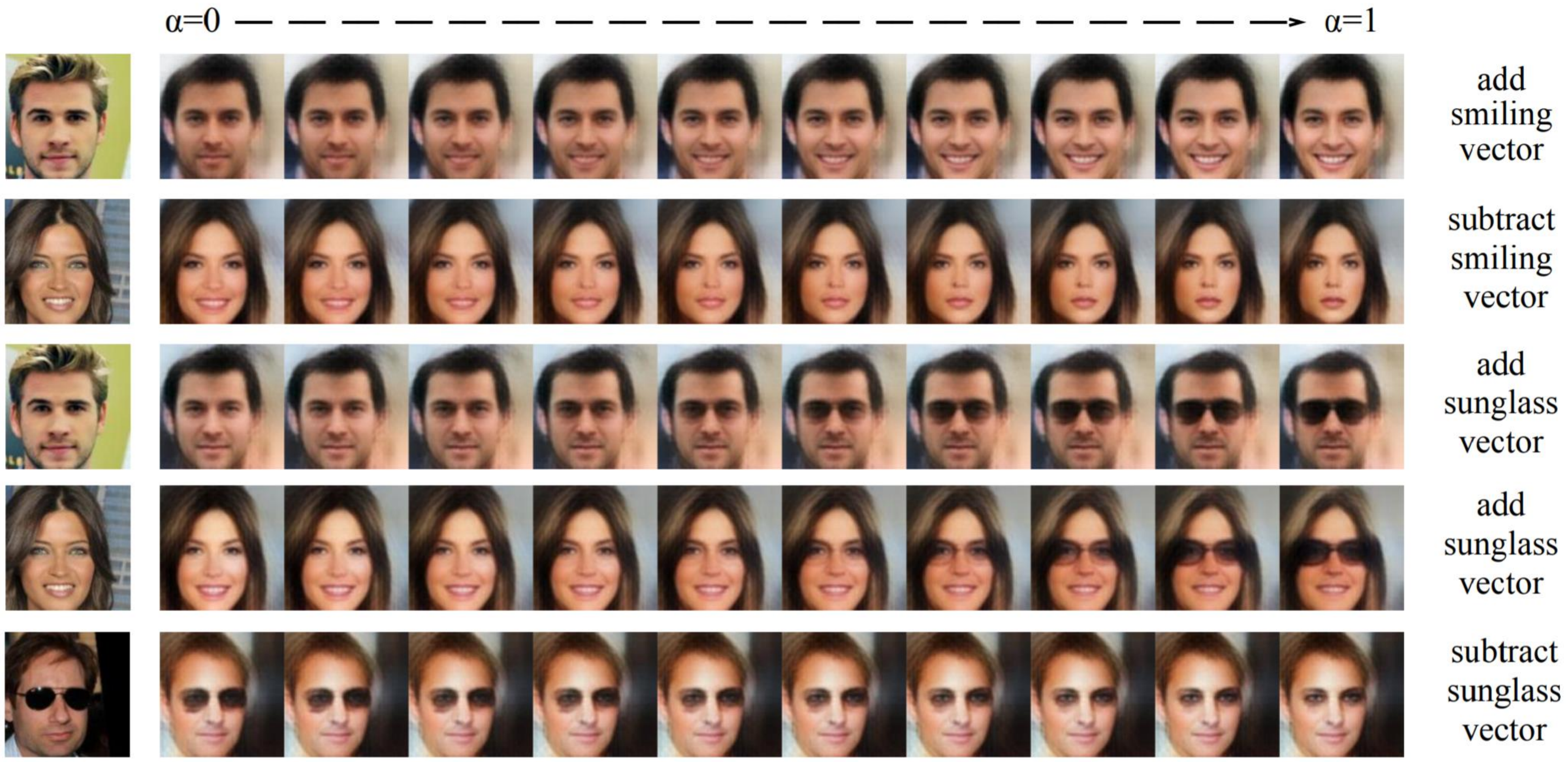
Regularization by a prior

- Looking at the form of $\mathcal{L}$ we used to justify $\tilde{\mathcal{L}}^B$ gives us additional insight
  $$\mathcal{L}(\phi, \theta, x) = -\mathrm{KL}\big(q(z|x, \phi) \,||\, p(z)\big) + \mathbb{E}_{q(z|x,\,\phi)}[\log p(x|z, \theta)]$$
- We are making the latent distribution as close as possible to a prior on z
- While maximizing the conditional likelihood of the data under our model
- In other words this is an approximation to **Maximum Likelihood Estimation regularized by a prior on the latent space**

Practical advantages of a VAE vs. an AE

- The prior on the latent space:
    - Allows you to inject domain knowledge
    - Can make the latent space more interpretable
- The VAE also makes it possible to estimate the variance/uncertainty in the predictions

Interpreting the latent space

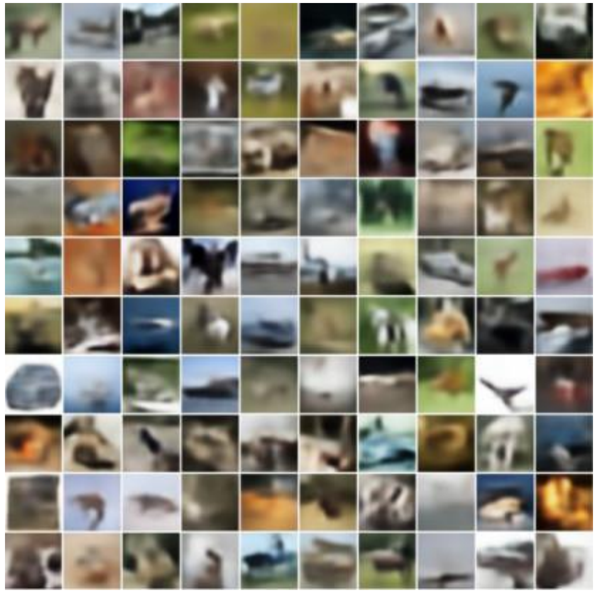


https://arxiv.org/pdf/1610.00291.pdf

Requirements of the VAE

- Note that the VAE requires 2 tractable distributions to be used:
  - The prior distribution $p(z)$ must be easy to sample from
  - The conditional likelihood $p(x|z, \theta)$ must be computable
- In practice this means that the 2 distributions of interest are often simple, for example uniform, Gaussian, or even isotropic Gaussian

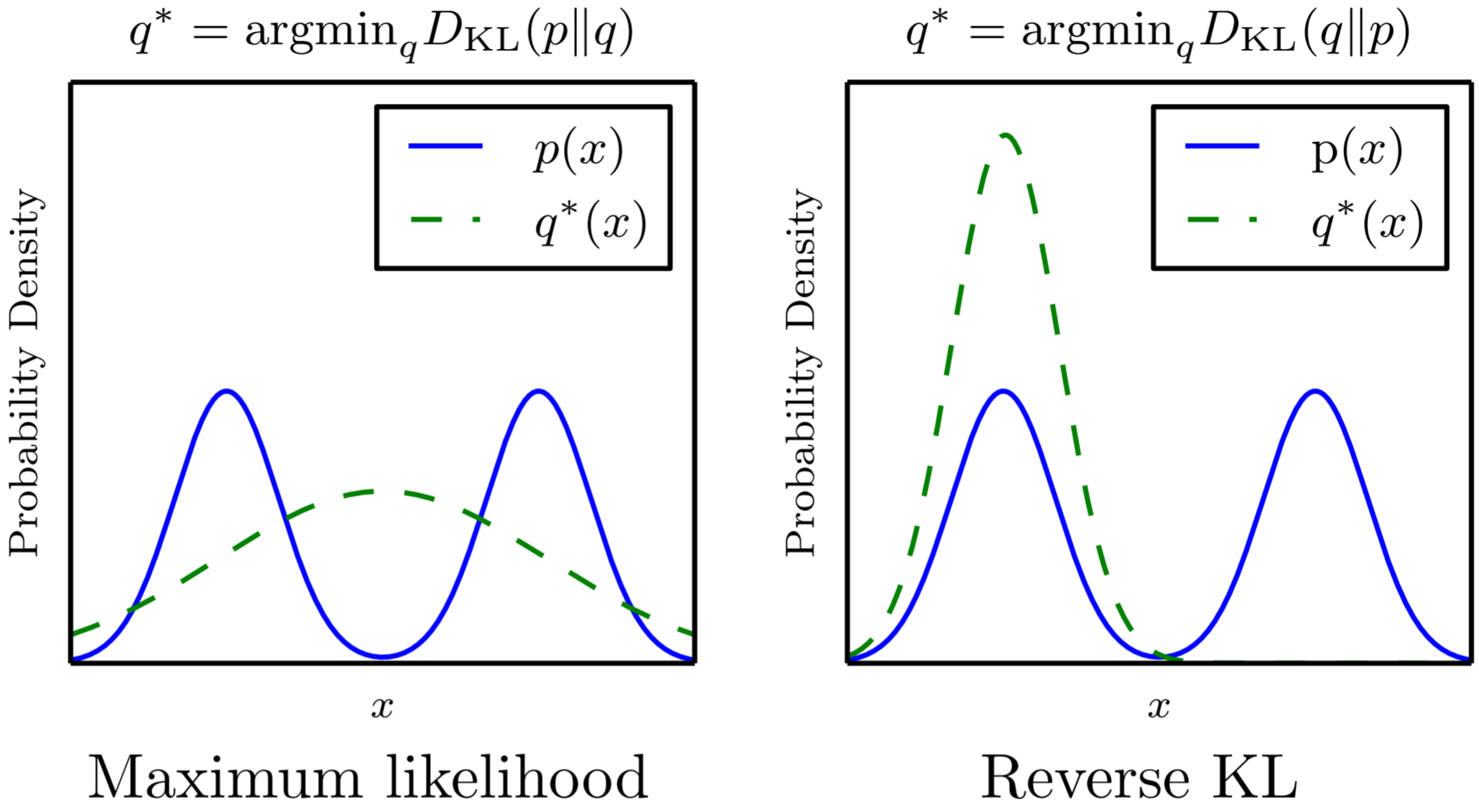
The blurry image problem



https://blog.openai.com/generative-models/

- The samples from the VAE look blurry
- Three plausible explanations for this
  - Maximizing the likelihood
  - Restrictions on the family of distributions
  - The lower bound approximation

The maximum likelihood explanation



Maximum likelihood

Reverse KL

- Recent evidence suggests that this is not actually the problem
- GANs can be trained with maximum likelihood and still generate sharp examples

https://arxiv.org/pdf/1701.00160.pdf

Investigations of blurriness

- Recent investigations suggest that both the simple probability distributions and the variational approximation lead to blurry images
- Kingma & colleages: Improving Variational Inference with Inverse Autoregressive Flow
- Zhao & colleagues: Towards a Deeper Understanding of Variational Autoencoding Models
- Nowozin & colleagues: f-gan: Training generative neural samplers using variational divergence minimization