EE-608: Deep Learning For Natural Language Processing: (Nonparametric) Variational Auto-Encoders

James Henderson

Idiap Research Institute

DLNLP, Lecture 4

Outline

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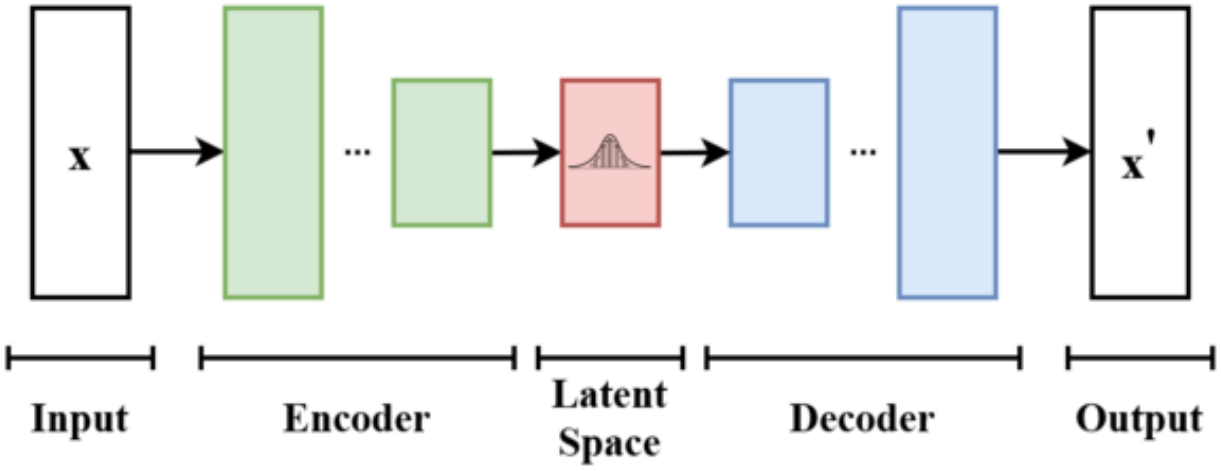
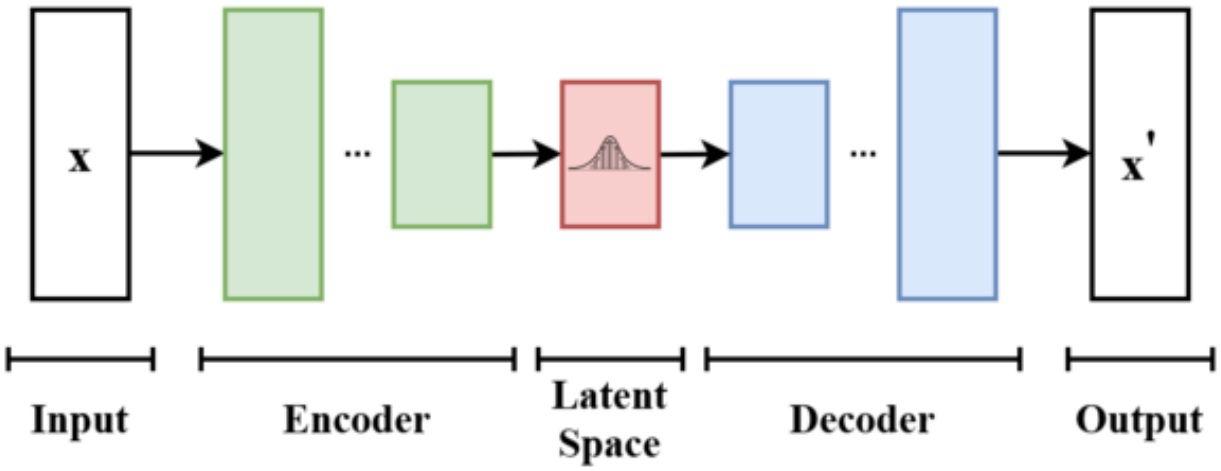
A Bayesian Approach to Auto-Encoders



- Auto-encoders learn to compress the observations into a smaller latent representation
- Thus learning a representation where underlying correlations are captured

But what does “smaller” mean? Can’t we encode an arbitrary amount of information in continuous values?

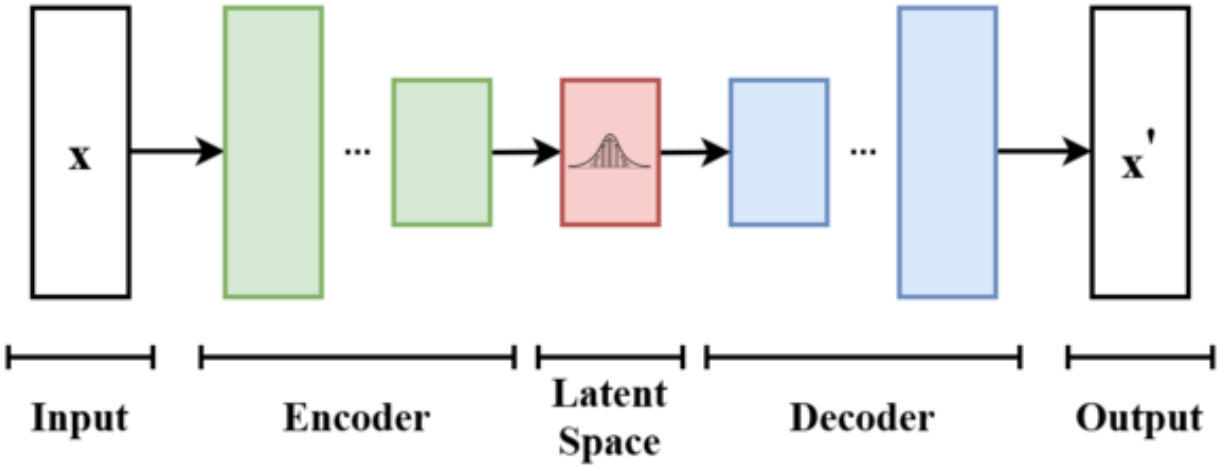
A Bayesian Approach to Auto-encoders

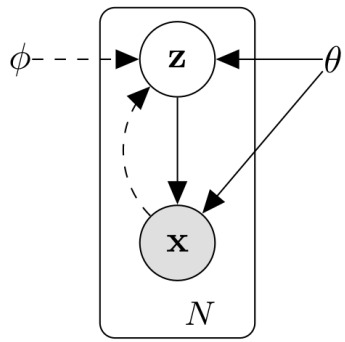


Adding noise to the latent representation controls the amount of information that can pass through it.

- **Information Bottleneck**: minimise the amount of information that passes through the latent representation
- **Reconstruction Loss**: ensure that enough information is passed to reconstruct the input

A Variational Bayesian Approach to Auto-Encoders



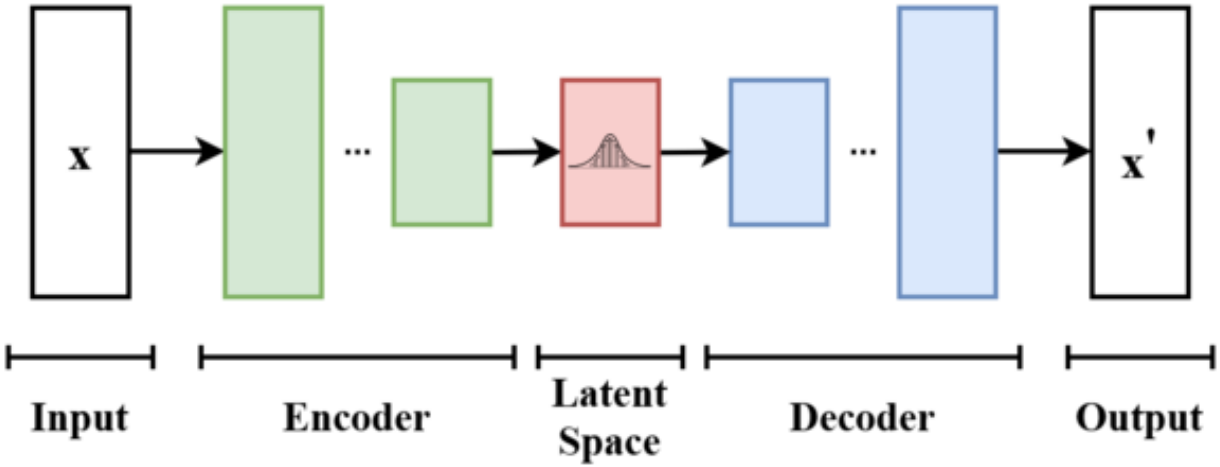


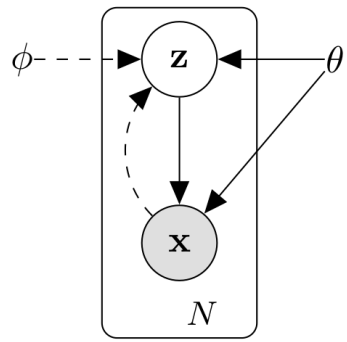
But Bayesian inference in deep models is intractable!

- **Variational Information Bottleneck**: train a deep variational approximation to the intractable parts of Bayesian inference

[Auto-Encoding Variational Bayes, Kingma and Welling, 2014]

A Variational Bayesian Approach to Auto-Encoders





But how can we backprop through a stochastic model?

- **Reparameterisation Trick**: move the noise to an input so that everything we need to backprop through is deterministic

[Auto-Encoding Variational Bayes, Kingma and Welling, 2014]

Taxonomy of Generative Models

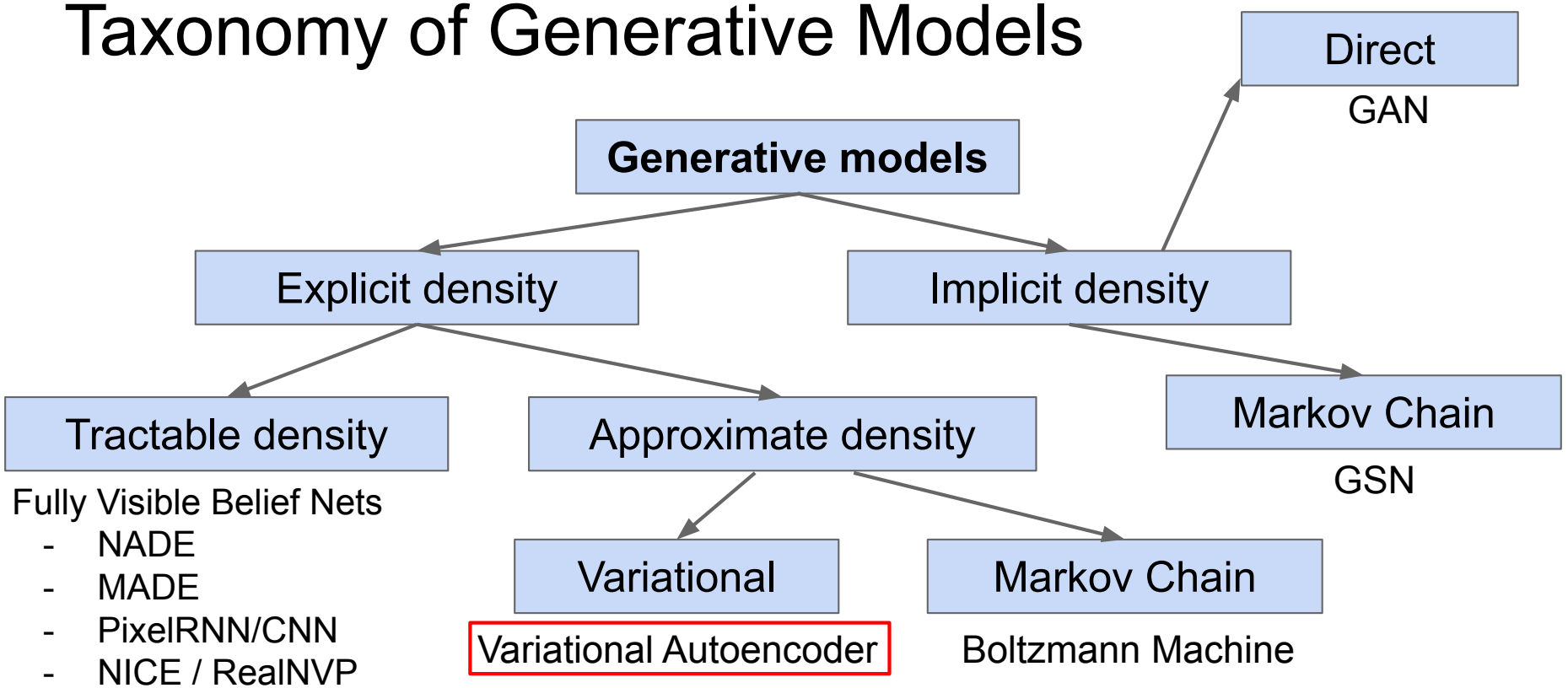
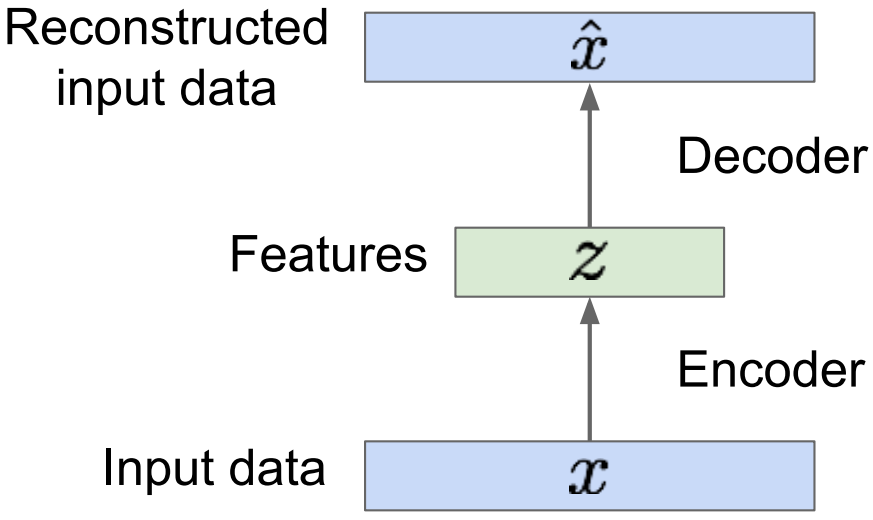


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Outline

Some background first: Autoencoders



Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data.

But we can't generate new images from an autoencoder because we don't know the space of z.

How do we make autoencoder a **generative model**?

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

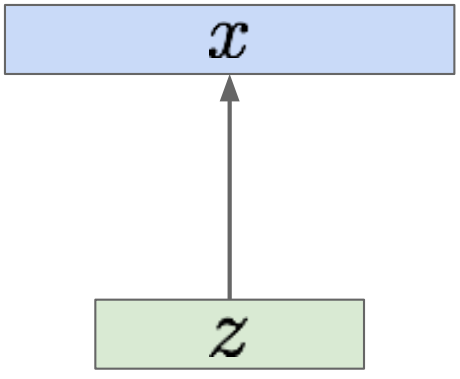
Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

Sample from true conditional $p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior $z^{(i)} \sim p_{\theta^*}(z)$



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

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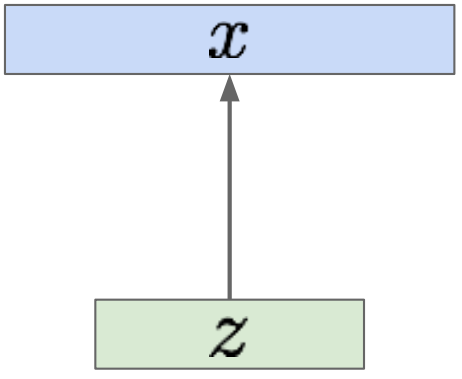

Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

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Variational Autoencoders

We want to estimate the true parameters θ^* of this generative model given training data x.

Sample from true conditional

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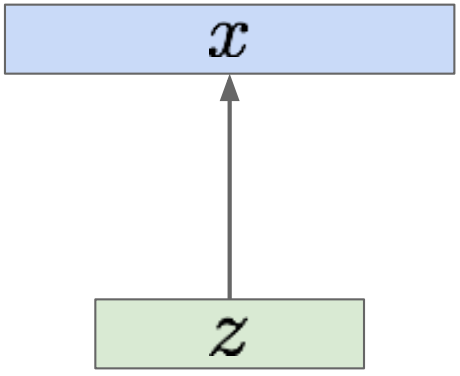

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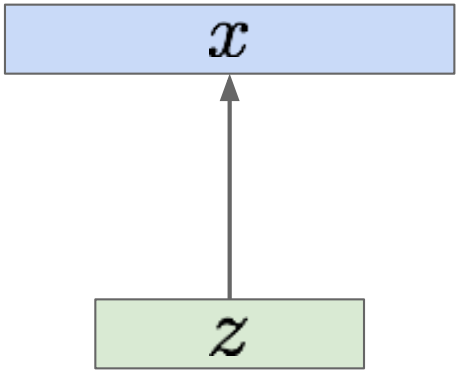

How should we represent this model?

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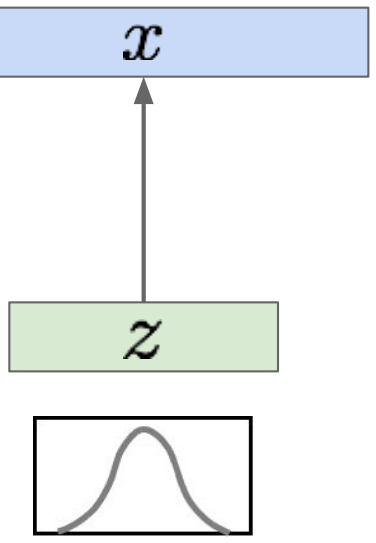

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How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

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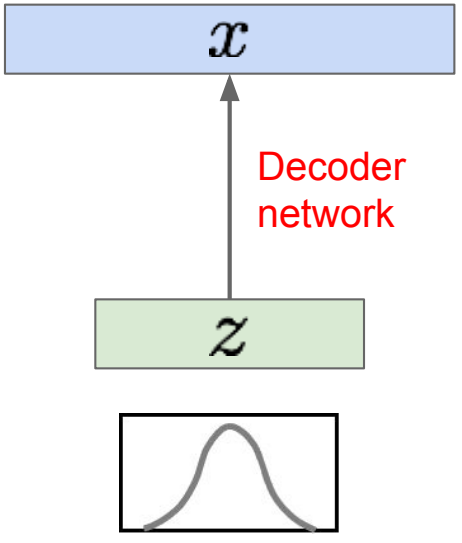

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Conditional p(x|z) is complex (generates image) => represent with neural network

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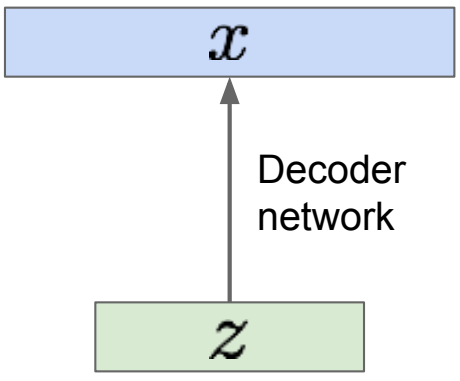

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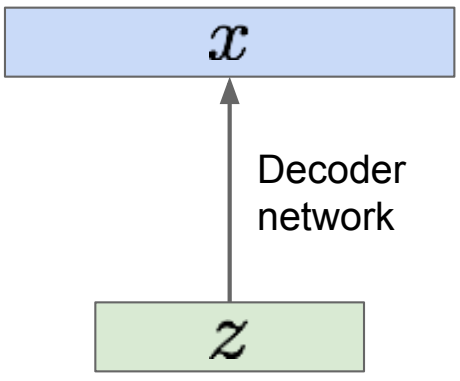

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How to train the model?

Learn model parameters to maximize likelihood of training data

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

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Variational Autoencoders

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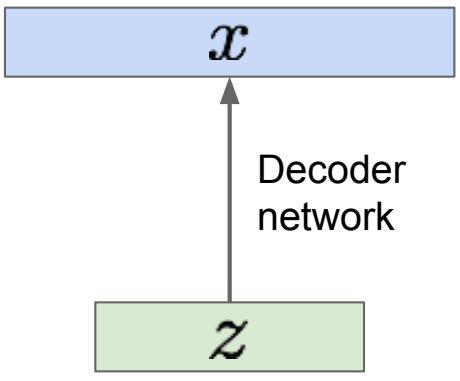

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Q: What is the problem with this?

Intractable!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

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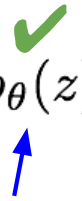

Simple Gaussian prior

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Variational Autoencoders: Intractability

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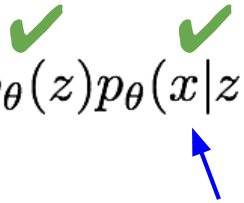

Decoder neural network

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Intractability

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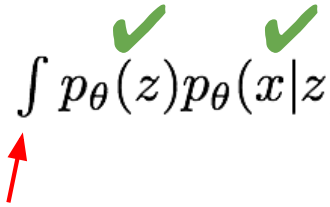

Intractable to compute p(x|z) for every z!

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Variational Autoencoders: Intractability

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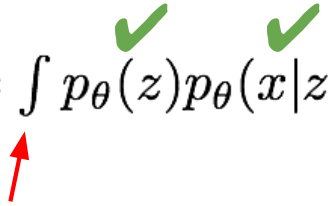

Intractable to compute p(x|z) for every z!

$$\log p(x) \approx \log \frac{1}{k} \sum_{i=1}^{k} p(x|z^{(i)}), \text{where } z^{(i)} \sim p(z)$$

Monte Carlo estimation is too high variance

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Posterior density: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Intractable data likelihood

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Solution: In addition to modeling $p_\theta(x|z)$, learn $q_\phi(z|x)$ that approximates the true posterior $p_\theta(z|x)$.

Will see that the approximate posterior allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize.

Variational inference is to approximate the unknown posterior distribution from only the observed data x

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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Taking expectation wrt. z (using encoder network) will come in handy later

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Variational Autoencoders

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\end{aligned}
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The expectation wrt. z (using encoder network) let us write nice KL terms

Variational Autoencoders

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Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling (need some trick to differentiate through sampling).

This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

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$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Bayes' Rule})$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant})$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Logarithms})$$

$$= \underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\geq 0}$$

Decoder: reconstruct the input data

Encoder: make approximate posterior distribution close to prior

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

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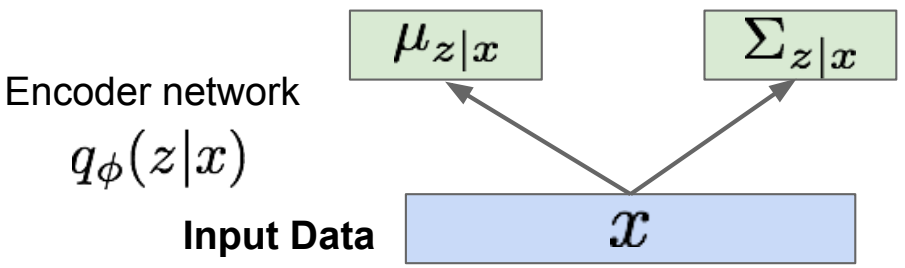
Let's look at computing the KL divergence between the estimated posterior and the prior given some data

Input Data x

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

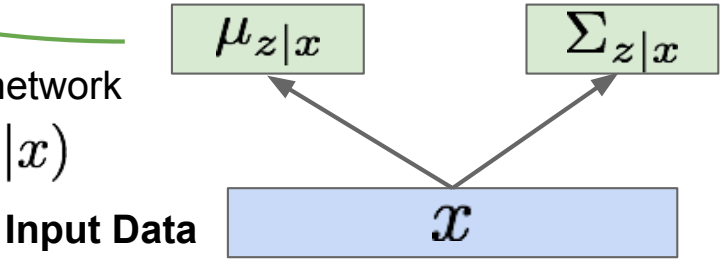
$$D_{KL}(\mathcal{N}(\mu_{z|x}, \Sigma_{z|x})||\mathcal{N}(0, I))$$

Have analytical solution

Make approximate posterior distribution close to prior

Encoder network

$q_\phi(z|x)$



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Not part of the computation graph!

Make approximate posterior distribution close to prior

Sample z from $z|x \sim \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$

z

$\mu_{z|x}$ $\Sigma_{z|x}$

Encoder network

$q_\phi(z|x)$

Input Data x

Variational Autoencoders

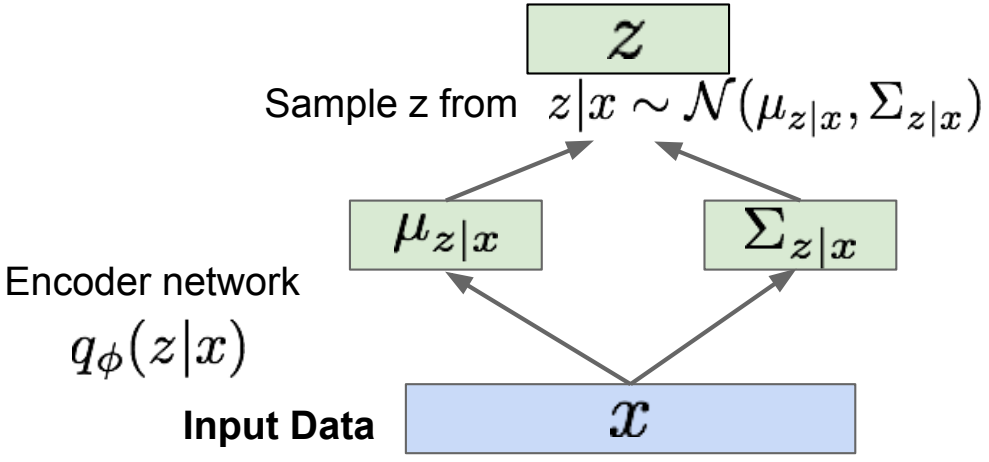
Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Reparameterization trick to make sampling differentiable:

Sample $\epsilon \sim \mathcal{N}(0, I)$

$$z = \mu_{z|x} + \epsilon \sigma_{z|x}$$



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

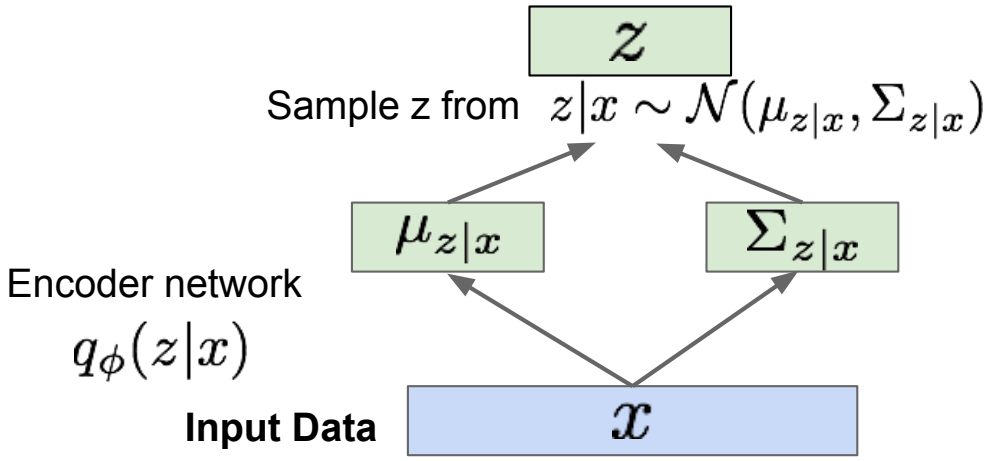
Reparameterization trick to make sampling differentiable:

Sample $\epsilon \sim \mathcal{N}(0, I)$

$$z = \mu_{z|x} + \epsilon \sigma_{z|x}$$

Input to the graph

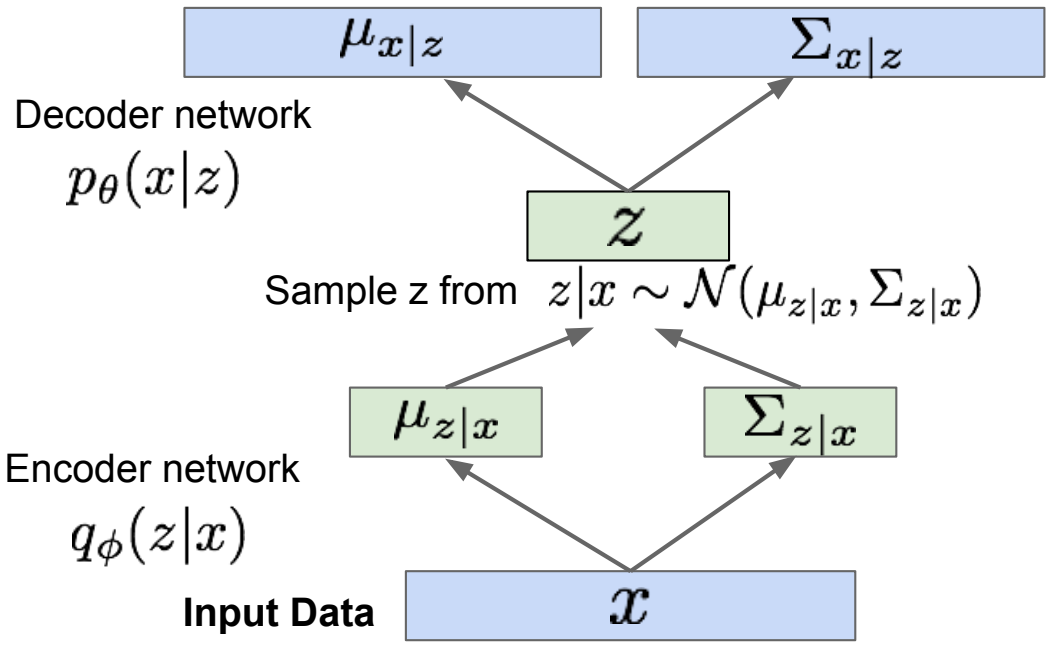
Part of computation graph



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

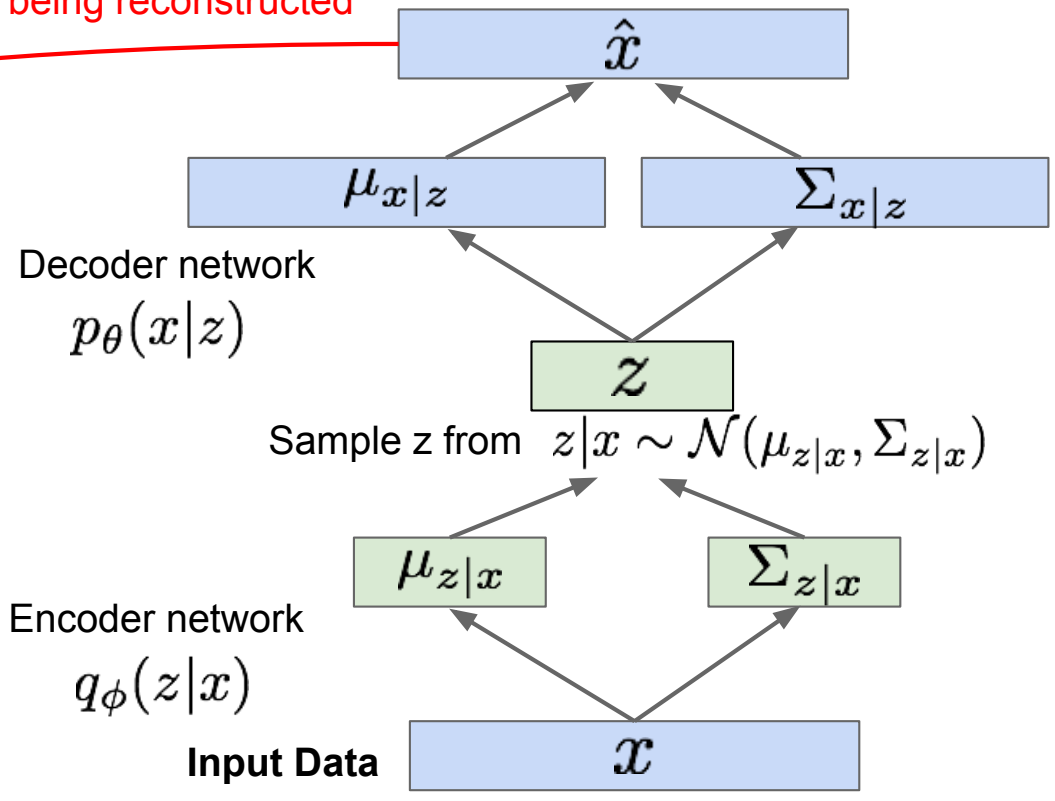


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\mathcal{L}(x^{(i)}, \theta, \phi) = \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))$$

Maximize likelihood of original input being reconstructed

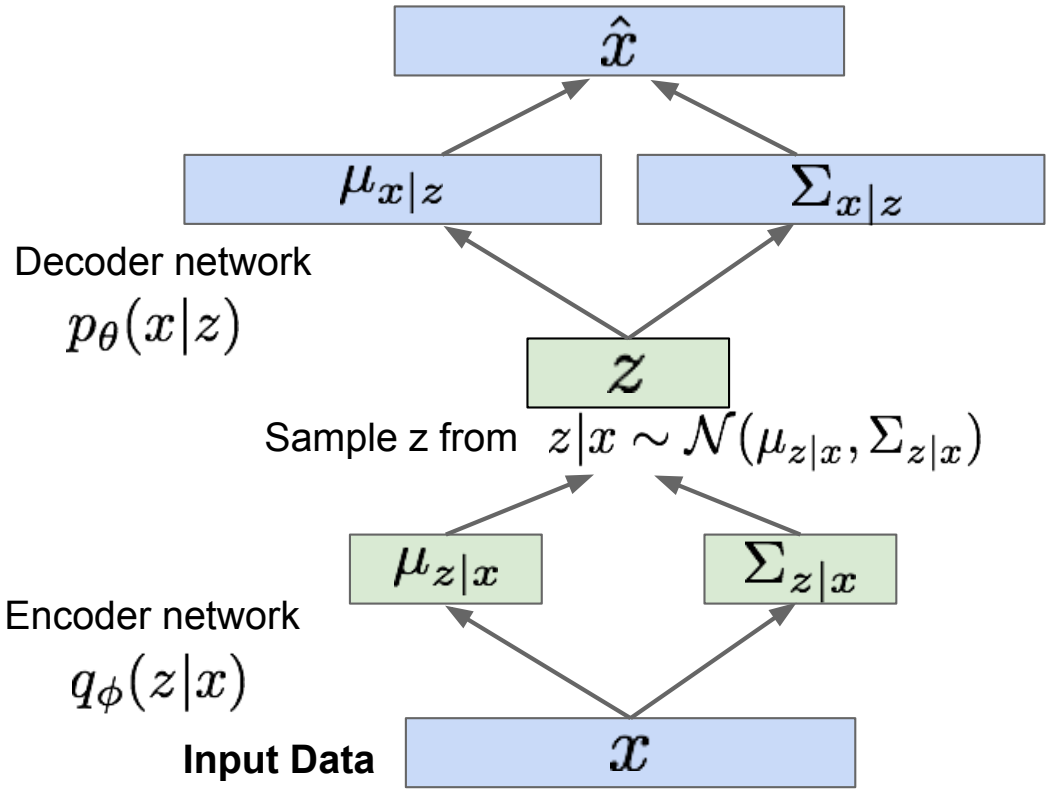


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

For every minibatch of input data: compute this forward pass, and then backprop!



Variational Autoencoders: Generating Data!

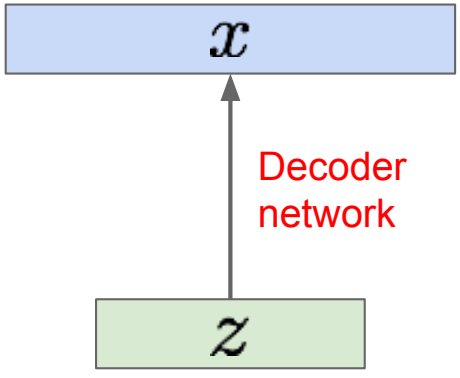
Our assumption about data generation process

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

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Sample from true conditional $p_{\theta^*}(x \mid z^{(i)})$

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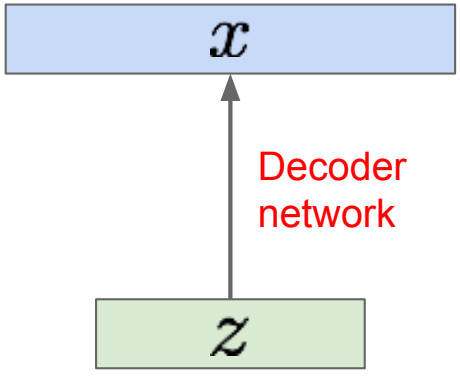
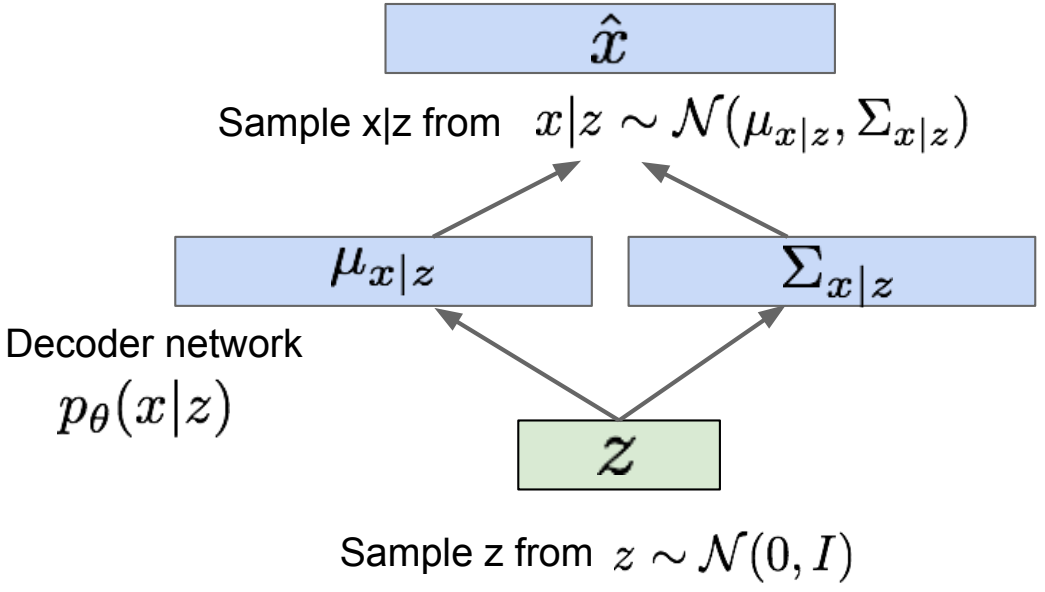


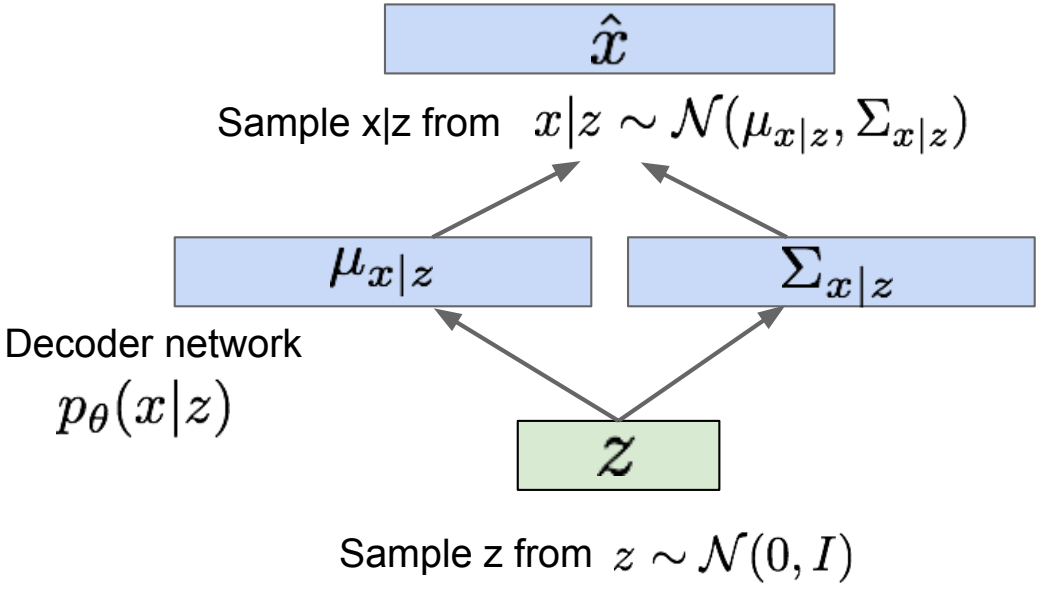
Now given a trained VAE: use decoder network & sample z from prior!

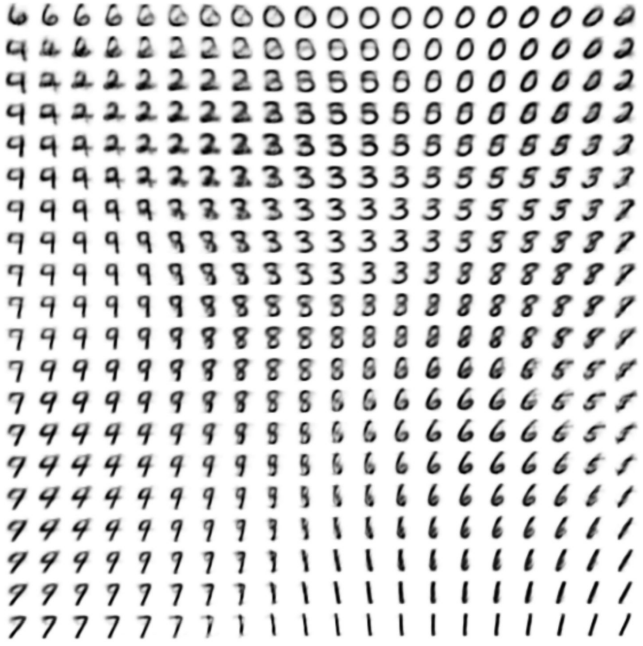


Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!





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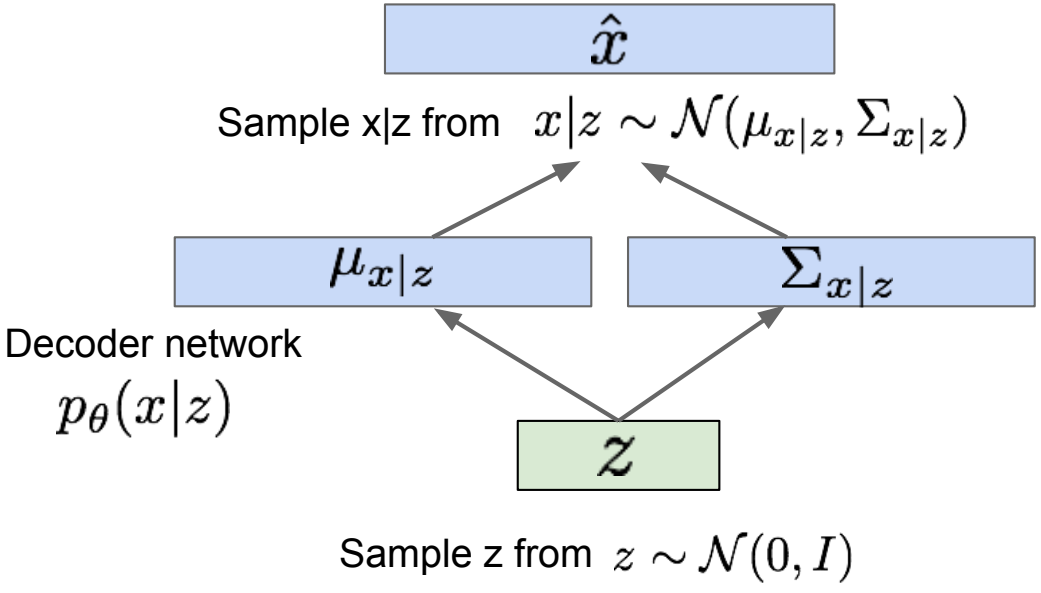
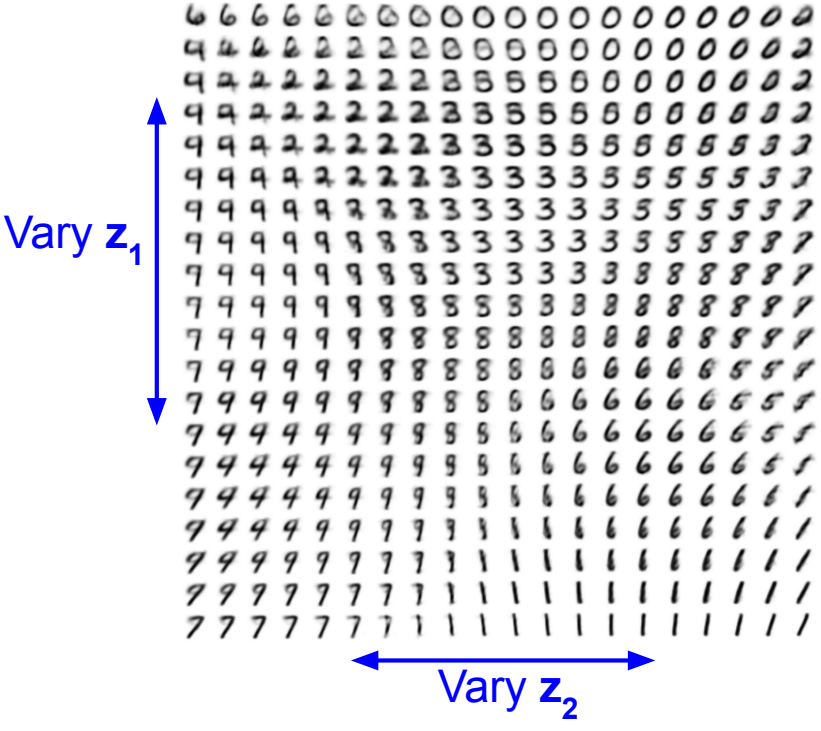
Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!



Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Data manifold for 2-d **z**



Variational Autoencoders: Generating Data!

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Also good feature representation that can be computed using $q_\phi(z|x)$!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Probabilistic spin to traditional autoencoders => allows generating data
Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Interpretable latent space.
- Allows inference of q(z|x), can be useful feature representation for other tasks

Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs), Categorical Distributions.
- Learning disentangled representations.

Backprop from Decoder to Encoder

The decoder and encoder are deep neural networks, so we know how to backprop through those.

- In between the encoder and decoder, we sample from the posterior distribution $q_\phi(z|x)$, so we need to backprop through this sampling step.
- In general, it is hard to get a good estimate of the derivative of a sampling step.
- But because $q_\phi(z|x)$ is a Gaussian, there is a simple solution.

Reparameterisation Trick: rewrite the sampling noise as an input ϵ, so that everything we need to backprop through is deterministic.

Outline

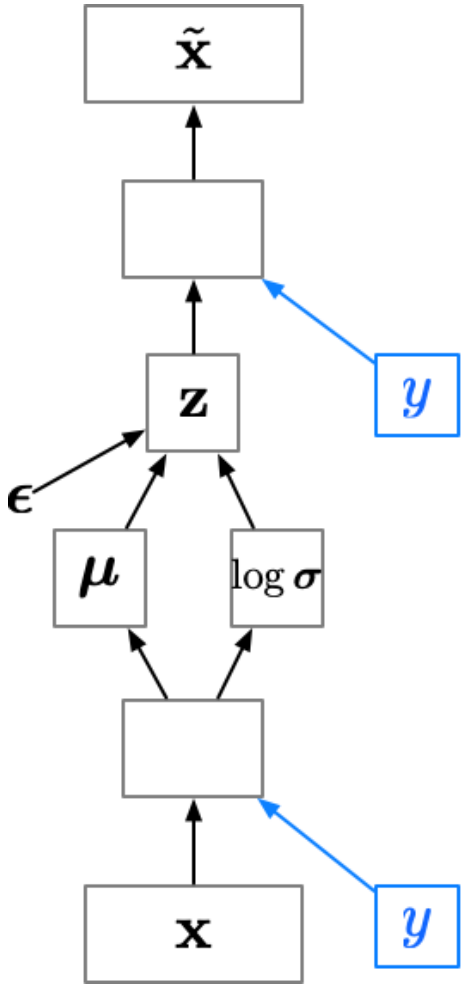
Conditional VAEs

What if we want to generate something which is appropriate for a given context?

- Condition the encoder and decoder on the context c, $p_\theta(x|z,c)$ $q_\phi(z|x,c)$
- Use a deep neural network to learn a representation of the context (if needed)
- Everything else stays the same

Class-Conditional VAE

- So far, we haven't used the labels y. A class-conditional VAE provides the labels to both the encoder and the decoder.
- Since the latent code $\mathbf{z}$ no longer has to model the image category, it can focus on modeling the stylistic features.
- If we're lucky, this lets us disentangle style and content. (Note: disentanglement is still a dark art.)
- See Kingma et al., "Semi-supervised learning with deep generative models."



Beta VAEs

- In practice, the two loss terms of a VEA are weighted by a hyperparameter β

$$L(\theta, \phi) = E_{z \sim q_\phi(z|x)} \log p_\theta(x|z) - \beta D_{KL}(q_\phi(z|x)||p_\theta(z))$$

- Reducing β below 1 can help prevent "mode collapse", where only the prior is learned
- Increasing β greater than 1 is used to force very compressed representations, which give more "disentangled" latent representations.

[beta-VAE: Learning Basic Visual Concepts with a Constrained Variational Framework. Irina Higgins, Loic Matthey, Arka Pal, Christopher Burgess, Xavier Glorot, Matthew Botvinick, Shakir Mohamed, Alexander Lerchner. 2017]

Vector-Space VAEs in NLP

Most work applying VAEs to language has focussed on generating text, particularly with conditional VAEs, or explainability.

- Generating Sentences from a Continuous Space. Samuel R. Bowman, Luke Vilnis, Oriol Vinyals, Andrew M. Dai, Rafal Jozefowicz, Samy Bengio. 2015
- Neural Variational Inference for Text Processing. Yishu Miao, Lei Yu, Phil Blunsom. 2015
- Educating Text Autoencoders: Latent Representation Guidance via Denoising. Tianxiao Shen, Jonas Mueller, Regina Barzilay, Tommi Jaakkola. 2019
- A transformer-based variational autoencoder for sentence generation. Danyang Liu, Gongshen Liu. 2019
- Variational Transformers for Diverse Response Generation. Zhaojiang Lin, Genta Indra Winata, Peng Xu, Zihan Liu, Pascale Fung. 2020
- Disentangling generative factors in natural language with discrete variational autoencoders. Giangiacomo Mercatali and André Freitas. 2021.

Summary of Variational Auto-Encoders

- Auto-encoders are an unsupervised approach to representation learning
- Deep Variational Bayesian approaches bring information and probability theory to representation learning
- Variational Auto-Encoders (VAE) are a variational Bayesian approach to auto-encoders
- VAEs have been widely applied, and are the basis of many approaches to disentanglement

Also see:
An Introduction to Variational Autoencoders,
Diederik P Kingma, 2019

Outline

Variational Auto-Encoders with an Attention-Based Latent Space

A **vector space is not an adequate latent represention** for language; we need an attention-based latent space.

- Texts vary widely in length, so a fixed dimensionality is often either too big or too small
- Attention-based models have a variable number of vectors in their latent spaces, depending on the number of tokens in the text
- Empirically, attention-based representations are much much better than fixed-dimentional representation

How do we define **distributions over attention-based latent representations**?

Outline

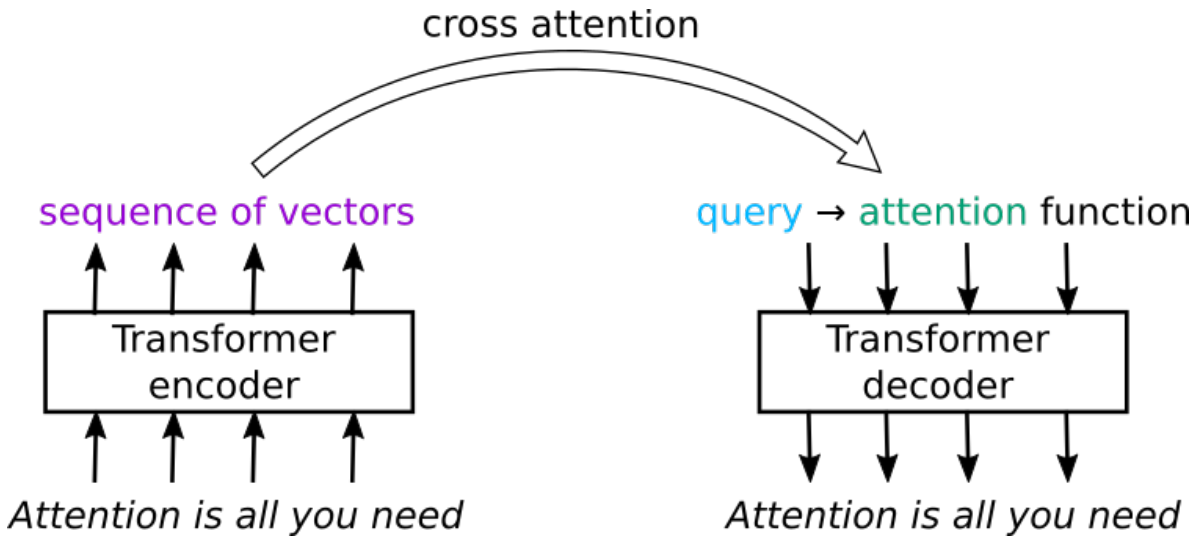
Attention-based Transformer Embeddings

A Transformer encoder passes information to a Transformer decoder using **attention**.

- Encoder embeds the input in a sequence of vectors
- Decoder issues a query to access the embedding
- Attention returns an average of the vectors near the query

$$Attn(\boldsymbol{u}, \boldsymbol{Z}) = \sum_{i=1}^{n} a_i \boldsymbol{z}_i$$

$$a_i = \frac{\exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}{\sum_{i=1}^{n} \exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}$$



where $\text{Attention}(\boldsymbol{u}', \boldsymbol{Z}\,;\ \boldsymbol{W}^Q, \boldsymbol{W}^K, \boldsymbol{W}^V) \ = \ \text{Attn}(\boldsymbol{u}'\boldsymbol{W}^Q(\boldsymbol{W}^K)^T,\ \boldsymbol{Z})\ \boldsymbol{W}^V$

The Latent Space of Transformers

- Attention function is **permutation invariant** in the vectors

$$Attn(\boldsymbol{u}, \boldsymbol{Z}) = \sum_{i=1}^{n} a_i \boldsymbol{z}_i$$

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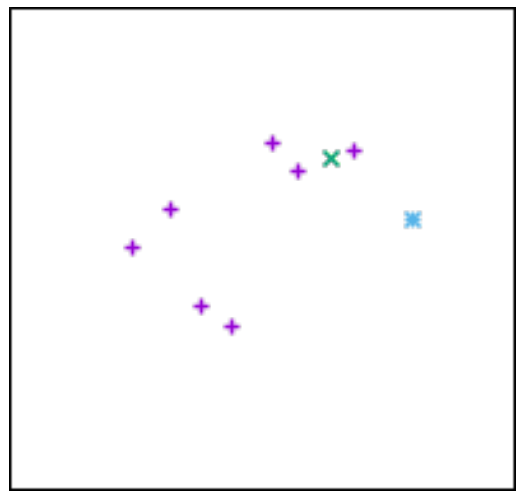

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- Attention imposes a **normalised weighting** over vectors

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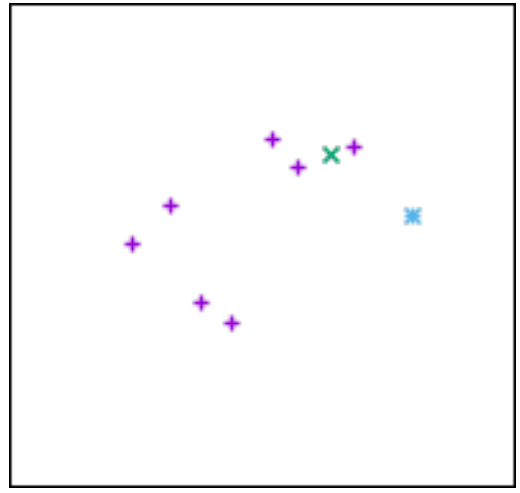
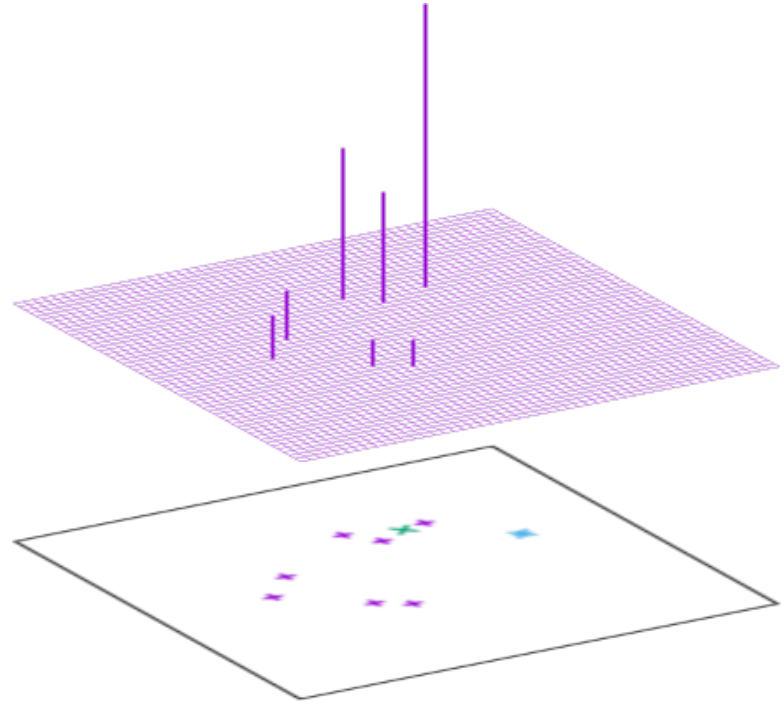


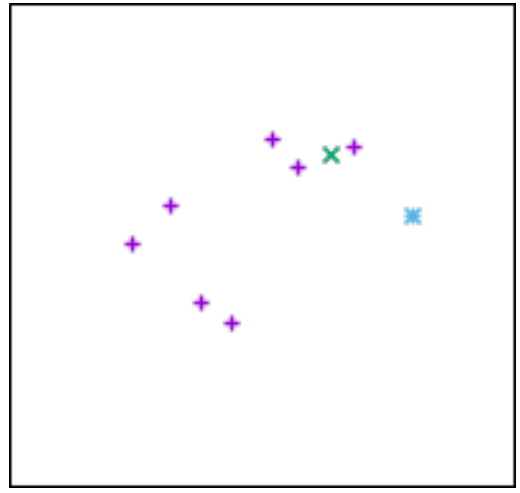


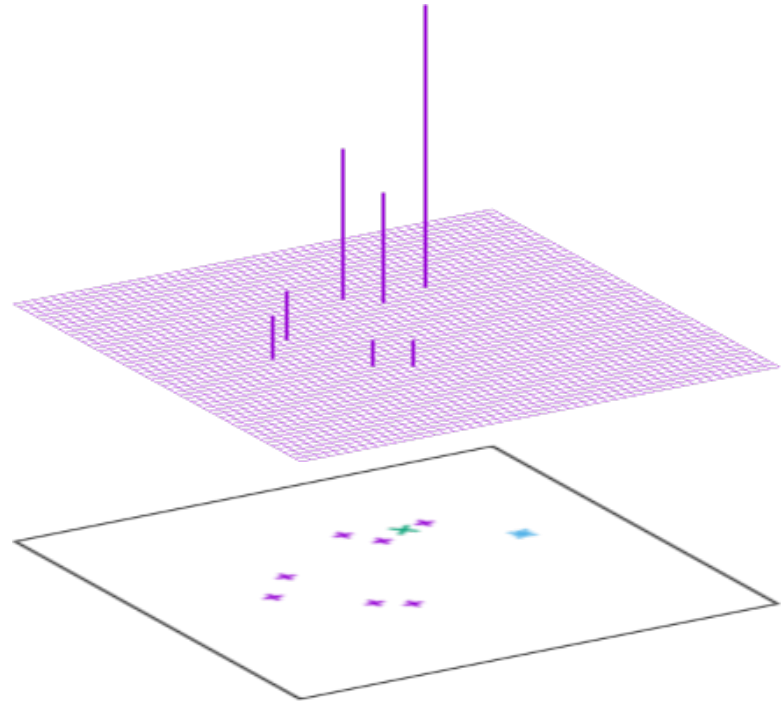
The Latent Space of Transformers

- Attention function is **permutation invariant** in the vectors
- Attention imposes a **normalised weighting** over vectors
- Attention supports a **variable number** of vectors

$$Attn(\boldsymbol{u}, \boldsymbol{Z}) = \sum_{i=1}^{n} a_i \boldsymbol{z}_i$$

$$a_i = \frac{\exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}{\sum_{i=1}^{n} \exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}$$





The Latent Space of Transformers

- Attention function is **permutation invariant** in the vectors
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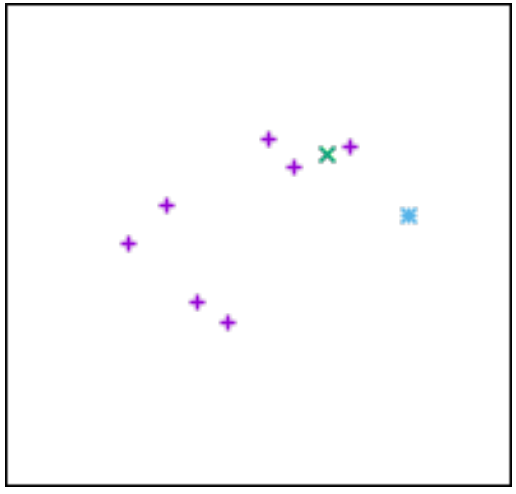
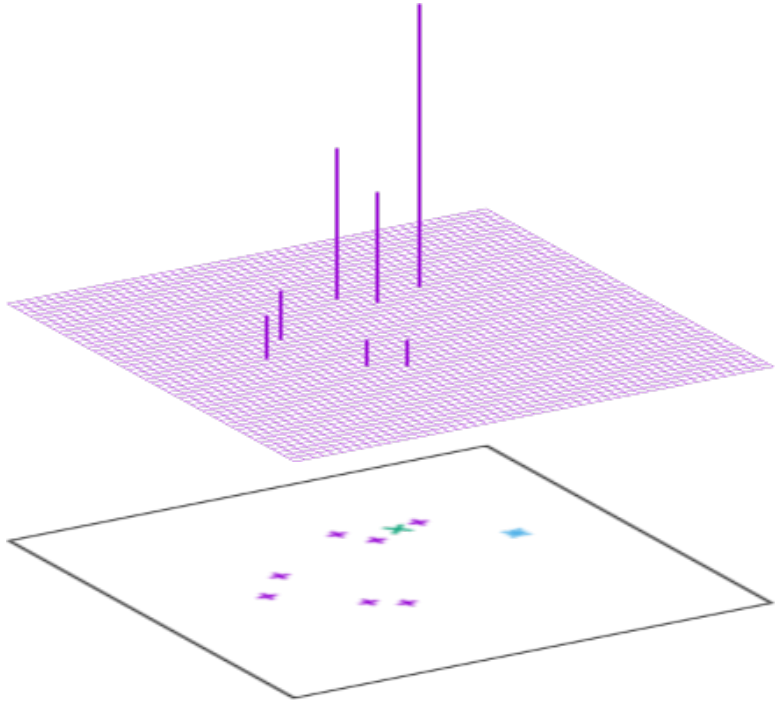
Like a **nonparametric** space of **mixture distributions**

$$Attn(\boldsymbol{u}, \boldsymbol{Z}) = \sum_{i=1}^{n} a_i \boldsymbol{z}_i$$

$$a_i = \frac{\exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}{\sum_{i=1}^{n} \exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}$$





The Latent Space of Transformers

Transformer embeddings are:

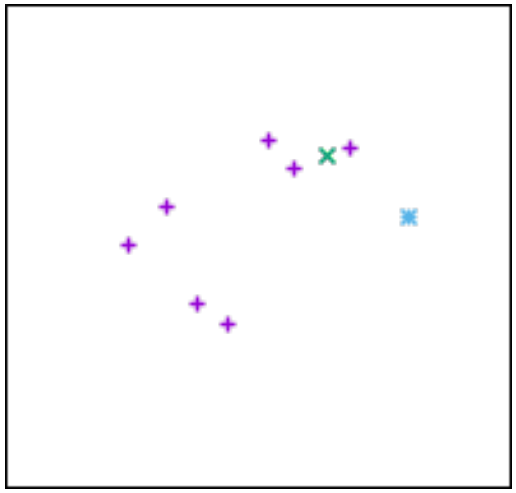
nonparametric mixtures of impulse distributions

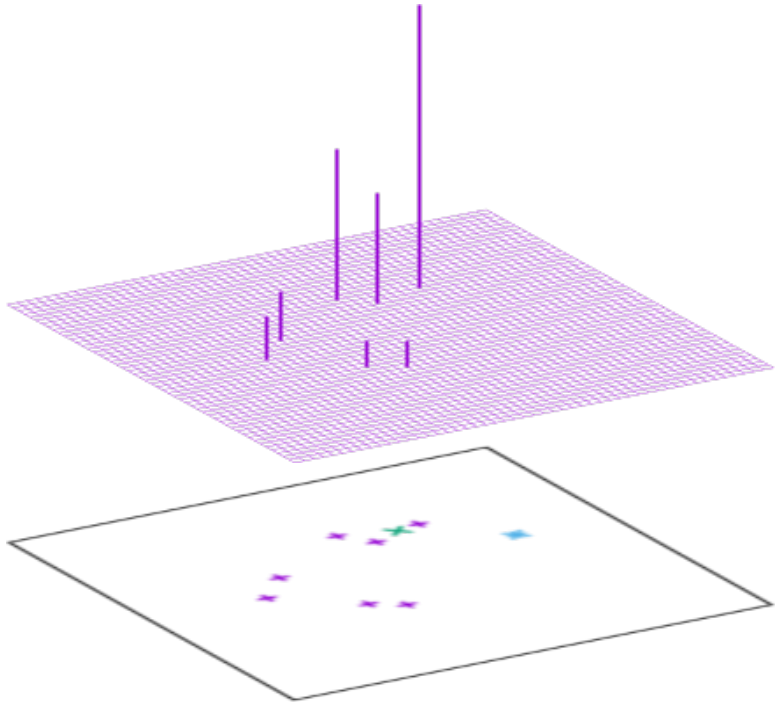
Attention function is:

Bayesian query denoising

$$Attn(\boldsymbol{u}, \boldsymbol{Z}) = \sum_{i=1}^{n} a_i \boldsymbol{z}_i$$

$$a_i = \frac{\exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}{\sum_{i=1}^{n} \exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}$$

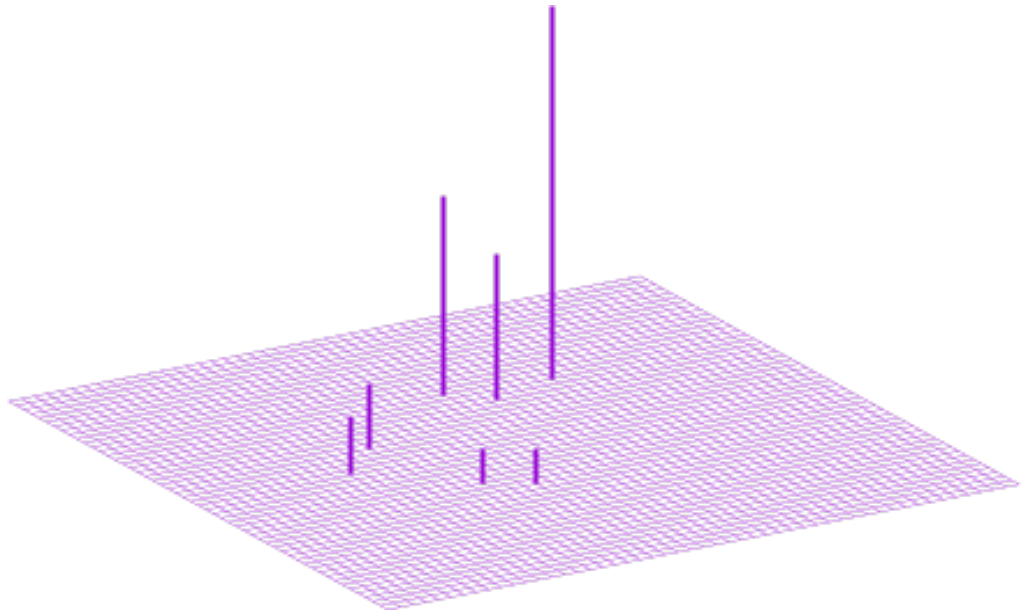




Query Denoising Attention Function

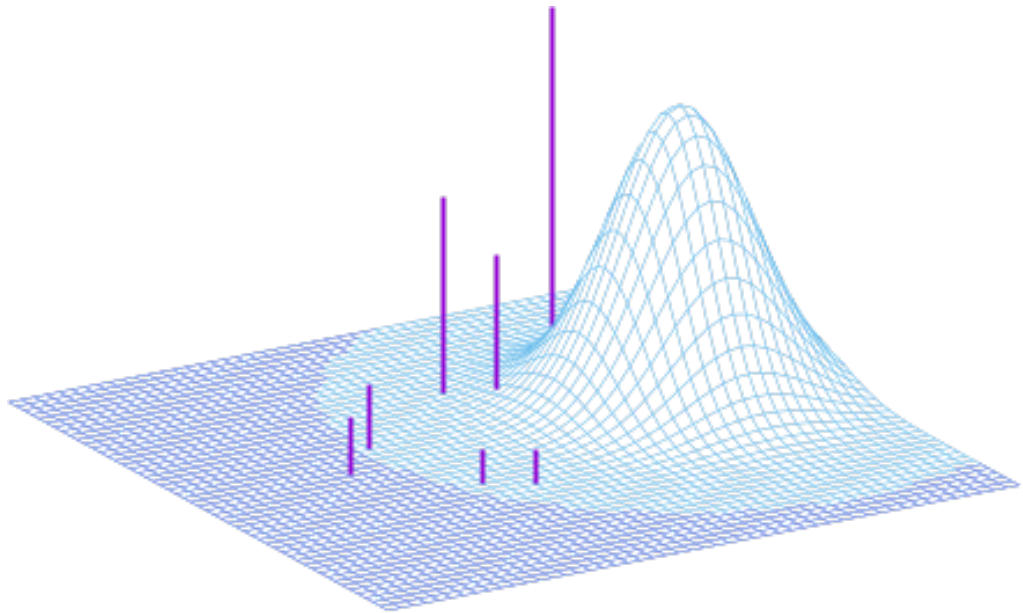
$$p_{\boldsymbol{Z}}(\boldsymbol{v}) \quad = \quad \sum_{i=1}^{n} \frac{\exp(\frac{1}{2\sqrt{d}}||\boldsymbol{z}_i||^2)}{\sum_{i=1}^{n}\exp(\frac{1}{2\sqrt{d}}||\boldsymbol{z}_i||^2)}\,\delta_{\boldsymbol{z}_i}(\boldsymbol{v})$$

$\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n$



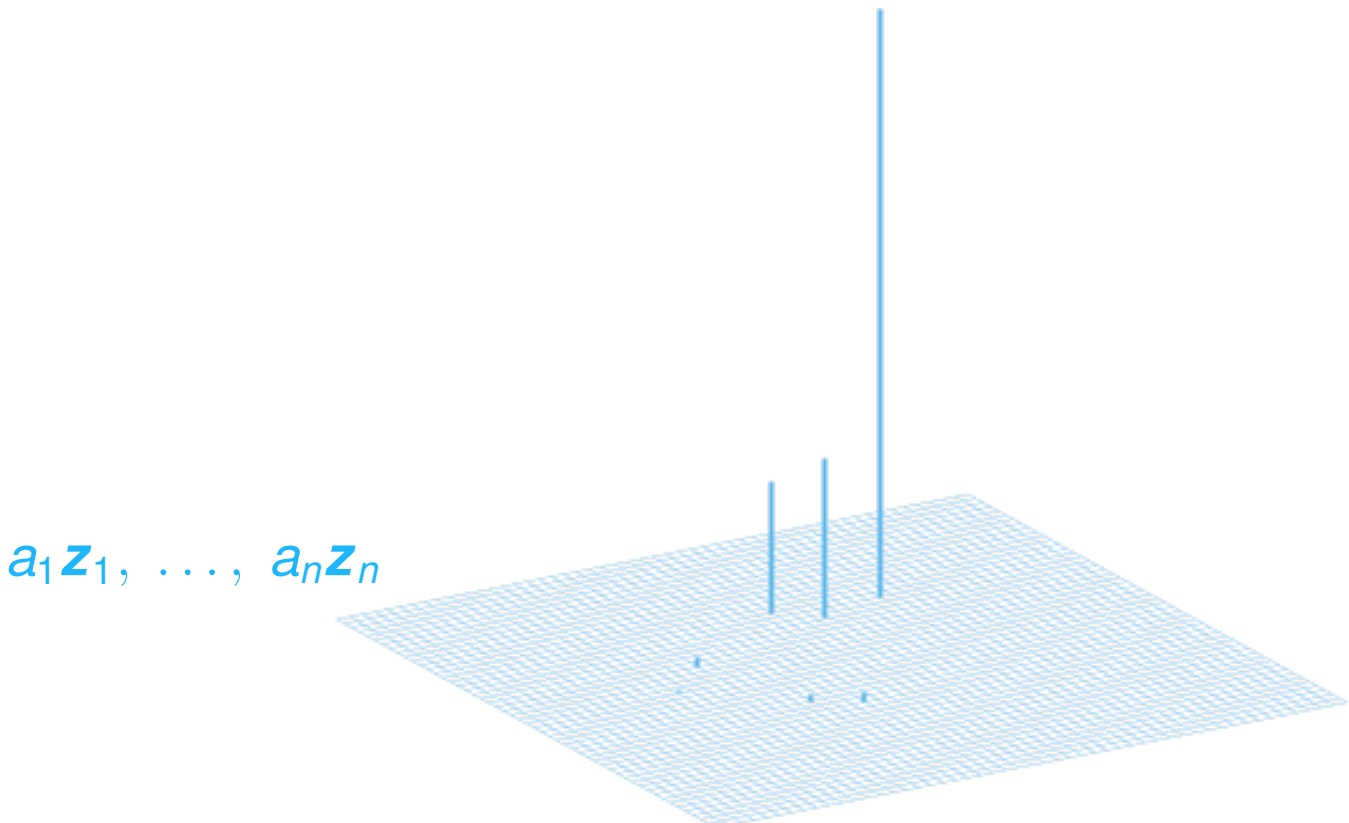
Query Denoising Attention Function

$$p(\boldsymbol{u} \mid \boldsymbol{v}) \quad = \quad g(\boldsymbol{u}\,;\ \boldsymbol{v}, \sqrt{d}\boldsymbol{I})$$



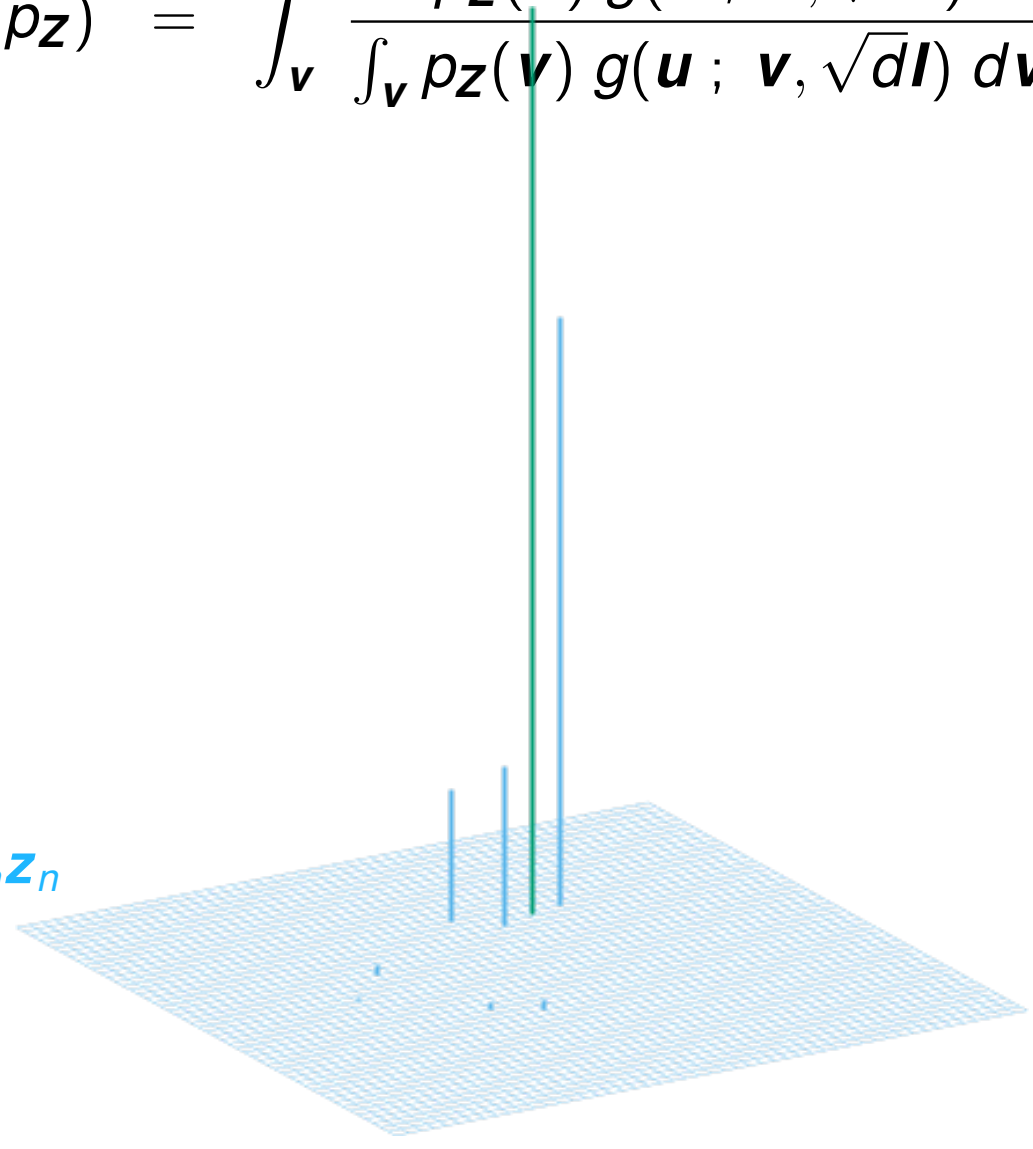
Query Denoising Attention Function

$$p_Z(\boldsymbol{v} \mid \boldsymbol{u}) \quad = \quad \frac{p_Z(\boldsymbol{v})\; g(\boldsymbol{u}\,;\; \boldsymbol{v}, \sqrt{d}\boldsymbol{I})}{\int_{\boldsymbol{v}} p_Z(\boldsymbol{v})\; g(\boldsymbol{u}\,;\; \boldsymbol{v}, \sqrt{d}\boldsymbol{I})\; d\boldsymbol{v}}$$



Query Denoising Attention Function

$$\mathrm{DAttn}(\boldsymbol{u}\,;\,p_{\boldsymbol{Z}}) \;=\; \int_{\boldsymbol{v}} \frac{p_{\boldsymbol{Z}}(\boldsymbol{v})\; g(\boldsymbol{u}\,;\;\boldsymbol{v}, \sqrt{d}\boldsymbol{I})}{\int_{\boldsymbol{v}} p_{\boldsymbol{Z}}(\boldsymbol{v})\; g(\boldsymbol{u}\,;\;\boldsymbol{v}, \sqrt{d}\boldsymbol{I})\; d\boldsymbol{v}}\; \boldsymbol{v}\; d\boldsymbol{v}$$



$a_1\boldsymbol{z}_1,\ \ldots,\ a_n\boldsymbol{z}_n$

$\sum_{i=1}^{n} a_i\boldsymbol{z}_i$

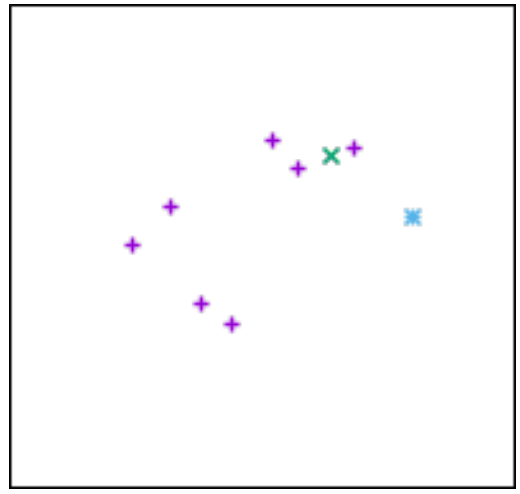
Denoising Attention

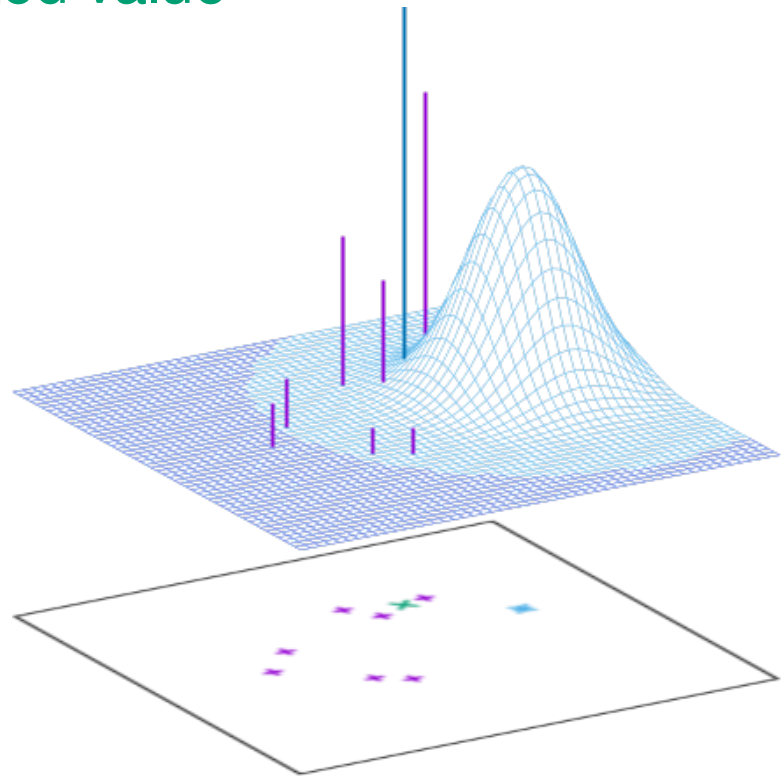
The **attention function** is **query denoising** using a mixture of impulses.

- Attention takes a sequence of vectors and a query vector and returns an attention vector
- Denoising takes a prior distribution and a noisy observation and returns its expected value

$$Attn(\boldsymbol{u}, \boldsymbol{Z}) = \sum_{i=1}^{n} a_i \boldsymbol{z}_i$$

$$a_i = \frac{\exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}{\sum_{i=1}^{n} \exp(\frac{1}{\sqrt{d}} \boldsymbol{u}\boldsymbol{z}_i)}$$

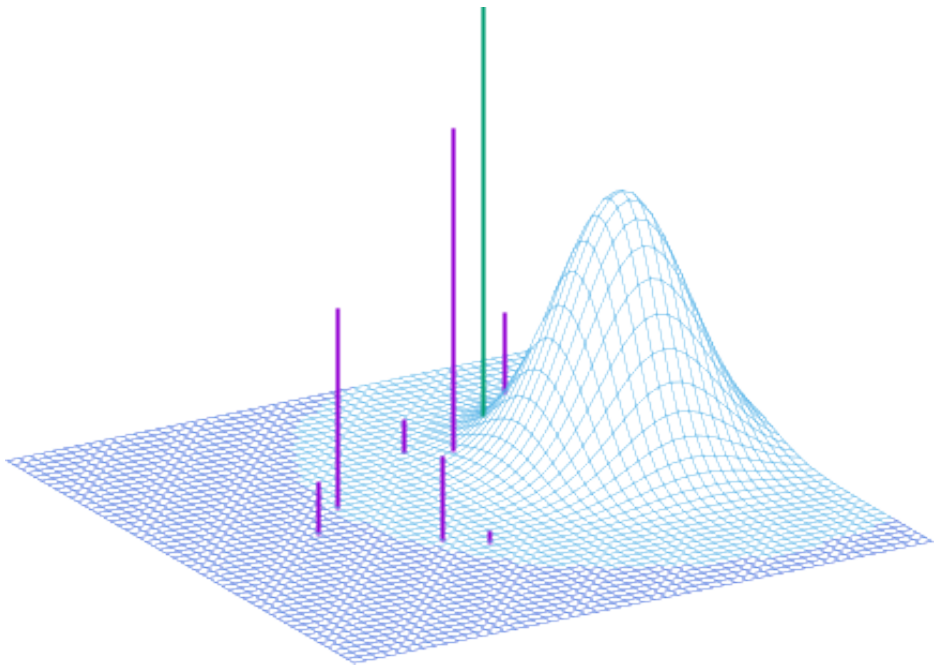


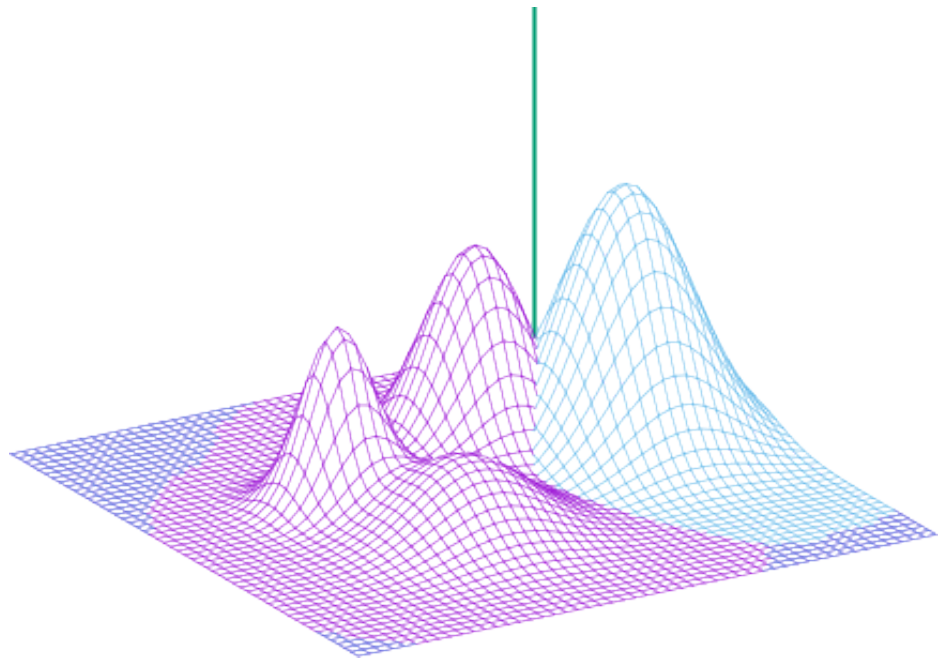


Denoising Attention

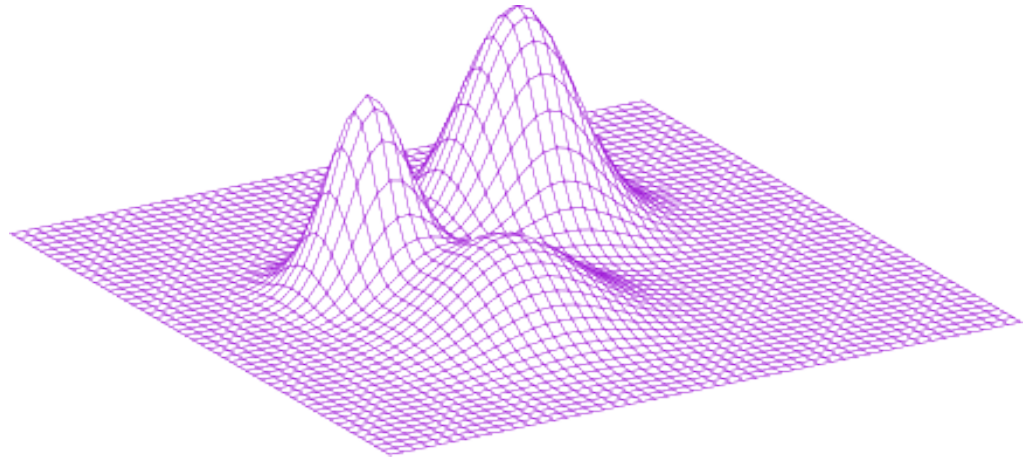
Query denoising is a **generalisation** of attention.

- The prior distribution can be **any mixture distribution**
- Gaussian mixtures make denoising easy to compute

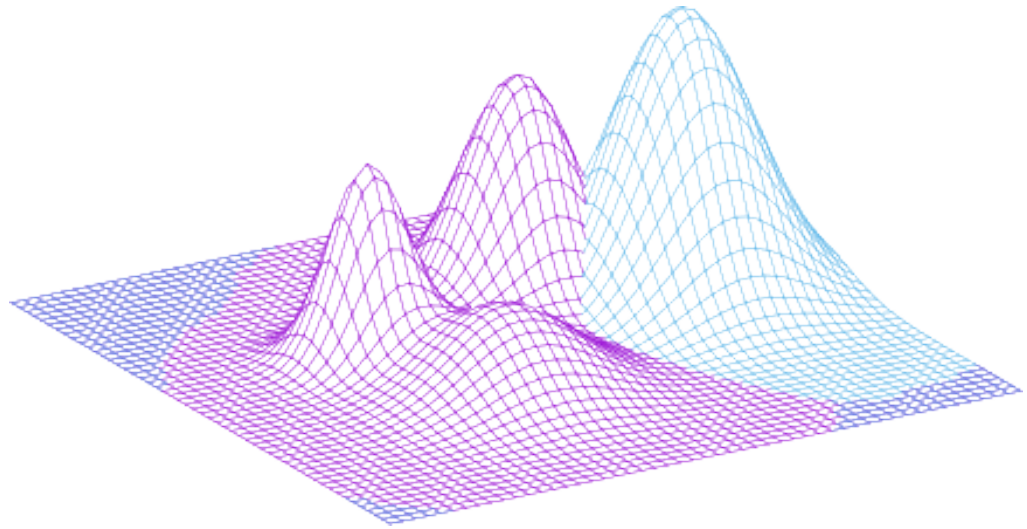




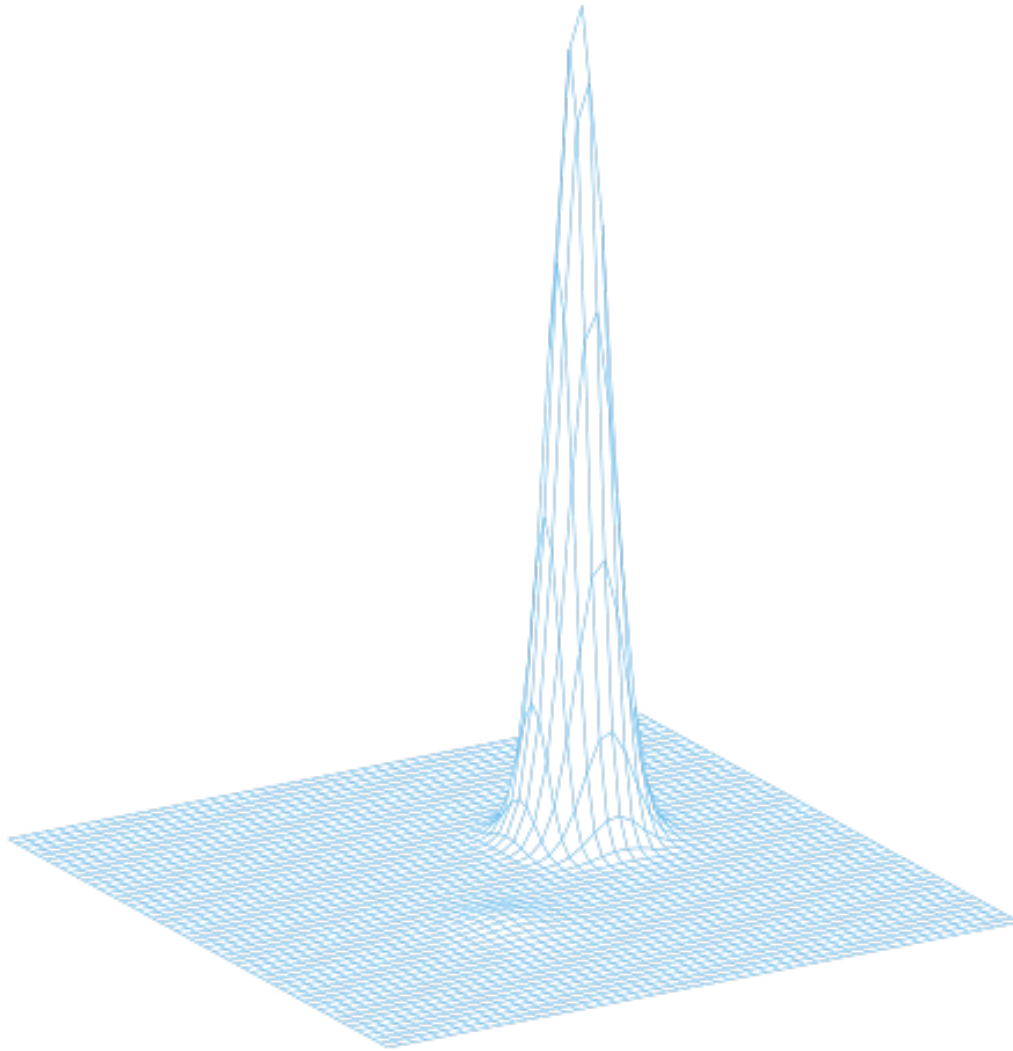
Denoising Attention



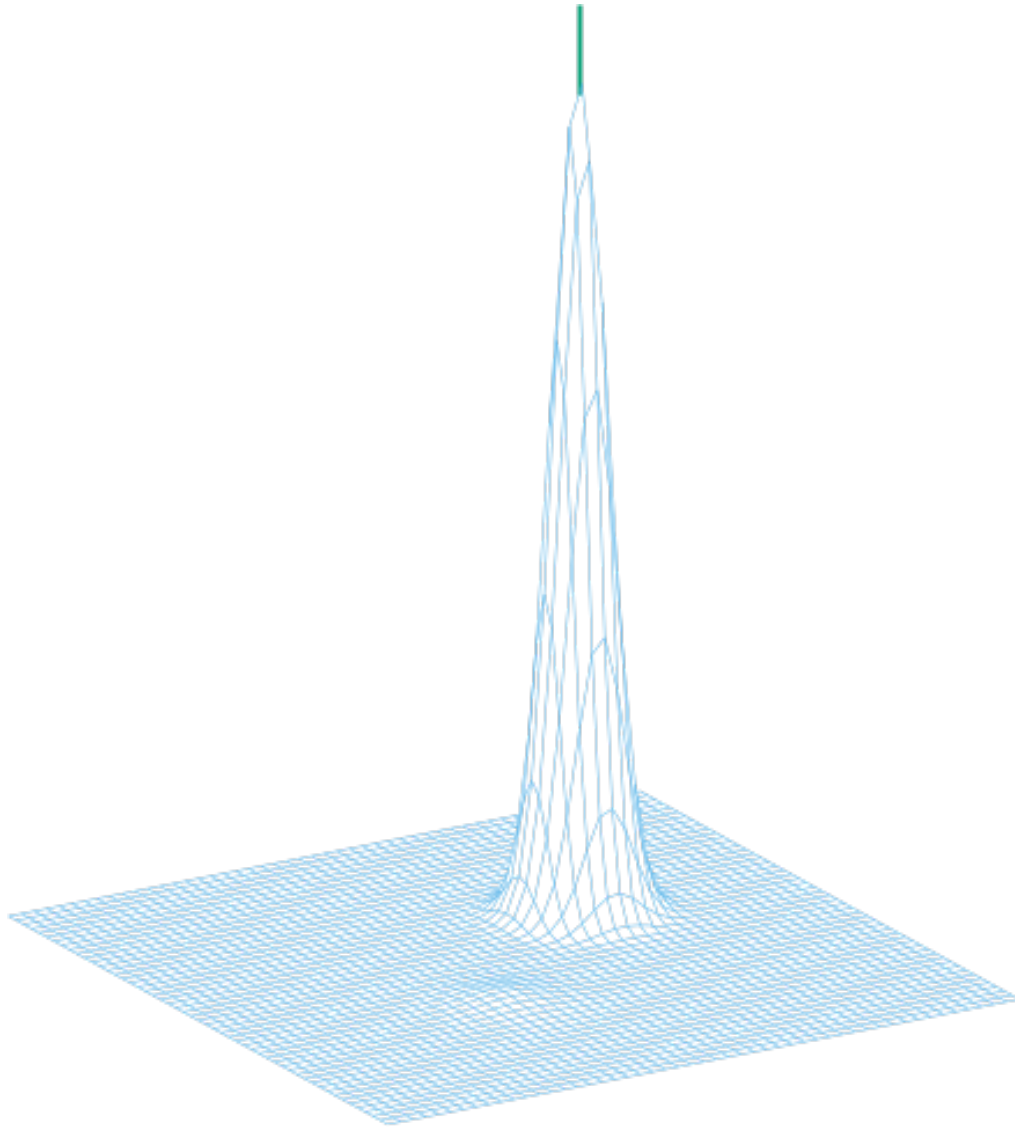
Denoising Attention



Denoising Attention



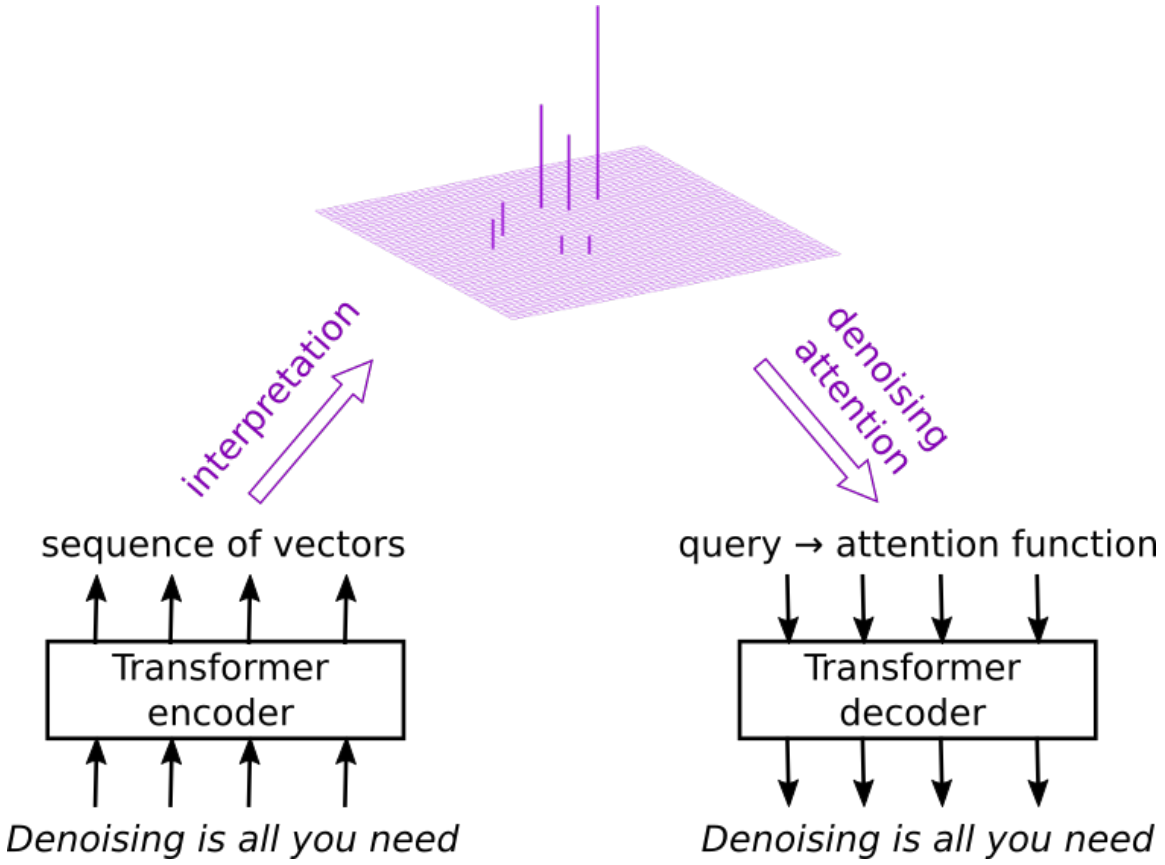
Denoising Attention



Attention-based Representation generalise to Mixture Distributions

Every attention-based representation has an **equivalent mixture distribution**.

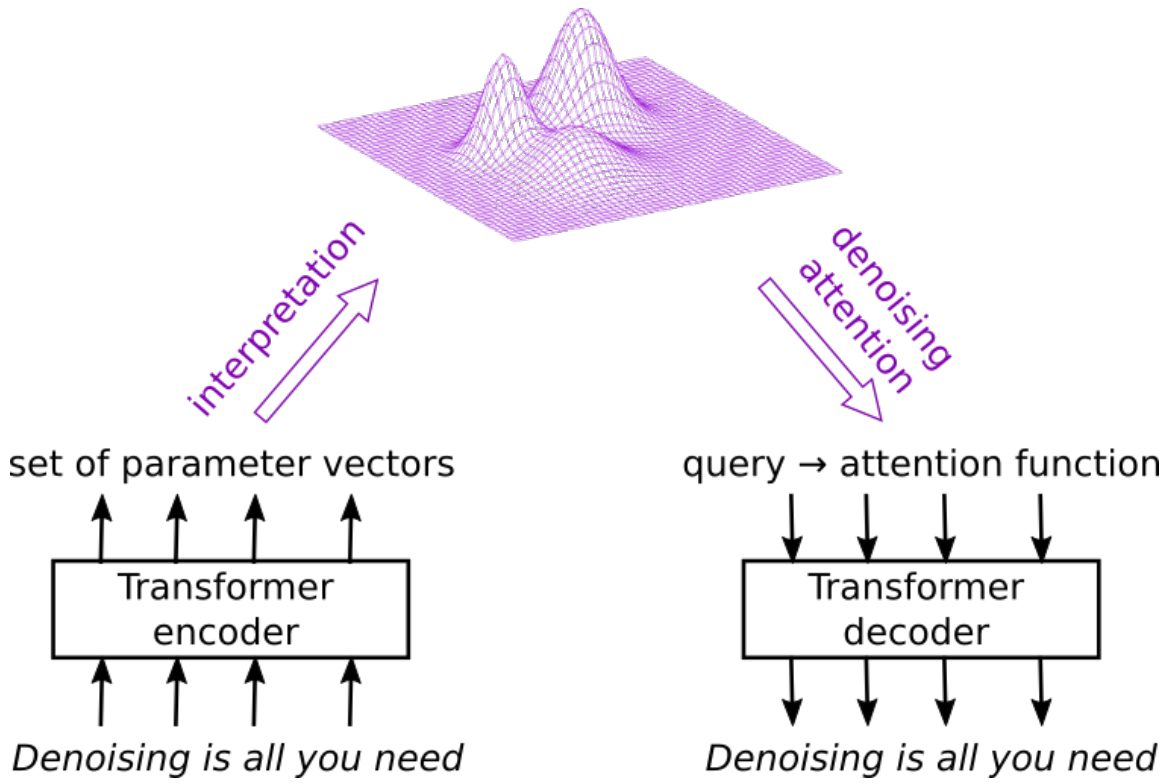
- Sets-of-vectors can be replaced by mixtures of impulse distributions
- Attention function can be replaced by denoising attention



Attention-based Representation generalise to Mixture Distributions

Mixture distribution are more general than set-of-vector representations.

- Sets-of-vectors can parameterise any mixture distribution
- Denoising attention function applies to **any mixture distribution**

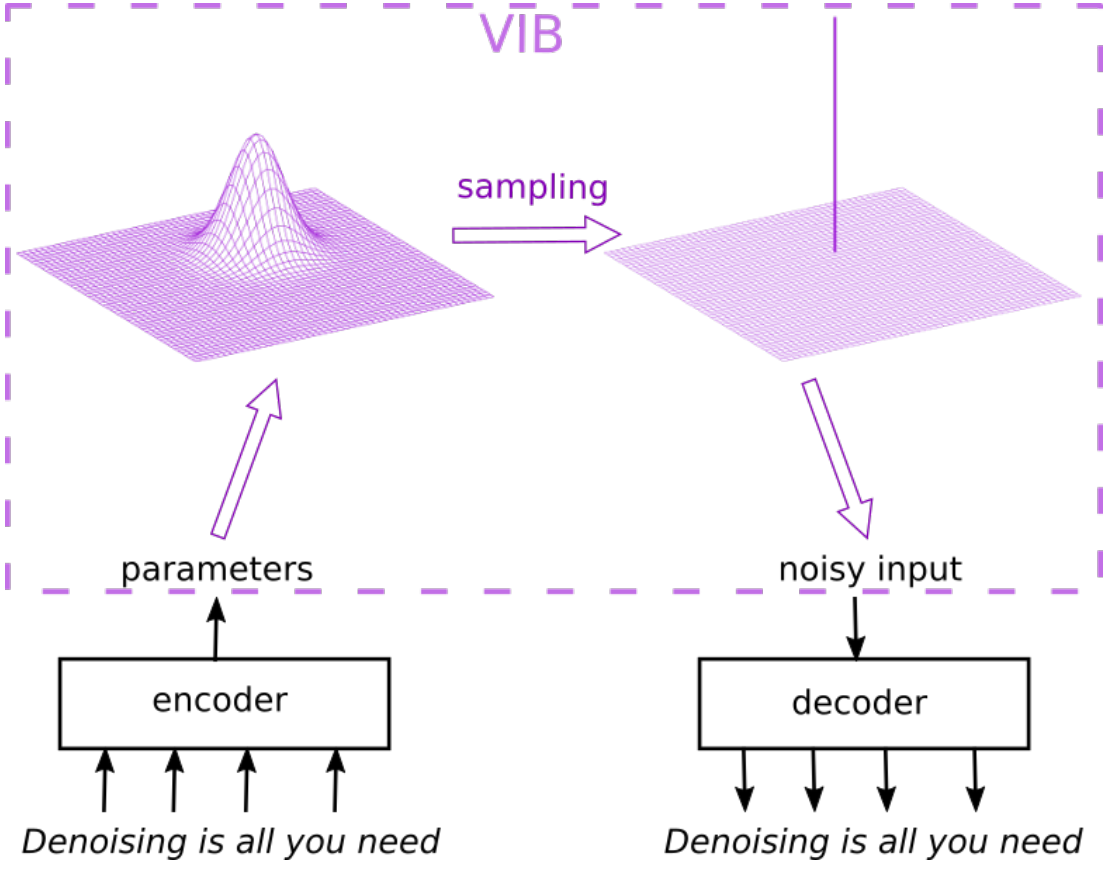


Outline

Variational Information Bottleneck

Variational Auto-Encoders use a Variational Information Bottleneck (VIB) to **regularise** their latent representation.

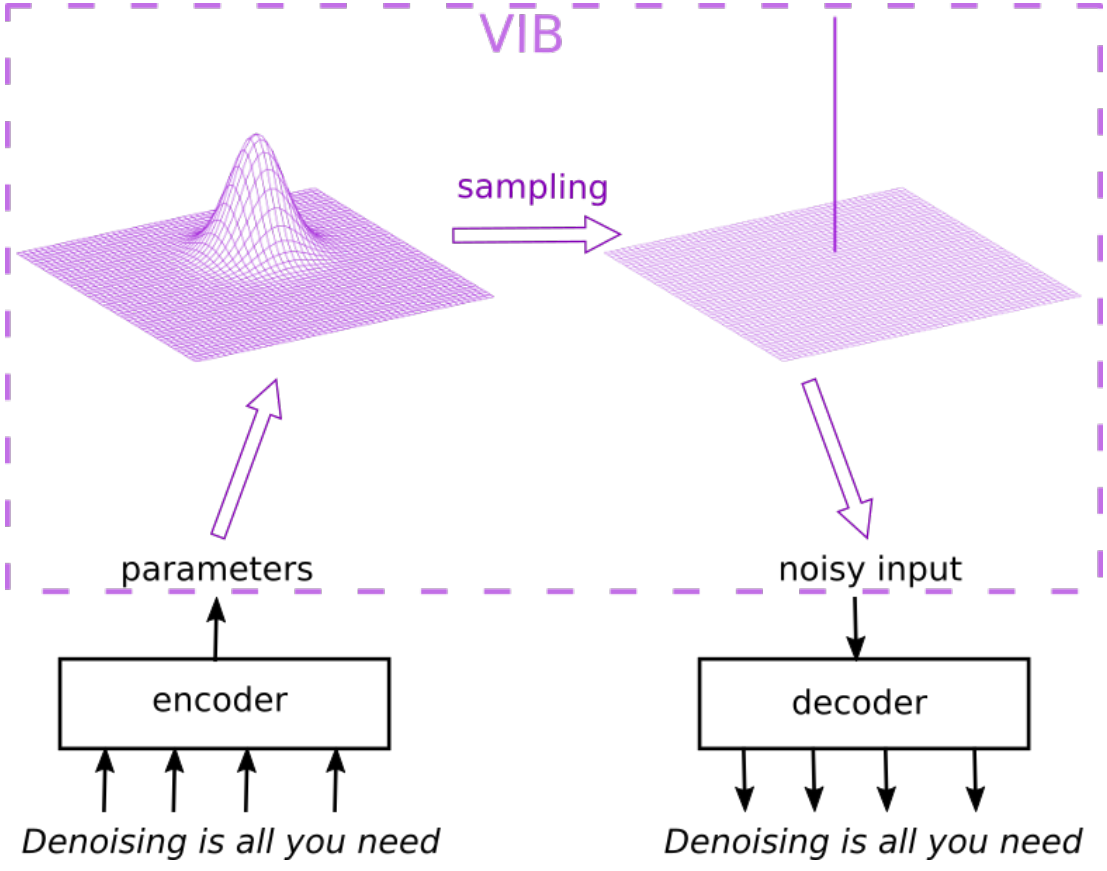
- Latent space is a vector space (previously)
- Encoder outputs a distribution over vectors



Variational Information Bottleneck

VIB only allows required information to pass from encoder to decoder.

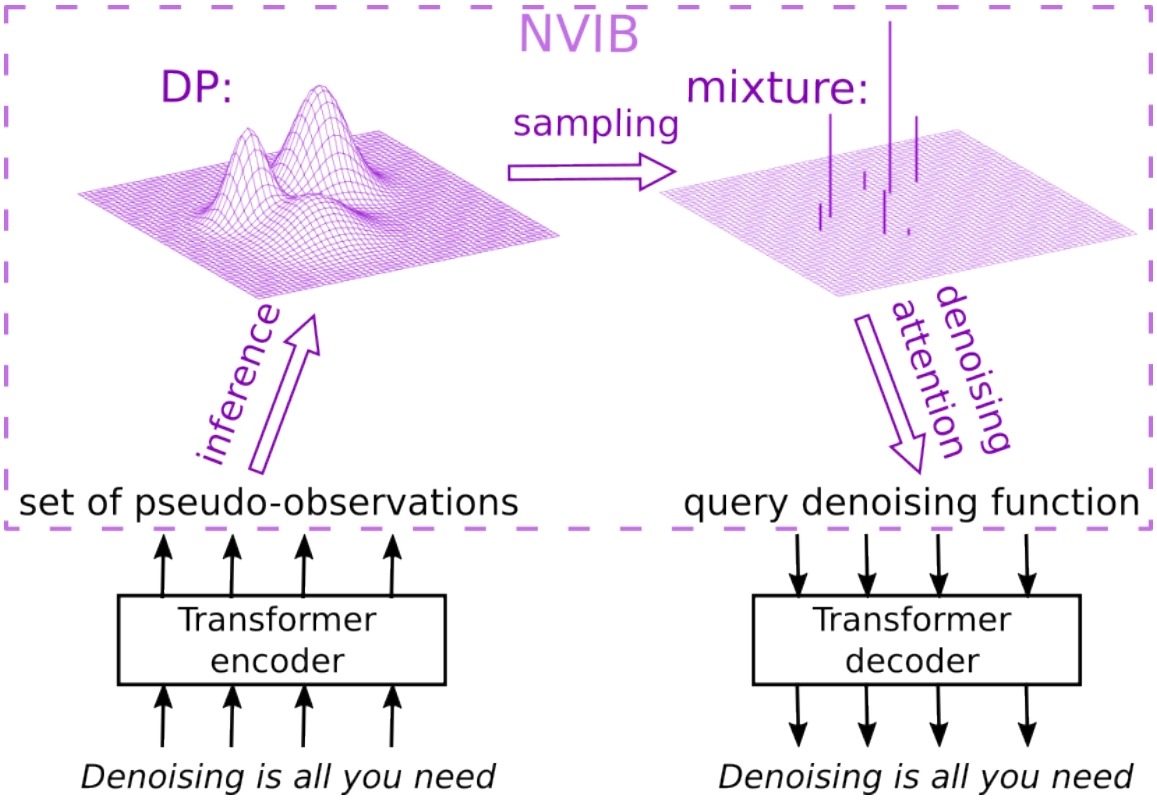
- Sampling noise controls the information that passes
- KL divergence with a prior regularises the noise level



Variational Information Bottleneck for Transformers

We can define a VIB for mixture distributions (NVIB) with **Bayesian nonparametrics**

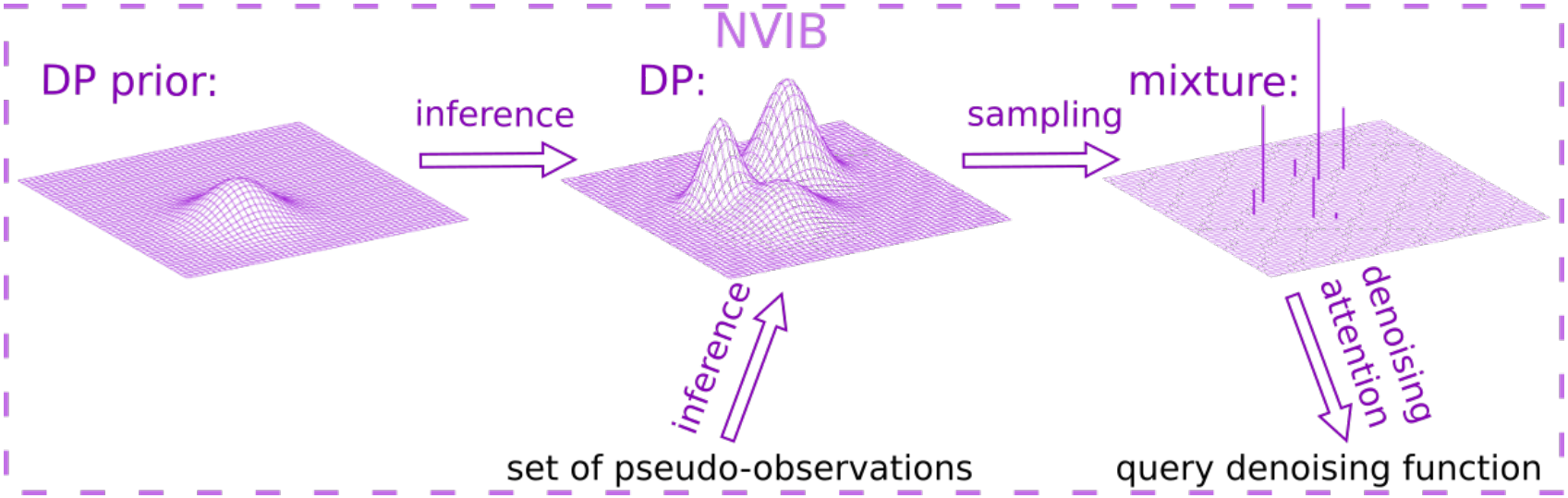
- Defines distributions over mixture distributions for the posterior and prior
- Defines sampling, means, and inference of the posterior



Nonparametric Variational Information Bottleneck

Bayesian nonparametrics provides an extensive theory on mixture distributions

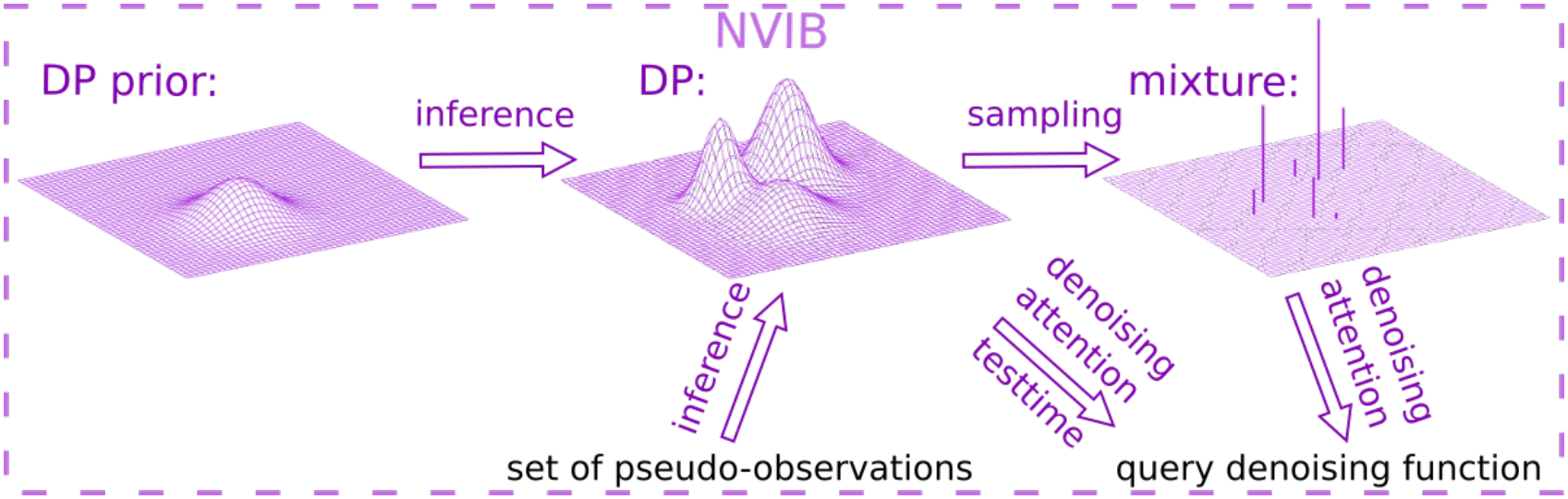
- **Dirichlet processes** specify distributions over mixtures of impulse distributions



Nonparametric Variational Information Bottleneck

Bayesian nonparametrics provides an extensive theory on mixture distributions

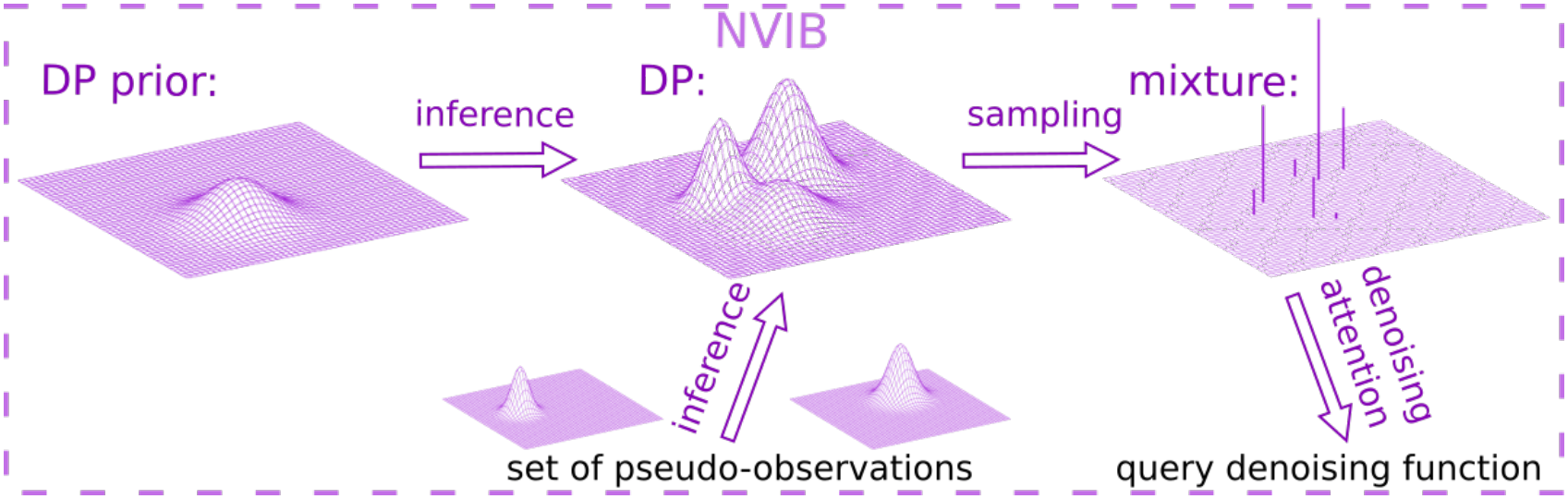
- Dirichlet processes specify distributions over mixtures of impulse distributions
- **Mean of the samples** is a continuous mixture distribution



Nonparametric Variational Information Bottleneck

Bayesian nonparametrics provides an extensive theory on mixture distributions

- Dirichlet processes specify distributions over mixtures of impulse distributions
- Mean of the samples is a continuous mixture distribution
- Dirichlet processes are **conjugate priors**



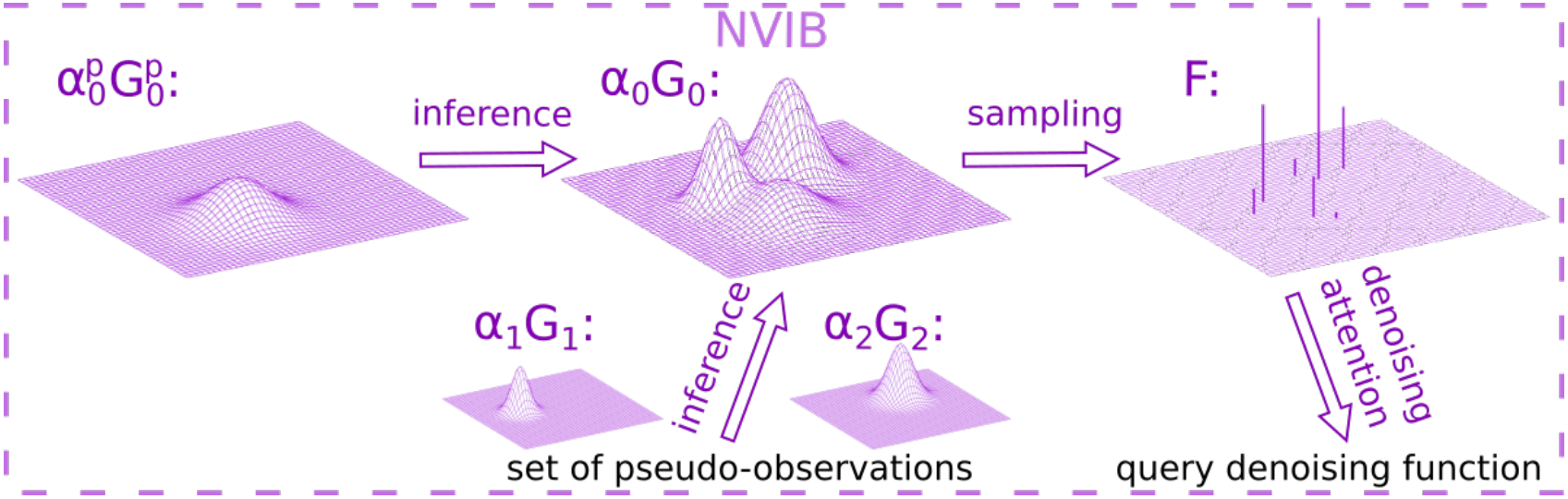
Inference of the Dirichlet Process Posterior

- One pseudo-observation per encoder token
- Each is a **Gaussian** G_i and its **pseudo-count** α_i
- Prior DP is a Gaussian G_0^p and its pseudo-count α_o^p
- Posterior DP is a mixture G_0 of the Gaussians and a total α_0 of the pseudo-counts

$$F \sim \mathrm{DP}(G_0, \alpha_0)$$

$$\alpha_0 = \alpha_0^p + \sum_{i=1}^{n} \alpha_i$$

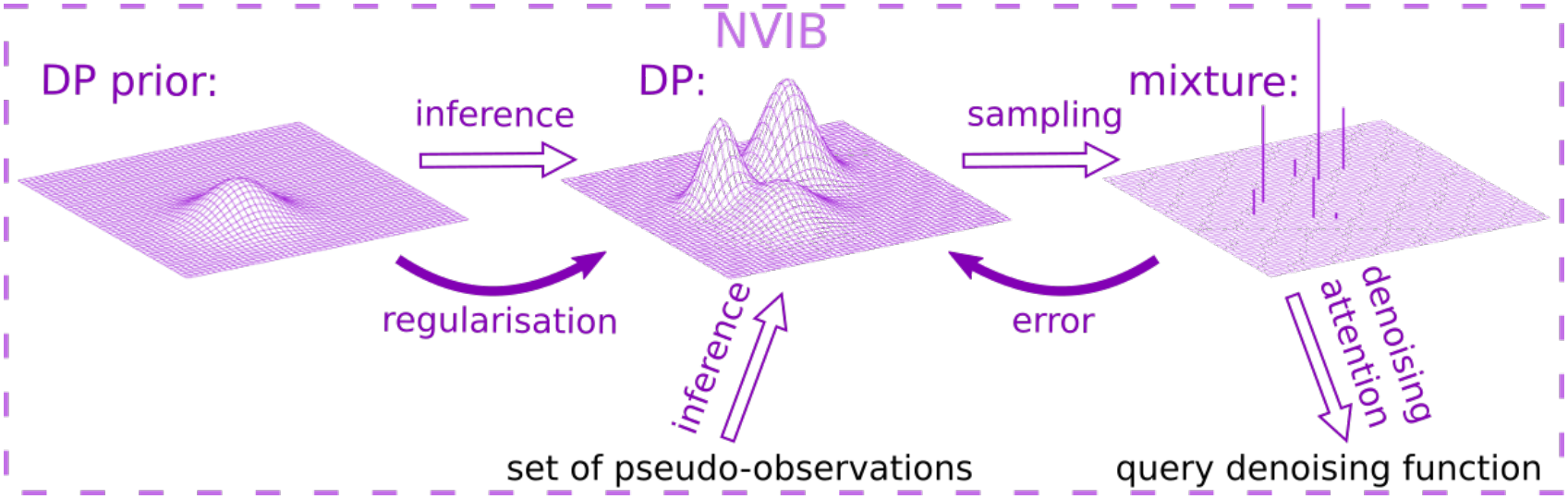
$$G_0 = \frac{\alpha_0^p}{\alpha_0} G_0^p + \sum_{i=1}^{n} \frac{\alpha_i}{\alpha_0} G_i$$



Nonparametric Variational Information Bottleneck

Our **Nonparametric Variational Information Bottleneck** required proposing some effective approximations:

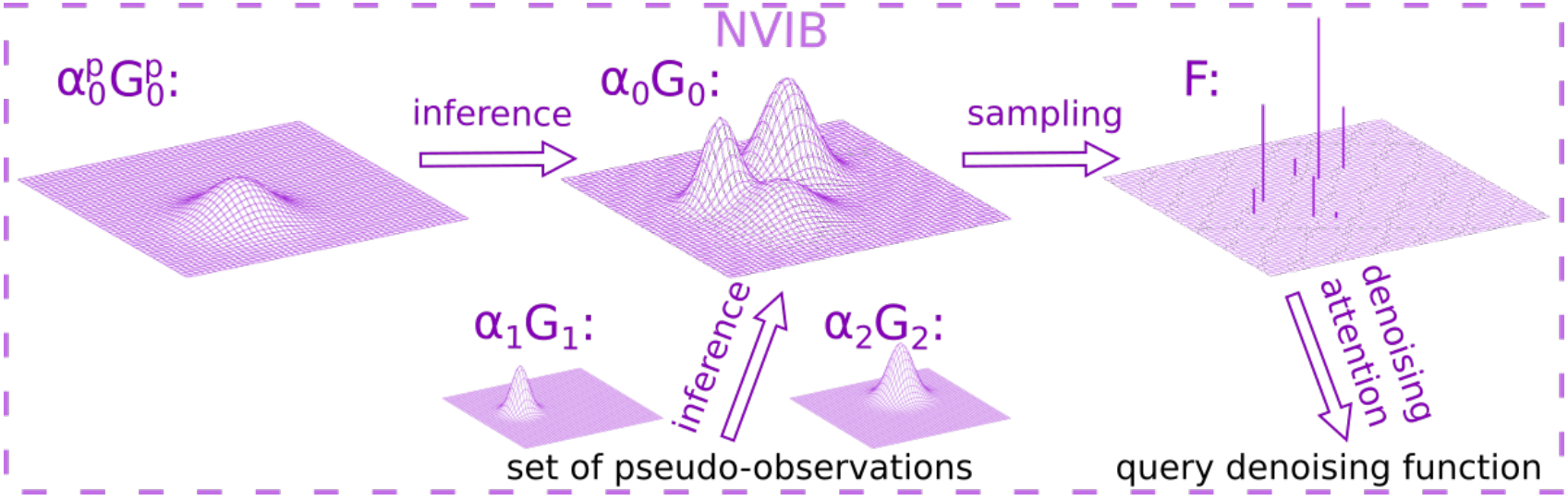
- the KL divergence between the posterior and prior DPs to regularise the posterior
- The reparameterisation trick for sampling from DPs with backpropagation through the sampling step



Sparseness of the Dirichlet Process Posterior

NVIB regularises the number of components.

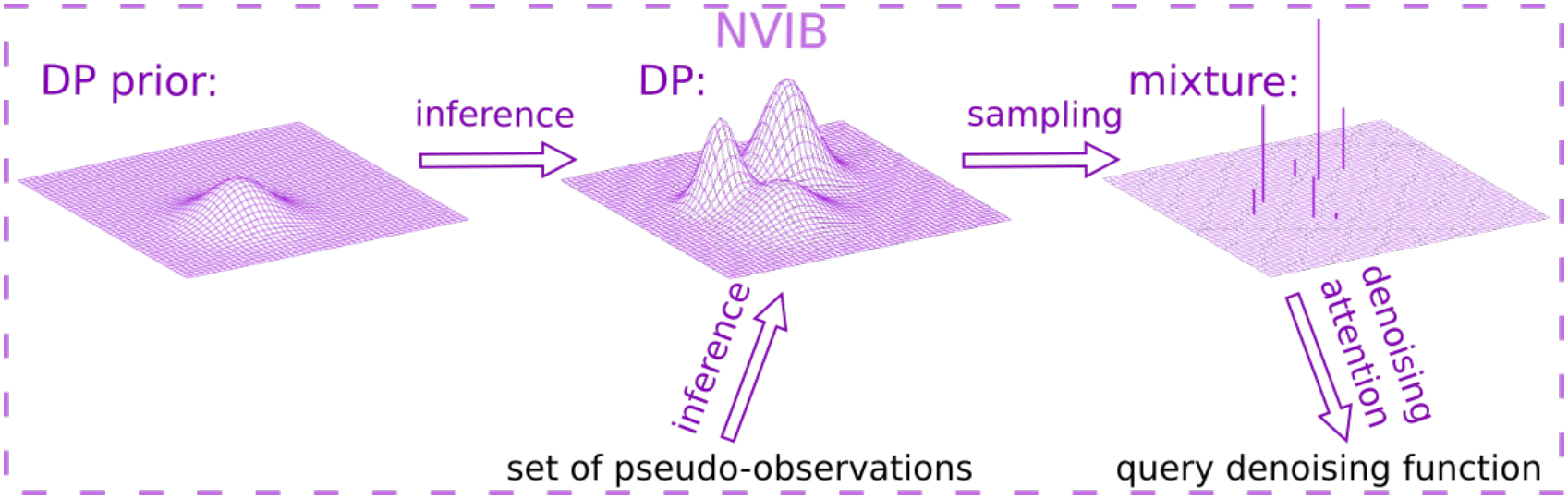
- Total pseudo-count α_0 determines the effective number of vectors in the sampled mixture, and thus its noise level
- KL divergence regularises the total pseudo-count to encourage more noise
- A **zero pseudo-count** removes that component



Nonparametric Variational Information Bottleneck

NVIB only allows required information to pass from encoder to decoder.

- Dirichlet processes define distributions over mixture distributions
- Sampled mixture is a noisy version of the base distribution
- Noise level is regularised by the effective number of vectors and their individual noise level

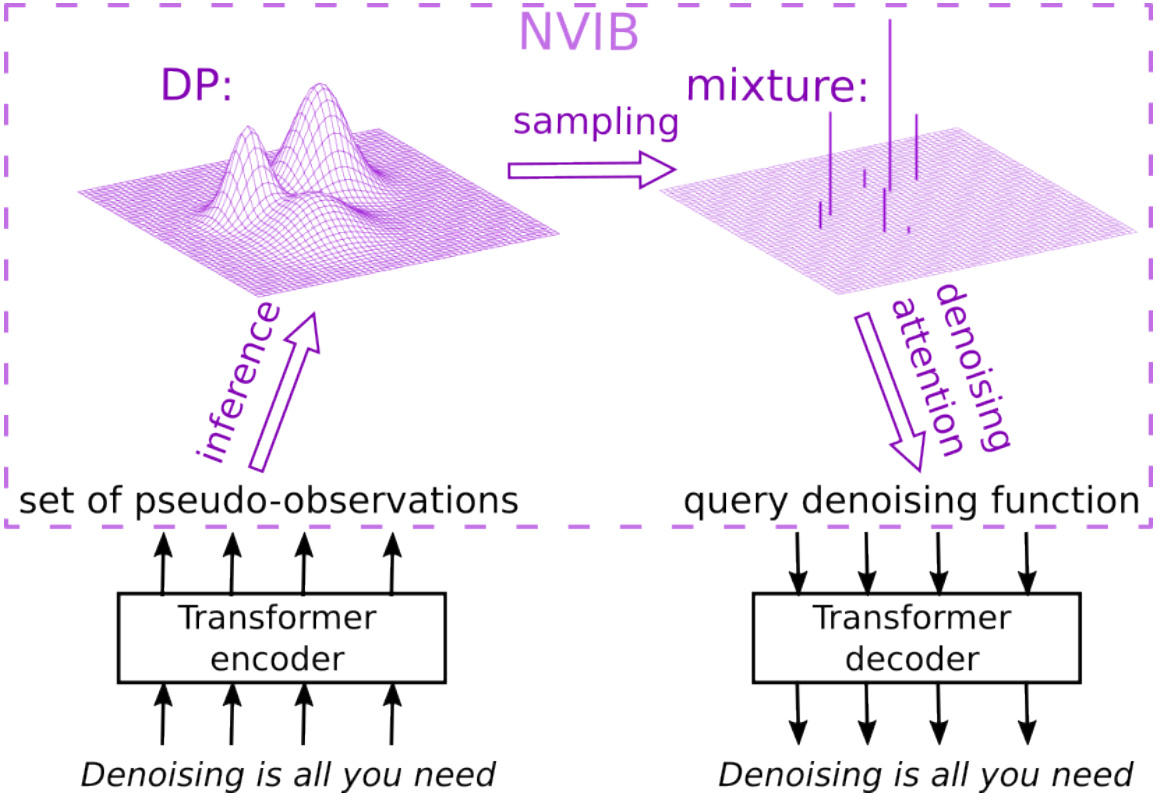


Outline

Nonparametric Variational Auto-Encoder

We can define a VAE for Transformers (NVAE) using NVIB.

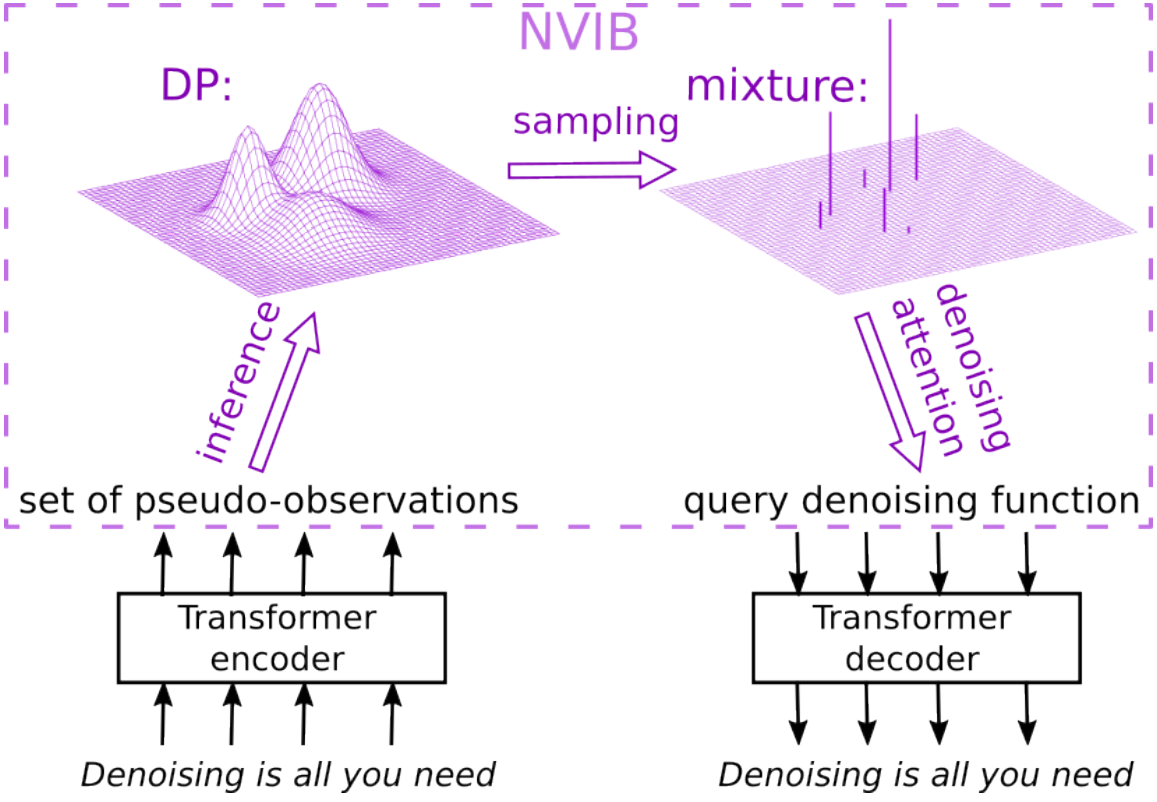
- **Transformer encoder** outputs pseudo-observations
- **NVIB** regularises the encoder-decoder interface
- **Transformer decoder** uses denoising attention



Nonparametric Variational Auto-Encoder

NVAE trained as an auto-encoder.

- Loss for cross-entropy of reconstructing the input sentence
- Loss for KL regulariser between the posterior and prior
- Hyperparameters to balance the **reconstruction** loss, and the two KL terms for the **Gaussians** and **pseudo-counts**

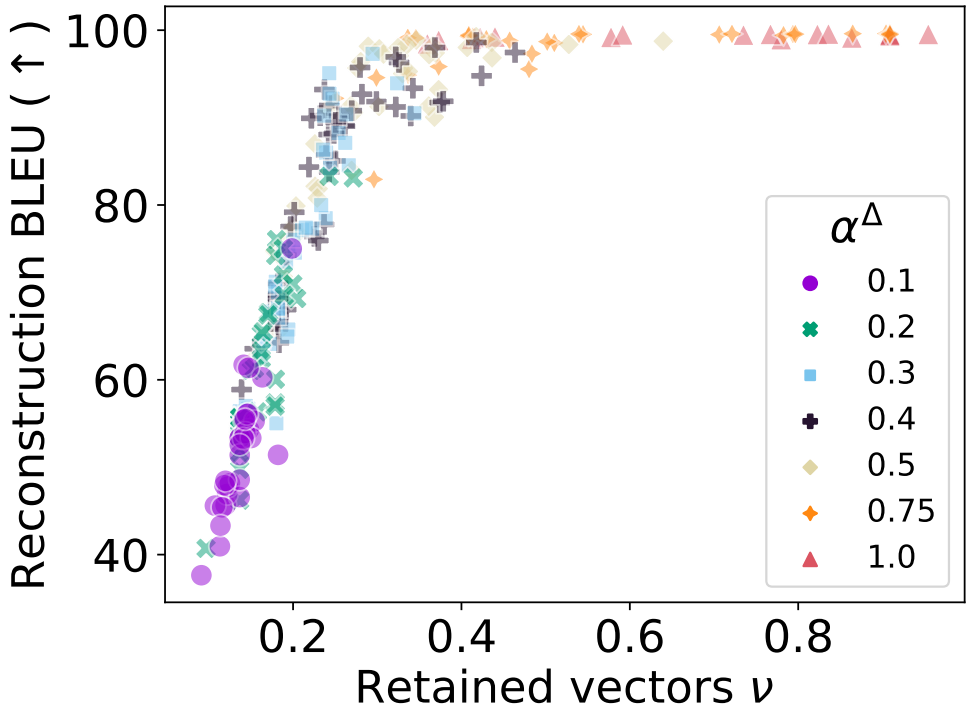


Outline

Inducing Representations of Text

We trained NVAE models on text data.

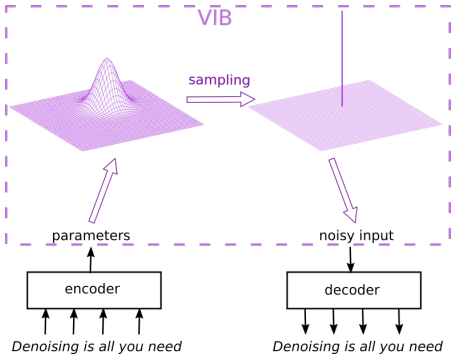
- Trained to reconstruct Wikipedia sentences
- Hyperparameter adjusts the sparsity rate
- Up to 2/3 of vectors can be dropped before reconstruction is degraded

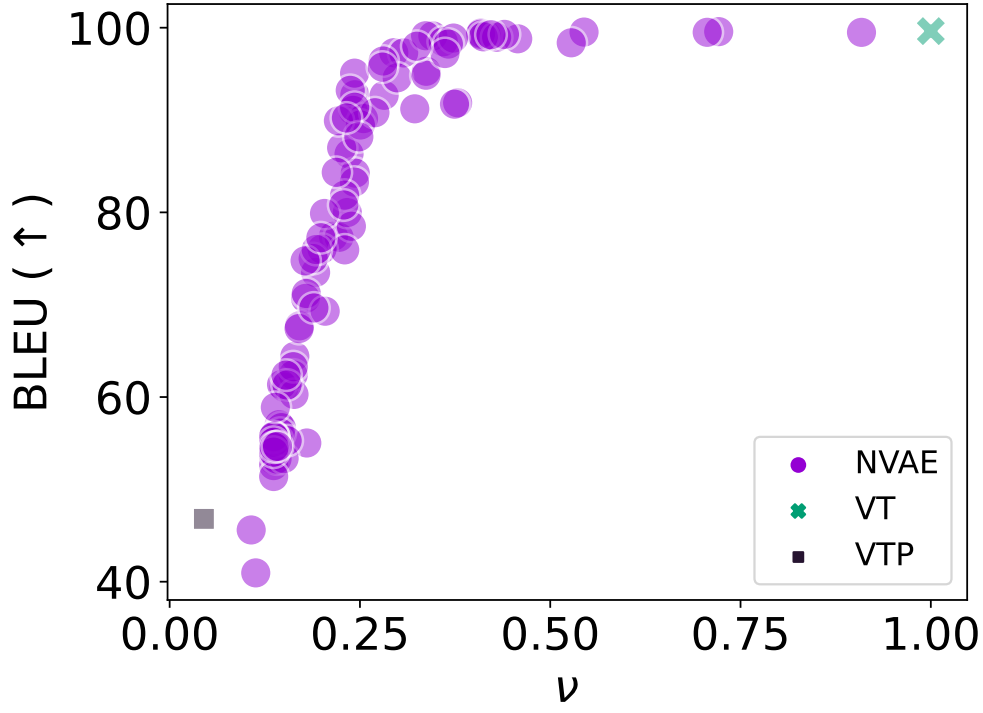


Inducing Compressed Representations

Baselines don't drop the right number of vectors.

- **V**ariational **T**ransformer **P**ooled only keeps one vector
- **V**ariational **T**ransformer keeps all the vectors
- NVAE can adjust the number of vectors

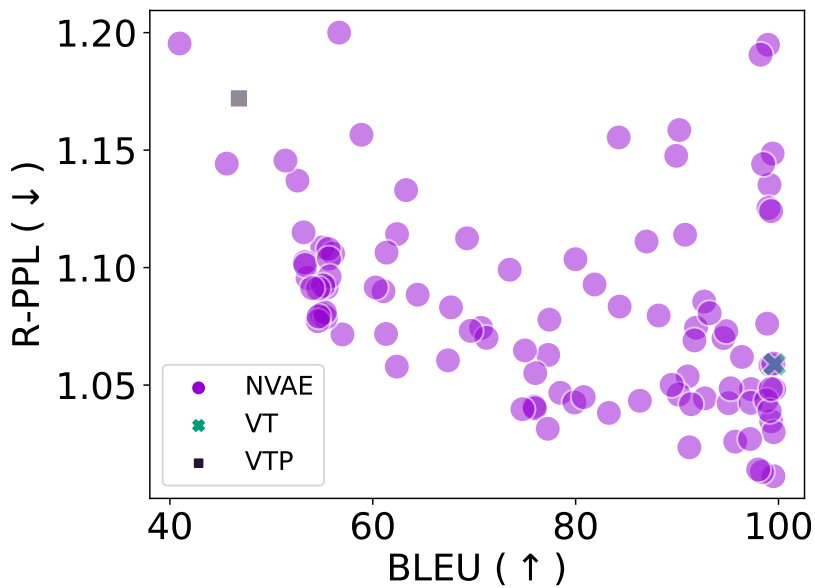




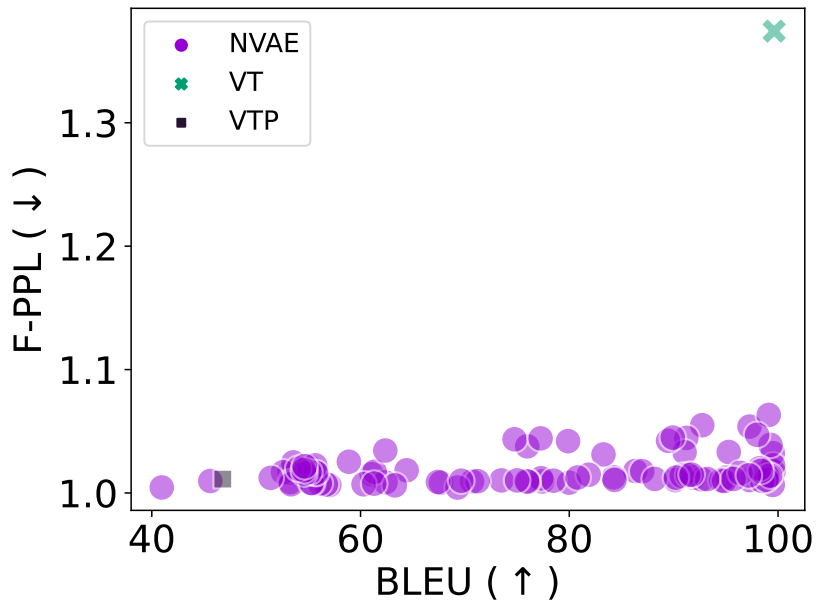
Inducing a Smooth Representation Space

Compressed representations generate text distributions better.

- Keeping all vectors
  - reconstructs text well
  - covers the space of texts well
  - many representations generate **garbage**
- NVIB compressed representations
  - reconstruct text well
  - cover the space of texts well
  - all representations generate good text



generation coverage vs reconstruction

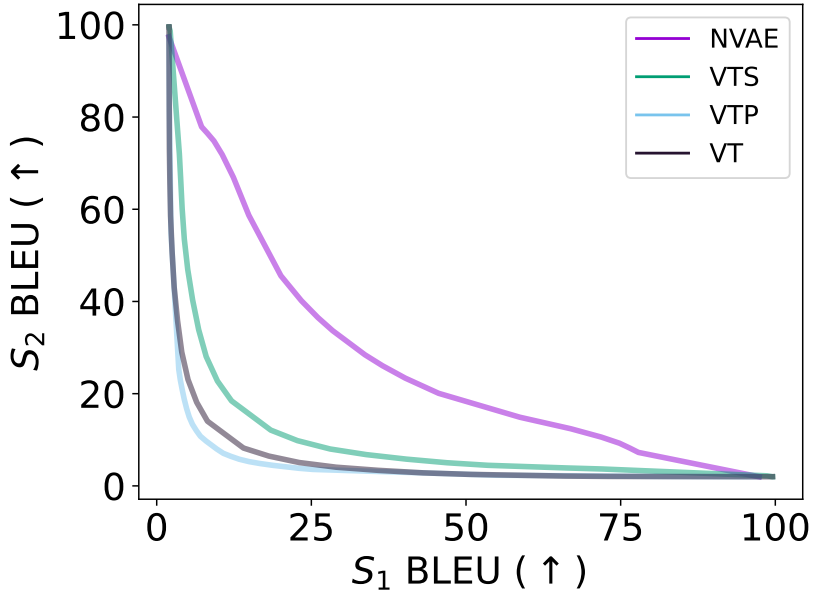


generation quality vs reconstruction

Inducing a Smooth Representation Space

Compressed representation space has smoother interpolation.

- Keeping all vectors does not interpolate well
  - decodes to the same sentence over a large region
  - generates unrelated text in between sentences
- NVIB induces a latent space with good interpolation
  - smoothly transitions between sentences
  - generates related sentences in between



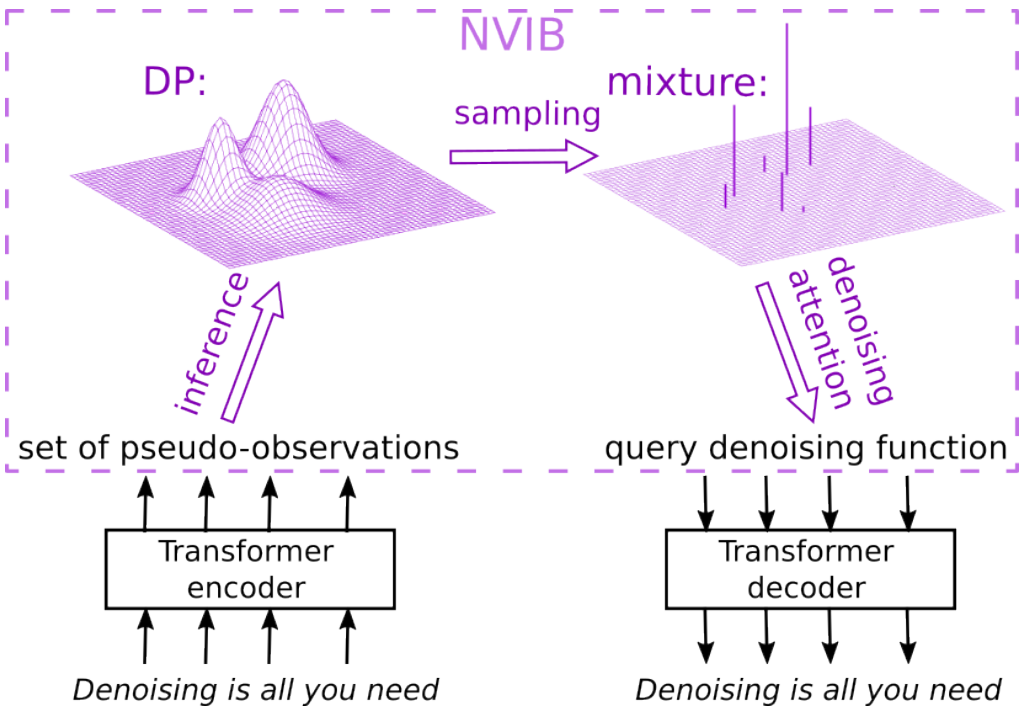
interpolation between sentences S1 and S2

Inducing Representations of Text

NVAE induces a better representation space.

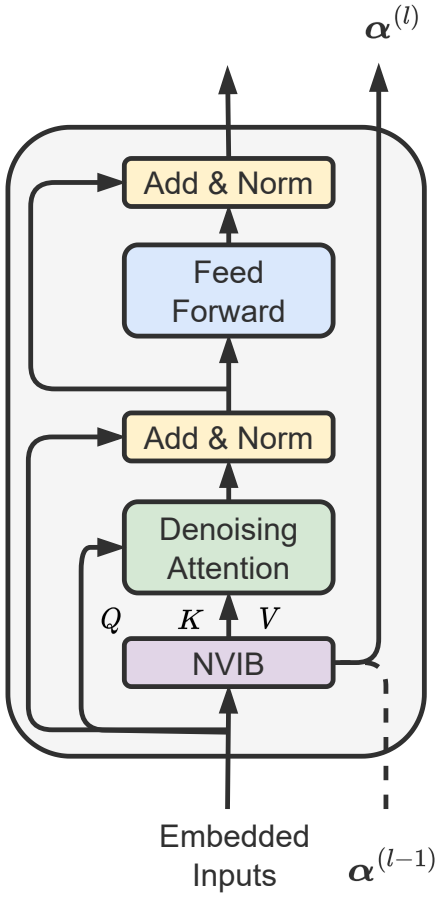
- Has an appropriate number of vectors
- Generates text distributions better
- Has smoother interpolation

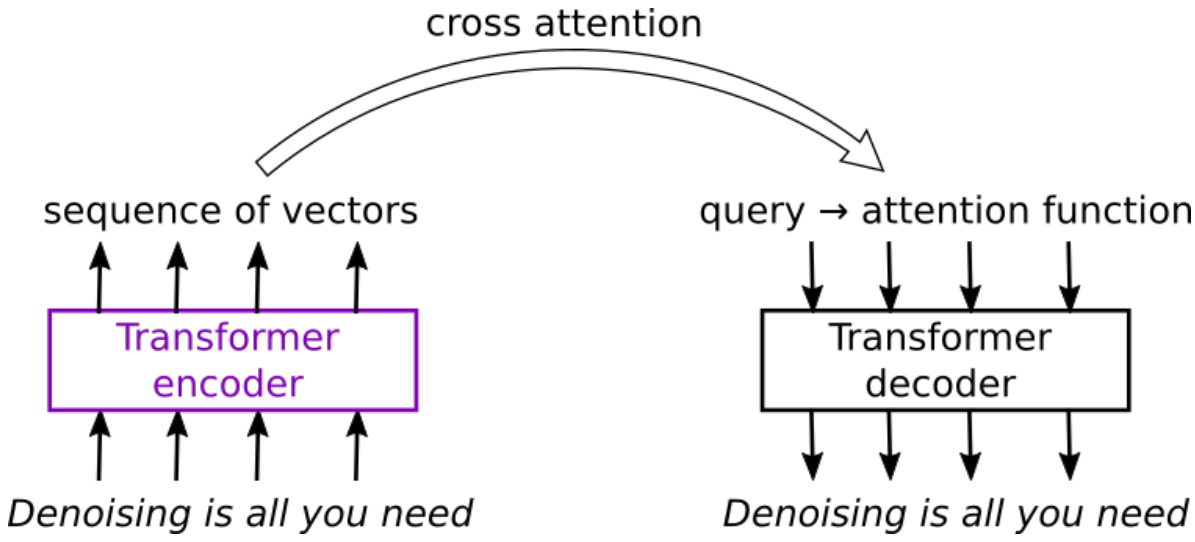
A better approximation to nonparametric variational Bayesian models gives a better induced representation space.



Learning to Abstract

We trained Transformer encoder-decoders with NVIB regularisation in the encoder's **stacked self-attention**.



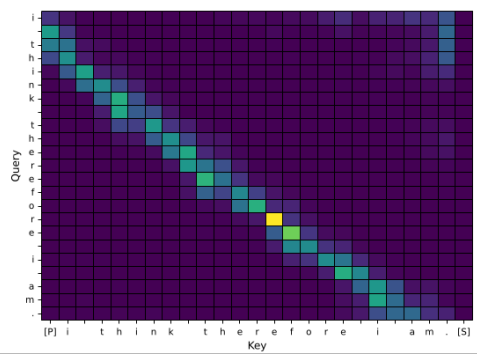


Learning to Abstract

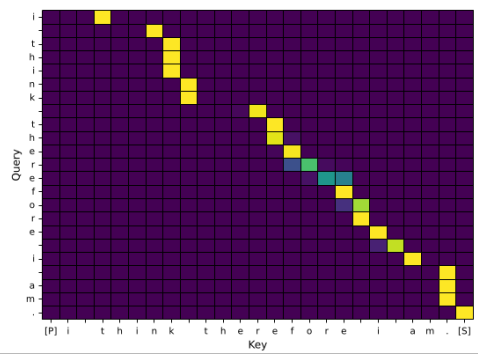
We trained Transformer encoder-decoders with NVIB regularisation in the encoder's stacked self-attention.

NVIB learns to group characters into meaningful units.

Normal Transformer



L-2



With NVIB

Learning to Abstract

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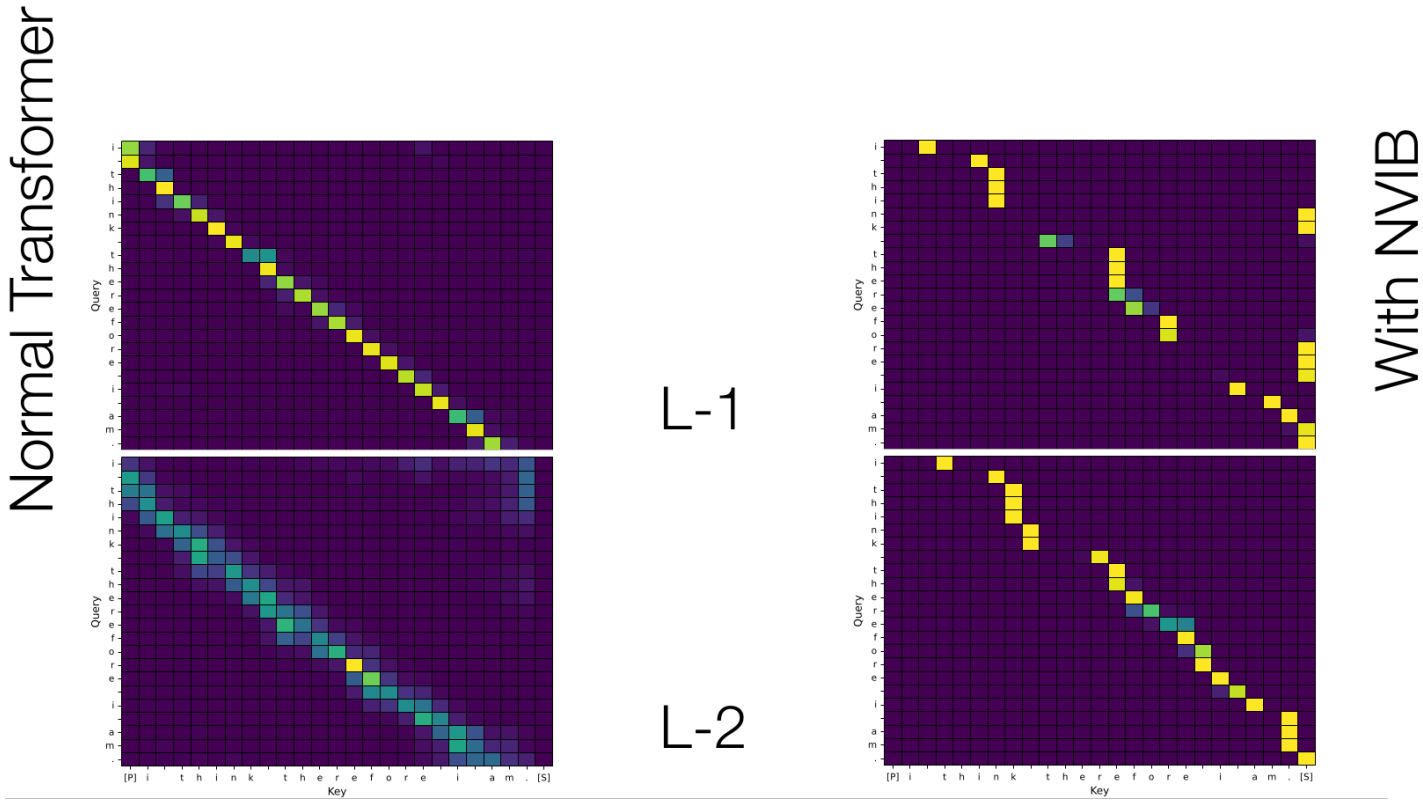

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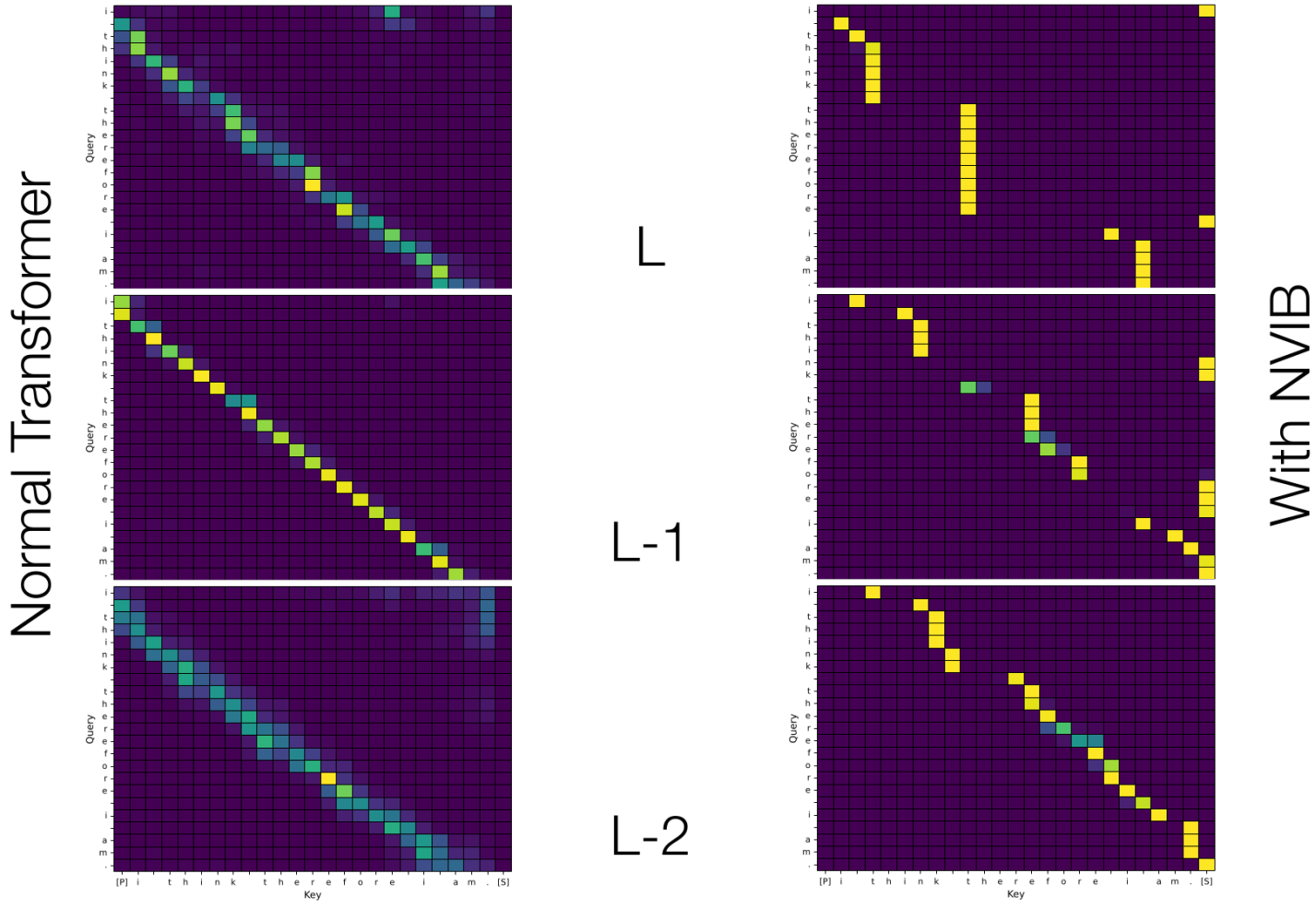

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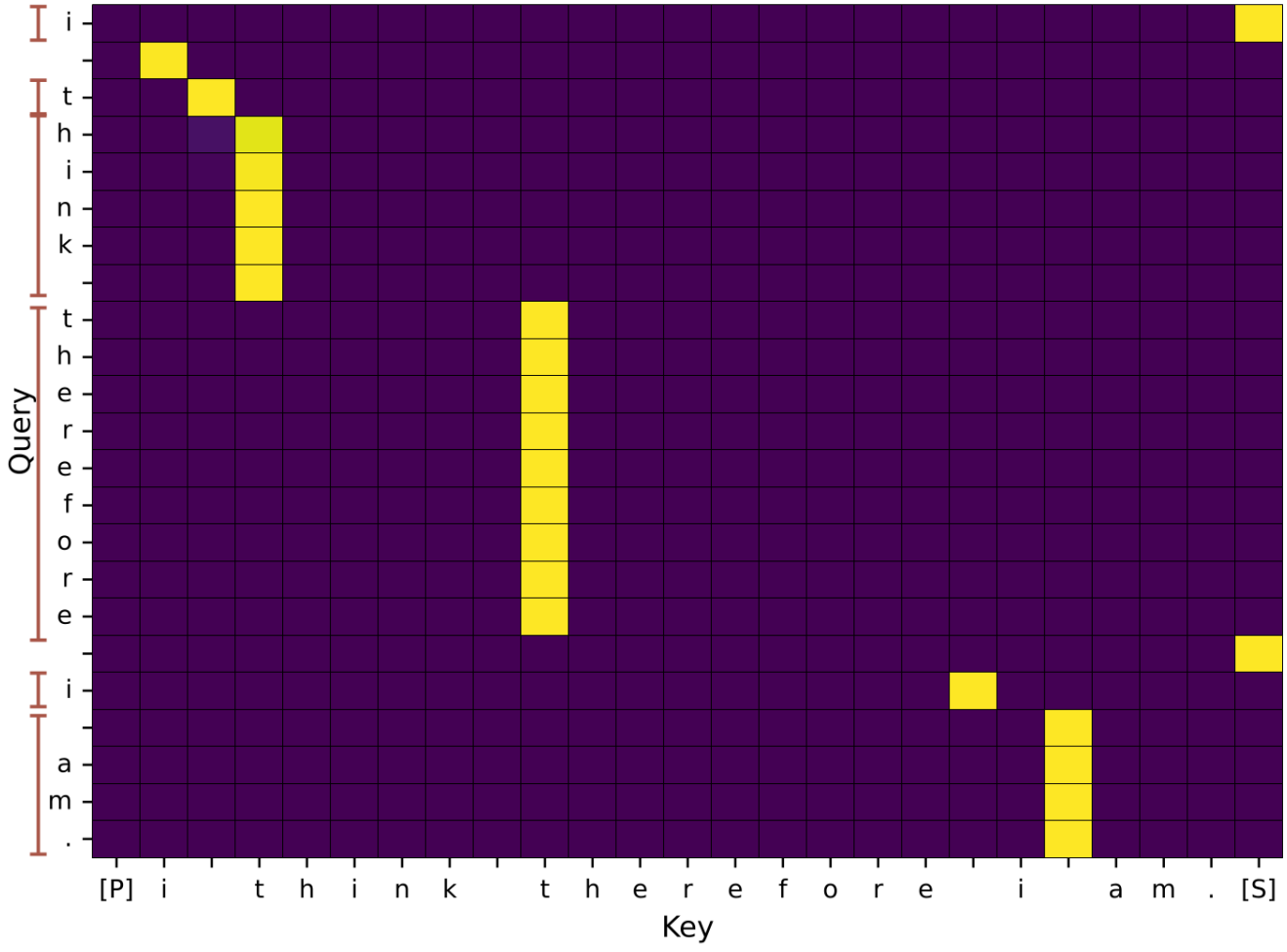
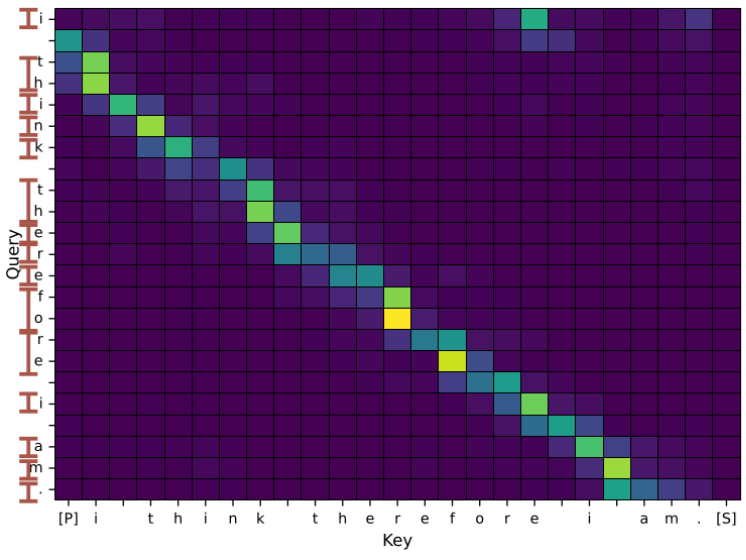


Learning to Abstract

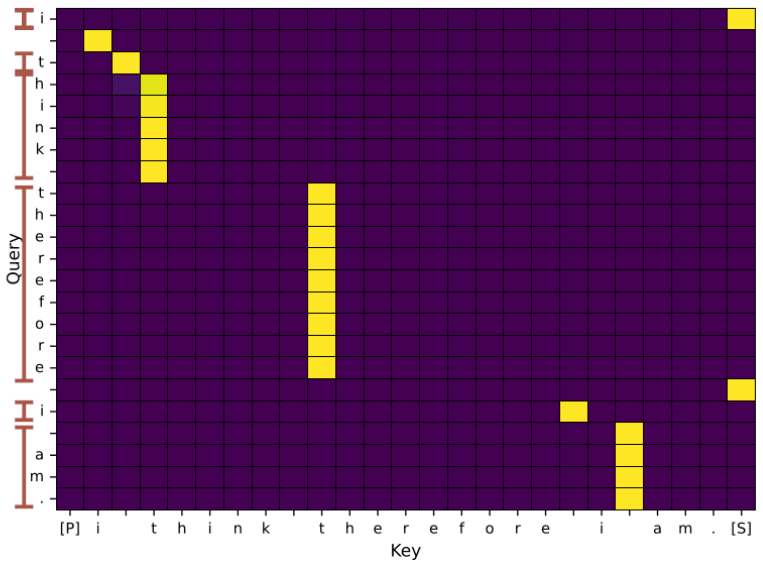
NVIB in encoder self-attention discovers words from characters.

F1=64.52%



Normal Transformer

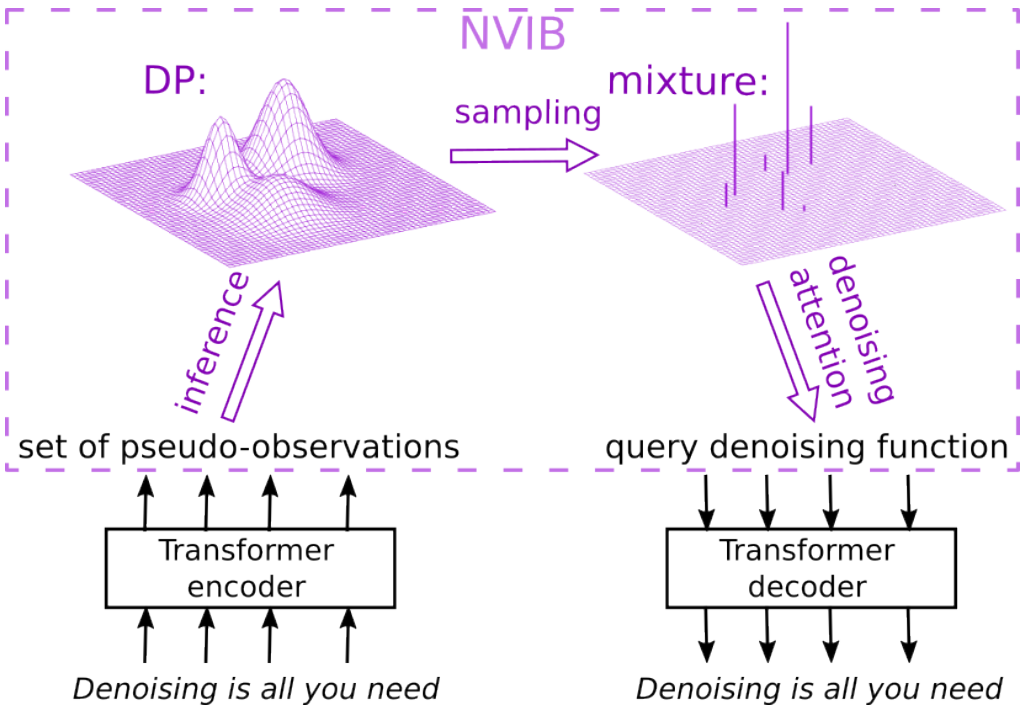
F1=78.86%



With NVIB

Summary of NVIB

- NVIB combines the effectiveness of **Transformers** with the regulariser of **Variational AutoEncoders**.
- NVIB has a good **inductive bias** for natural language.

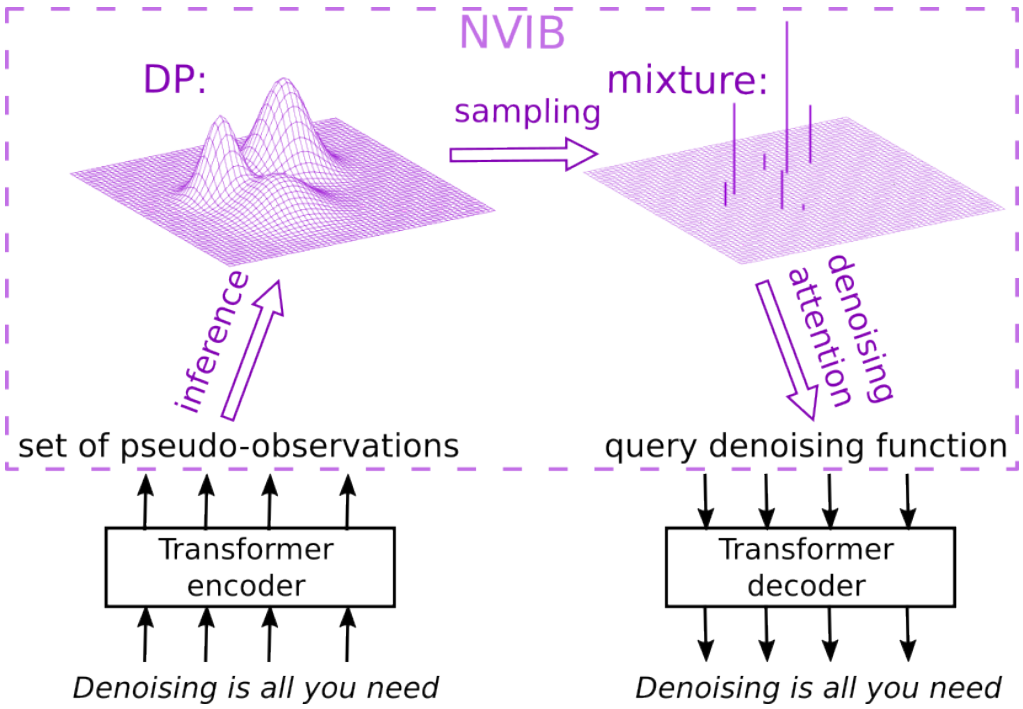


A VAE for Transformers with Nonparametric Variational Information Bottleneck. James Henderson and Fabio Fehr. ICLR 2023.

Why do Transformers work so well?

Transformers are **nonparametric variational Bayesian** models.

- Their latent representations are **nonparametric mixture distributions**
- Their encoders approximate **nonparametric variational Bayesian inference**
- Thier decoders approximate **nonparametric Bayesian generative models**



Why do Transformers work so well?

Hypothesis: Transformers work well ***because*** human thoughts are Dirichlet processes.

- Transformers are models of Dirichlet processes.
- Transformers are astoundingly good models of language.
- Language is (approximately) isomorphic to thought.