Deep Probabilistic Models (2)

Piyush Rai

Probabilistic Machine Learning (CS772A)

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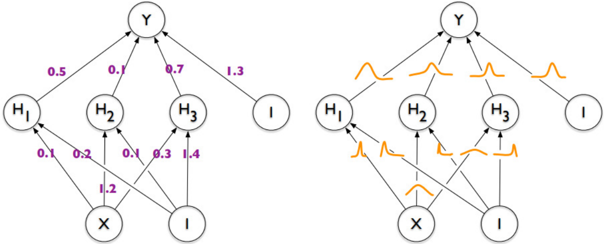
Recap: Bayesian Neural Networks

- Responses modeled via a suitable prob. distribution whose params are outputs of an NN, e.g.,

$$y_n \sim \mathcal{N}(\text{NN}(\boldsymbol{x}_n; \mathbf{W}), \sigma^2) \qquad \text{(for real-valued responses)}$$



- $\text{NN}(\boldsymbol{x}_n; \mathbf{W})$ is a neural network with features $\boldsymbol{x}_n$ as its inputs and parameters $\mathbf{W}$

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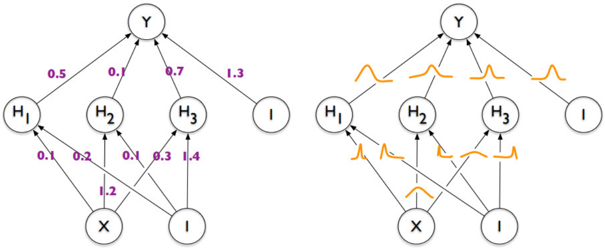

- $\text{NN}(\boldsymbol{x}_n; \mathbf{W})$ is a neural network with features $\boldsymbol{x}_n$ as its inputs and parameters $\mathbf{W}$
- Unlike standard neural networks, we learn the posterior over the unknowns
  - Non-conjugate model. MCMC or VB with Monte Carlo approximations typically used

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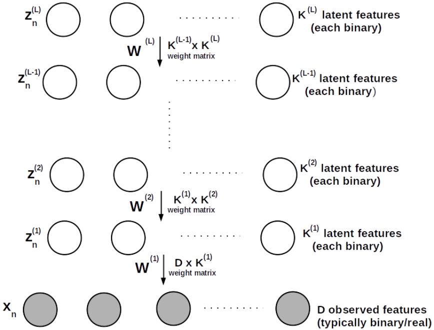
Recap: Sigmoid Belief Network

- An unsupervised generative model for the inputs $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$
- Assumes data generated by successive nonlinear transformations of multiple layers of latent features



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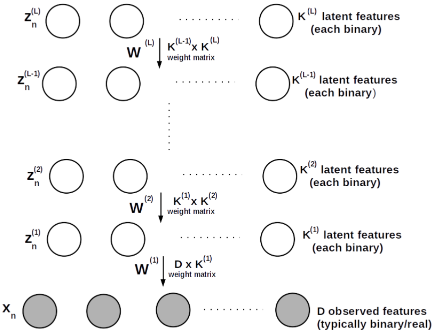

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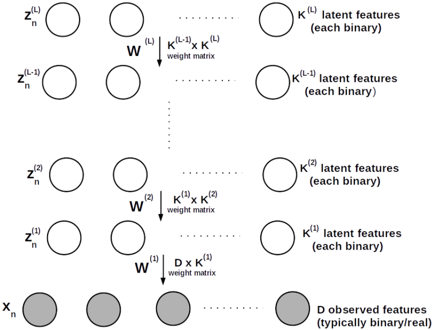
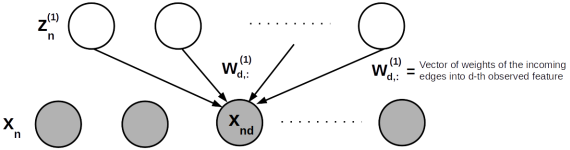


- In SBN, the latent features in each hidden layer are assumed to be binary-valued
- The goal is to infer $\mathbf{Z}^{(1)}, \ldots, \mathbf{Z}^{(L)}$ and the other parameters of the network (MCMC or VB with Monte Carlo approximations is needed since the model is non-conjugate)

Recap: Sigmoid Belief Network (A Zoomed-in Look)

- Layer 1 hidden nodes (latent features) generate each observed feature (assuming binary) as



$$p(x_{nd} = 1 | \boldsymbol{z}_n^{(1)}) = \text{sigmoid}(\boldsymbol{w}_{d,:}^{(1)\top} \boldsymbol{z}_n^{(1)} + b_d)$$

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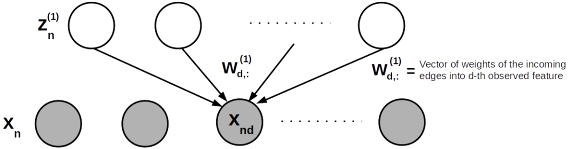

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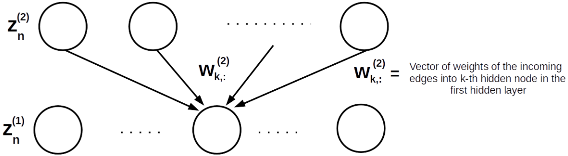
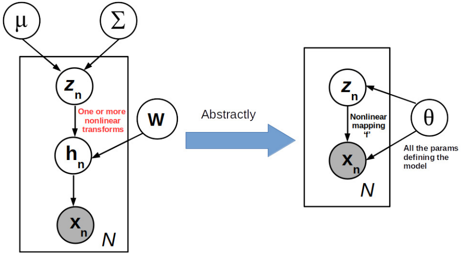
- Each hidden layer generates the nodes of hidden layer below it as (e.g., L2 $\rightarrow$ L1 in fig. below)



$$p(z_{nk}^{(1)} = 1|\boldsymbol{z}_n^{(2)}) \quad = \quad \text{sigmoid}(\boldsymbol{w}_{k,:}^{(2)\top}\boldsymbol{z}_n^{(2)} + c_k)$$

Recap: Deep Latent Gaussian Models

- Assume that a Gaussian latent variable $\boldsymbol{z}_n$ is pushed through a (deep) NN to generate $\boldsymbol{x}_n$



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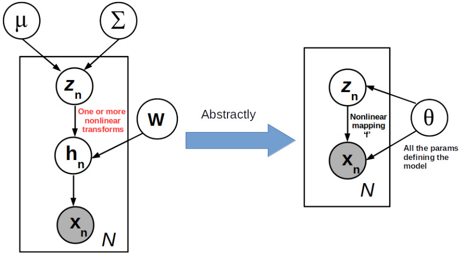

- A simple example with $\boldsymbol{z}_n \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_K)$ and assuming $\boldsymbol{x}_n \in \mathbb{R}^D$ with Gaussian likelihood

$$\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{h}_n, \sigma^2 \mathbf{I}_D)$$

where $\boldsymbol{h}_n$ is a deterministic nonlinear transform of $\boldsymbol{z}_n$, e.g., $\boldsymbol{h}_n = \mathbf{W}\underbrace{\sigma(\mathbf{V}\boldsymbol{z}_n)}_{\text{sigmoid}}$ or $\boldsymbol{h}_n = \mathbf{W}\underbrace{\max\{\mathbf{0}, \mathbf{V}\boldsymbol{z}_n\}}_{\text{ReLU}}$

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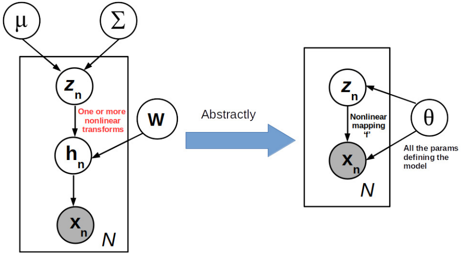

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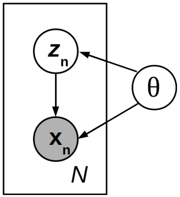
Inference for Deep Latent Gaussian Models



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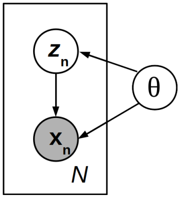

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- Initialize θ. Then iterate until converence
  - For $n = 1, \ldots, N$
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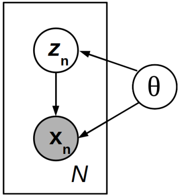

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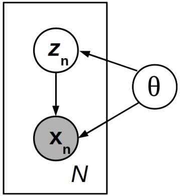

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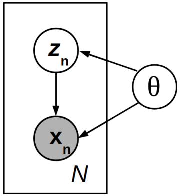

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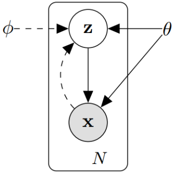
- This iterative approach can be slow for large N
- Also, inferring $\boldsymbol{z}$ for new data point(s) $\boldsymbol{x}$ would require using the same iterative procedure

Variational Auto-encoder (VAE)

- Esseentially a DLGM, i.e., the $\boldsymbol{z}$ to $\boldsymbol{x}$ mapping $p(\boldsymbol{x}|\boldsymbol{z})$ is defined by a neural net. Proposed almost simultaneously by Kingma & Welling (2013), and Rezende *et al* (2014)



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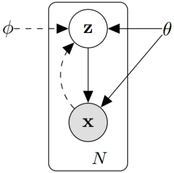

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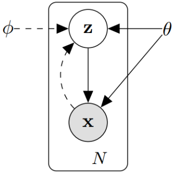

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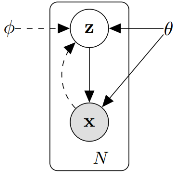

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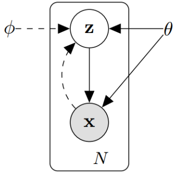

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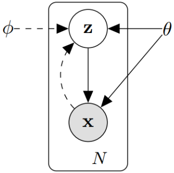

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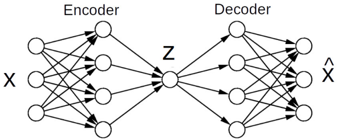
- $p(\boldsymbol{x}|\boldsymbol{z})$ is known as decoder and $q(\boldsymbol{z}|\boldsymbol{x})$ is known as encoder

Standard Auto-encoder vs Variational Auto-encoder

- A standard auto-encoder learns to (nonlinearly) compress and uncompress an input



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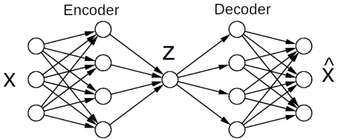

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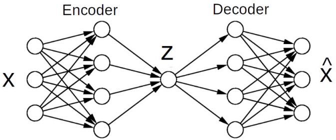

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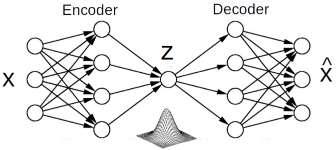

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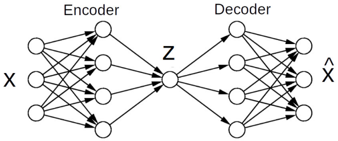

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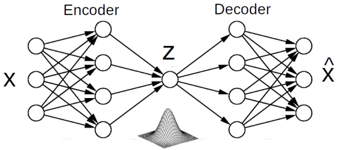
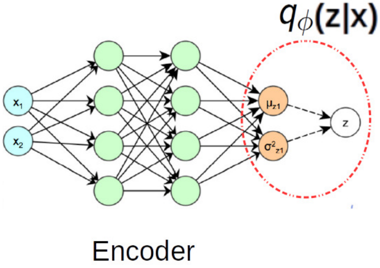


- Note: Simple generative models like PPCA or factor analysis also have this ability to generate data from random $\boldsymbol{z}$ but the linear map from $\boldsymbol{z}$ to $\boldsymbol{x}$ limits the type of data that can be generated well

VAE: The Encoder

- Role of encoder: Take $\boldsymbol{x}$ as input and generate an encoding $\boldsymbol{z}$



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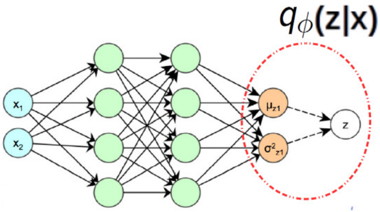

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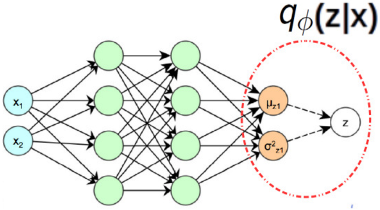

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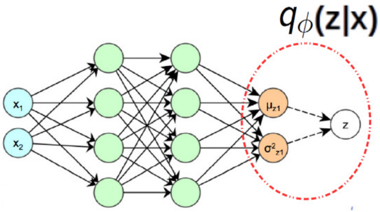

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- Since μ_z, σ_z are outputs of neural networks, the $\boldsymbol{x}$ to $\boldsymbol{z}$ mapping is nonlinear

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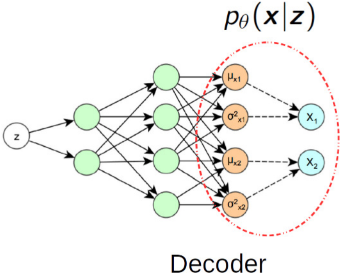
- Role of decoder: Generate $\boldsymbol{x}$ given $\boldsymbol{z}$. Defined by the likelihood model $p_\theta(\boldsymbol{x}|\boldsymbol{z})$



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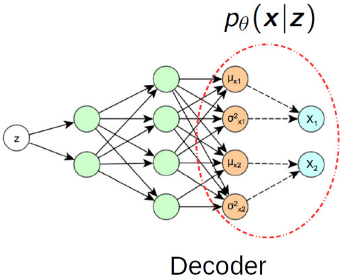

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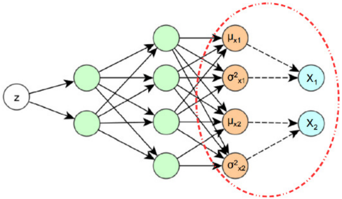

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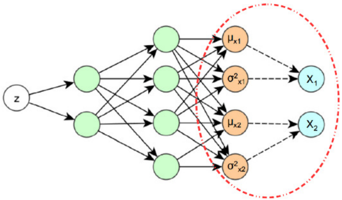
VAE: The Decoder

- Role of decoder: Generate $\boldsymbol{x}$ given $\boldsymbol{z}$. Defined by the likelihood model $p_\theta(\boldsymbol{x}|\boldsymbol{z})$



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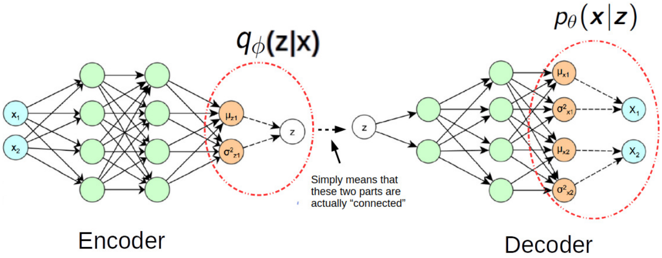
- Thus in the VAE, both $\boldsymbol{x}$ to $\boldsymbol{z}$ (encoder) and $\boldsymbol{z}$ to $\boldsymbol{x}$ (decoder) mappings are nonlinear

Inference for VAE

- VAE uses variational inference (hence the name!) to learn the model parameters θ and ϕ



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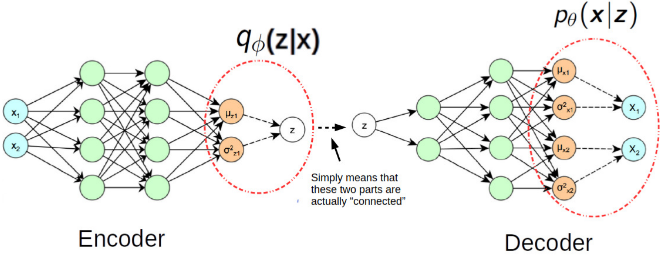

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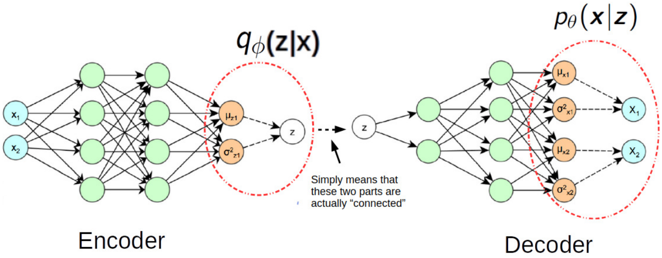

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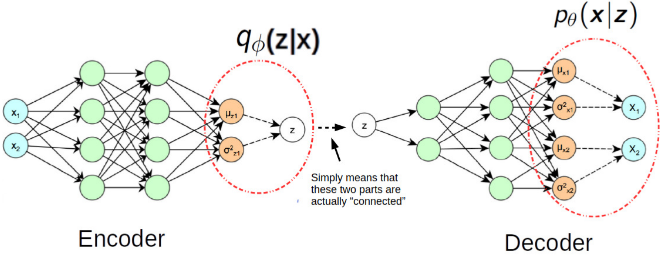

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- ELBO intuition: Maximizing it will learn latent code $\boldsymbol{z}_n$ that will give good reconstruction for $\boldsymbol{x}_n$ (in expectation) and will keep $q(\boldsymbol{z}_n|\boldsymbol{x}_n)$ to be close to the prior $p(\boldsymbol{z}_n)$ (i.e., regularization)

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$$\nabla_\phi \mathbb{E}_q[f(\boldsymbol{z}_n)] = \mathbb{E}_q[f(\boldsymbol{z}_n)\nabla_\phi \log q(\boldsymbol{z}_n)] \approx \frac{1}{L}\sum_{\ell=1}^{L} f(\boldsymbol{z}_n^{(\ell)})\nabla_\phi \log q(\boldsymbol{z}_n^{(\ell)})$$

where $f(\boldsymbol{z}_n)$ denotes all the difficult terms in the ELBO expression

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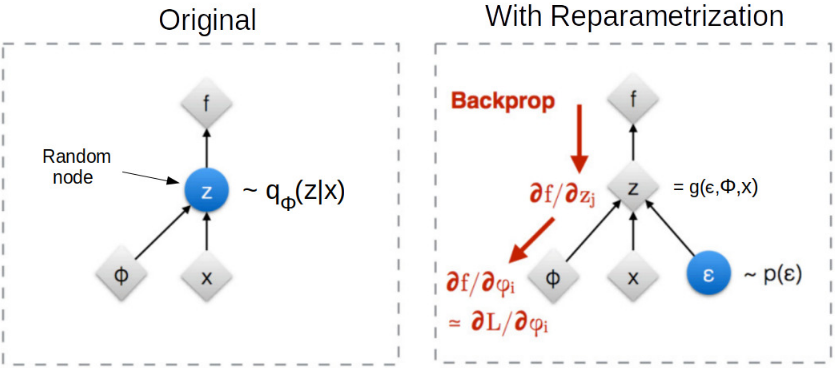
- Given samples from $p(\epsilon)$, can easily approximate the ELBO (these samples don't depend on ϕ)

Reparametrization Trick

- Decoupling the randomness of $\boldsymbol{z}$ from ϕ using the reparametrization $z = g(\epsilon, \phi, x)$ also helps backpropagate easily through $\boldsymbol{z}$ when taking derivatives



VAE Architecture: An Example

- Assume a generative model (decoder) of the form $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ as specified below

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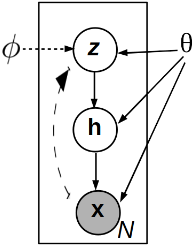

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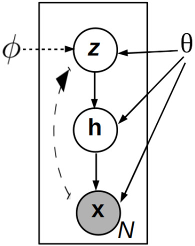

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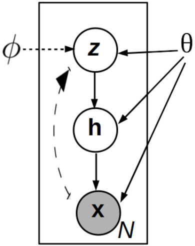

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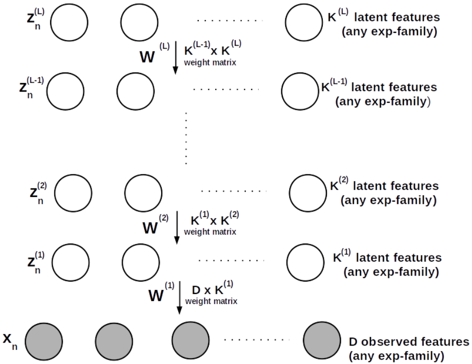
- Note: Recent work on VAE uses richer priors $p(\boldsymbol{z})$ as well as richer variational approx. $q(\boldsymbol{z}|\boldsymbol{x})$
  - For standard VAEs, these are simple Gaussians with diagonal covariances

Other Architectures: Deep Exponential Families

- Similar in architecture to sigmoid belief networks
- However, latent variables in every layer, as well as observations, are from exp. family distributions



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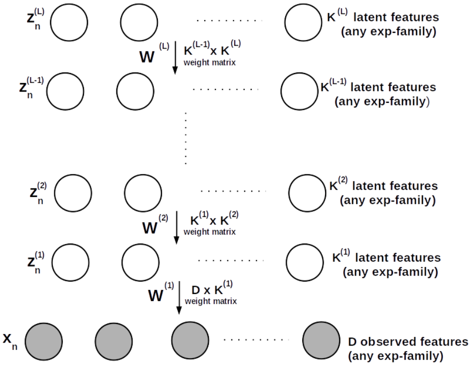
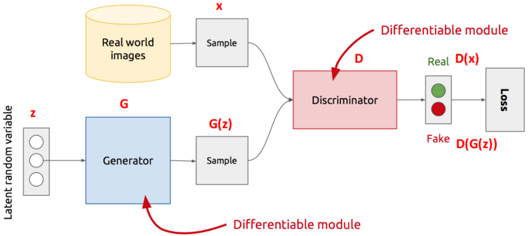


- Overall model not conjugate but BBVI (Ranganath et al, 2013) or MCMC methods can be used

Other Architectures: Generative Adversarial Networks

- Based on a game between a generator and a discriminator (Goodfellow et al, 2013)



https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

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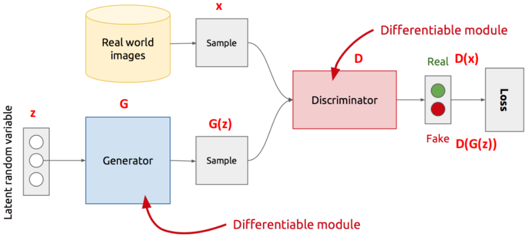

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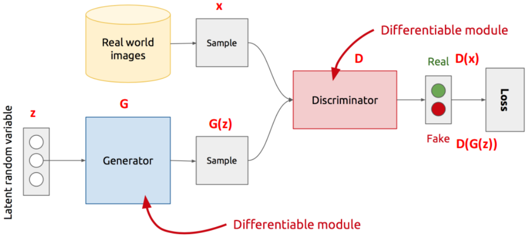

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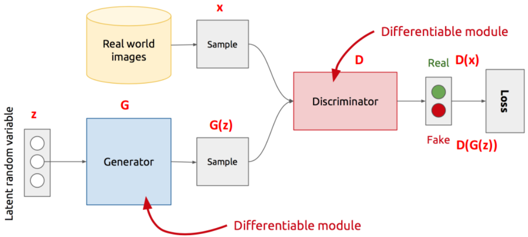

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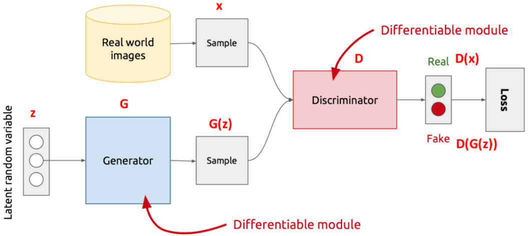

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- Originally designed mainly for synthetic data generation tasks but recent work extends GANs for many other problems such as latent variable inference, semi-supervised learning, etc.

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