Probabilistic Modeling meets Deep Learning

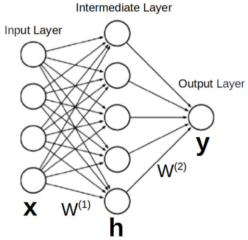
Piyush Rai

Topics in Probabilistic Modeling and Inference (CS698X)

April 3, 2019

Neural Networks

- A simple neural network with one intermediate (also called “hidden”) layer and a single output



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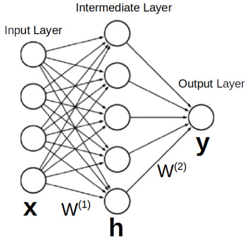

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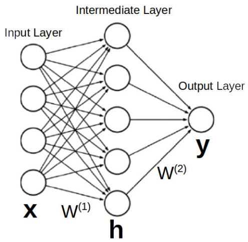

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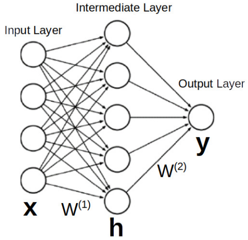

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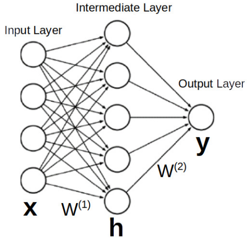

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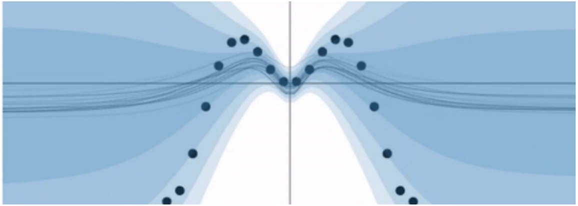
  - Do not provide uncertainty estimates

What We Want..

- Neural networks with additional benefits of probabilistic/Bayesian modeling



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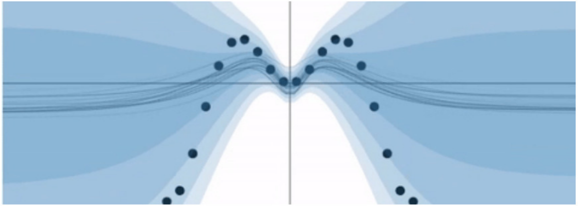

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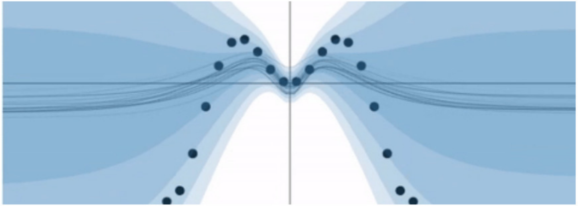

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- Note: We already have seen something that accomplishes this - Gaussian Processes
- Probabilistic/Bayesian neural nets are another alternative to this

Probabilistic/Bayesian Neural Networks

- A probabilistic model for neural network for supervised learning

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y_n &\sim \mathcal{N}(\mathrm{NN}(\boldsymbol{x}_n;\mathbf{W}),\beta^{-1}) && \text{(for real-valued responses)}\\
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where $\mathrm{NN}(\boldsymbol{x}_n;\mathbf{W})$ is a neural network with features $\boldsymbol{x}_n$ as inputs and parameters $\mathbf{W}$

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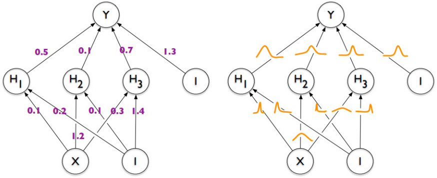
- We can perform point estimation or fully Bayesian inference for such probabilistic neural networks



Left: Standard NN or NN with point estimation, Right: Bayesian Neural Network

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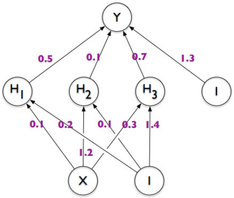
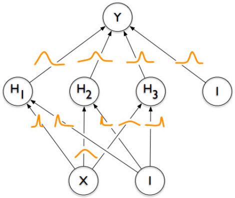
Learning Bayesian Neural Networks





- Computing posterior over $\mathbf{W}$ or computing posterior predictive is intractable in general

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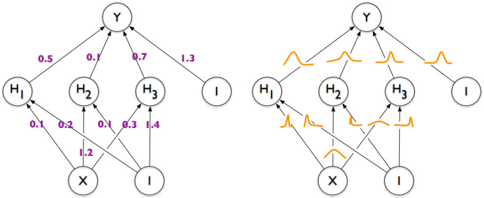

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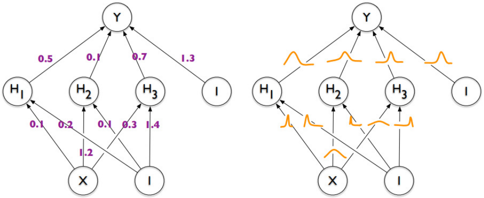

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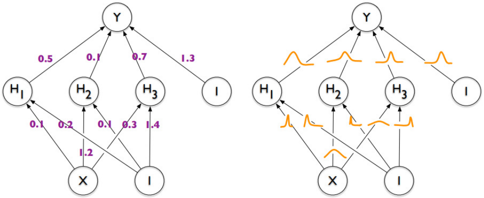

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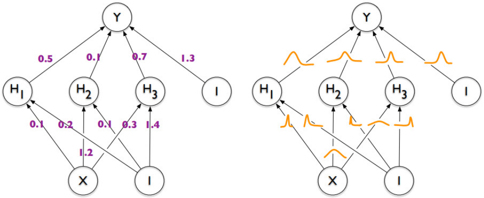

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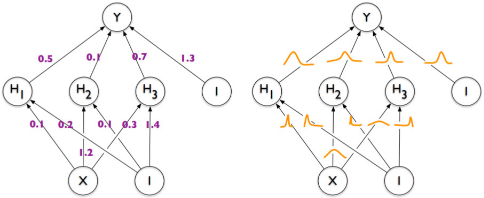

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  - Scalable versions of classic approximations, e.g., Laplace with diag/block-diag approx. of Hessian*

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Regularization in Deep Neural Nets: A Bayesian View

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- Basic idea: Perturb each NN weight or activations using multiplicative noise, e.g.,
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- The above stoch. grad. is the same as the stoch. grad of (verify using reparam trick)

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\nabla_{\mathbf{W}} \int \mathcal{N}(\hat{\mathbf{W}}|\mathbf{W}, \alpha\mathbf{W}^2) \log p(\boldsymbol{y}|\mathbf{X}, \hat{\mathbf{W}}) d\hat{\mathbf{W}} = \nabla_{\mathbf{W}} \mathbb{E}[\log p(\boldsymbol{y}|\mathbf{X}, \hat{\mathbf{W}})]
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where $\mathcal{N}(\hat{\mathbf{W}}|\mathbf{W}, \alpha\mathbf{W}^2) = \prod_{ij} \mathcal{N}(\hat{w}_{ij}|w_{ij}, \alpha w_{ij}^2)$

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- Sparse variational dropout: If we use $q(\hat{\mathbf{W}}|\mathbf{W},\alpha) = \prod_{ij}\mathcal{N}(\hat{w}_{ij}|w_{ij},\alpha_{ij}w_{ij})$

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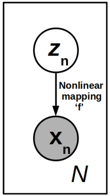

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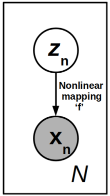

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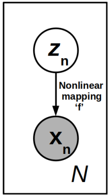

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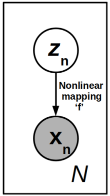

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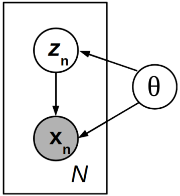
- The NN enables learning a nonlinear latent variable to data mapping f
- If $\boldsymbol{z}_n$ has a Gaussian prior, such models are called "Deep Latent Gaussian Models" (DLGM)

Inference for Deep Latent Gaussian Models

- Assume θ to be the global parameters of the model (params defining $p(\boldsymbol{z})$, $p(\boldsymbol{x}|\boldsymbol{z})$, etc.)



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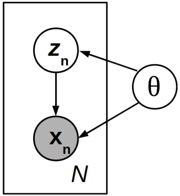

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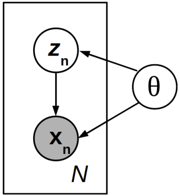

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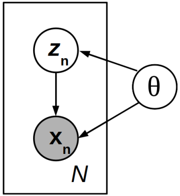

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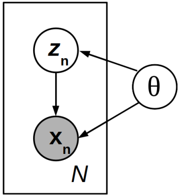

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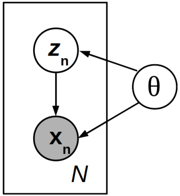

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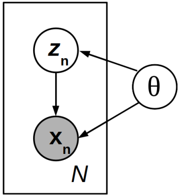

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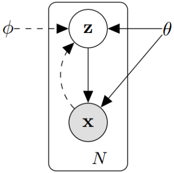
- Also, inferring $\boldsymbol{z}$ for new data point(s) $\boldsymbol{x}$ would require using the same iterative procedure

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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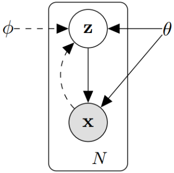

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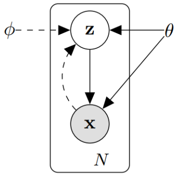

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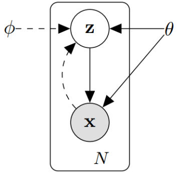

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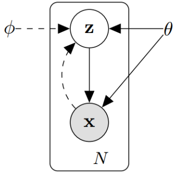

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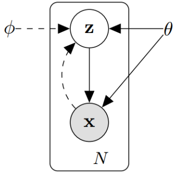

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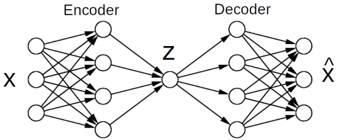
Standard Auto-encoder vs Variational Auto-encoder

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



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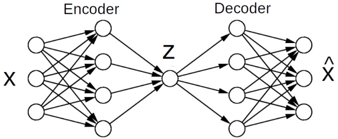

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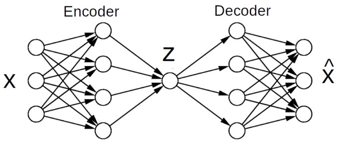

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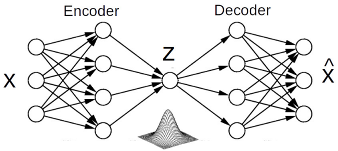

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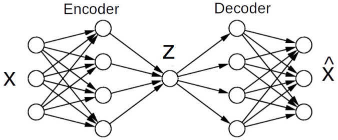

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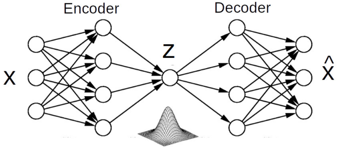
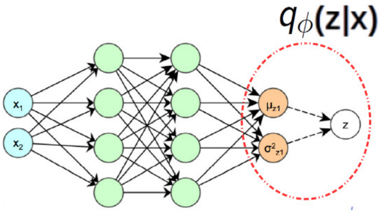


- Note: Simple generative models like PPCA or factor analysis also have this ability to generate data from random $\boldsymbol{z}$ but the linear map from $\boldsymbol{z}$ to $\boldsymbol{x}$ limits the type of data that can be generated well

VAE: The Encoder

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



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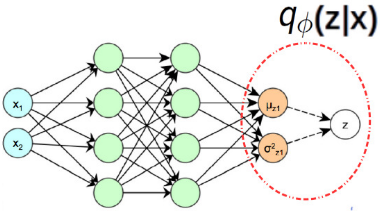

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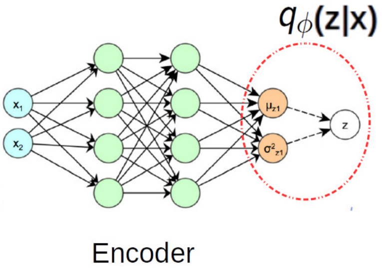

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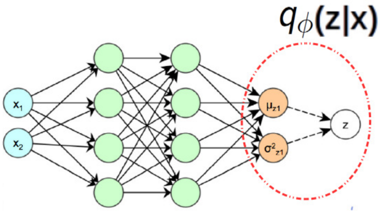

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- Since μ_z, σ_z are outputs of neural networks, the $\boldsymbol{x}$ to $\boldsymbol{z}$ mapping is nonlinear

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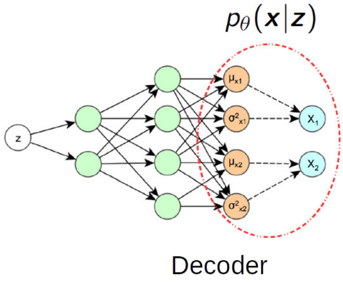

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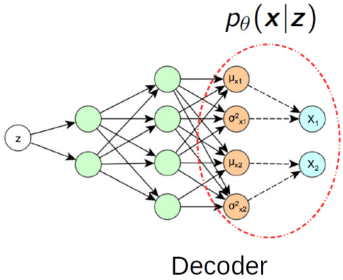

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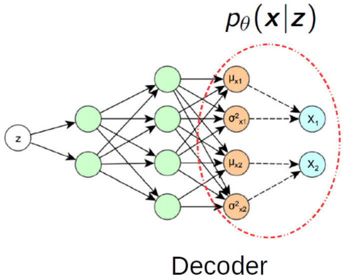

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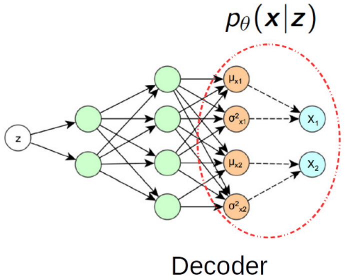

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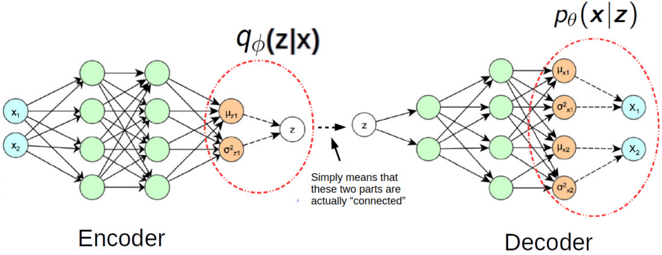
- Thus in the VAE, both $\boldsymbol{x}$ to $\boldsymbol{z}$ (encoder) and $\boldsymbol{z}$ to $\boldsymbol{x}$ (decoder) mappings are nonlinear

Inference for VAE

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



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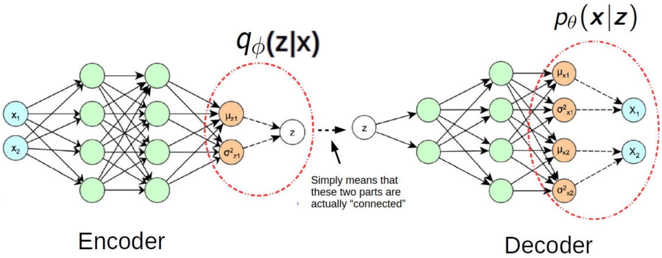

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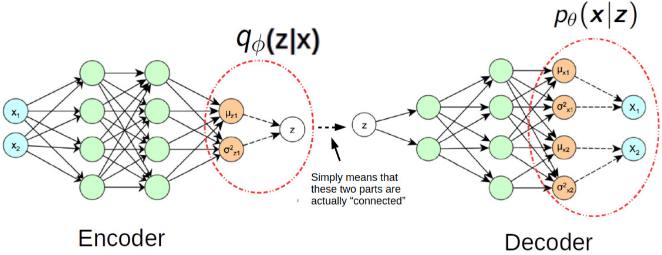

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- Variational inference uses the reparametrization trick† for computing ELBO derivatives

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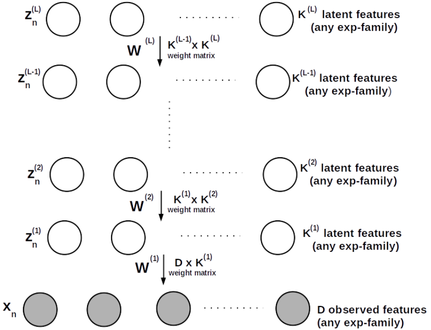

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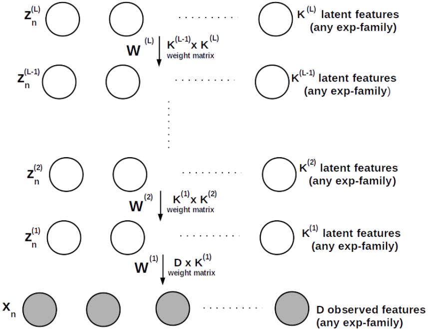

- Overall model not conjugate but BBVI (Ranganath et al, 2013) or MCMC methods can be used

Learning the right size of a deep neural network

- How to decide the number of layers and width of each layer?
- Nonparametric Bayesian methods can help here

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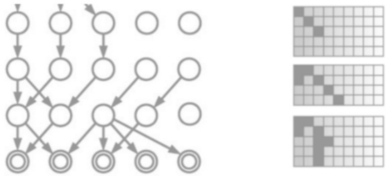

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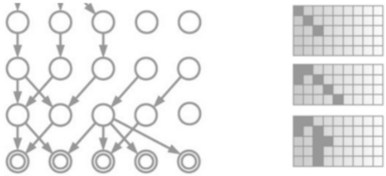

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  - The bottom-most layer is the data layer (fixed/known size)
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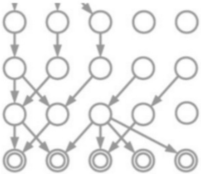
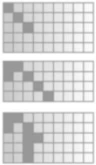
"Learning the Structure of Deep Sparse Graphical Models" (Adams et al, 2009), "Model Selection in Bayesian Neural Networks via Horseshoe Priors", Ghosh and Doshi-Velez (2017)

Learning the right size of a deep neural network

- How to decide the number of layers and width of each layer?
- Nonparametric Bayesian methods can help here





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- Another option is to use sparsity inducing priors on the connection weights

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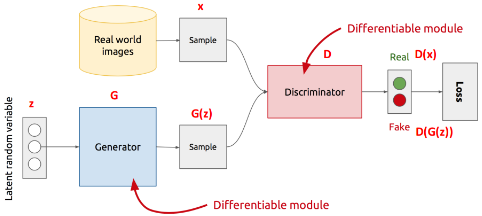

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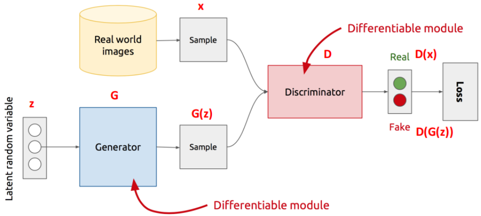

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$$\min_G \max_D V(D, G) = \mathbb{E}_{\boldsymbol{x} \sim p_{data}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z}))]$$

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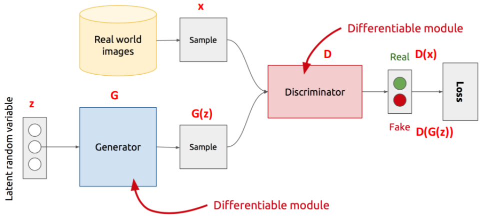

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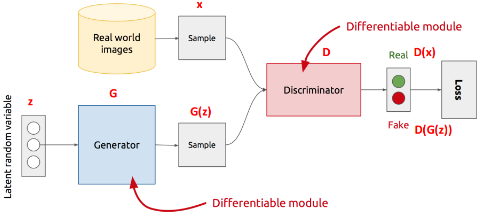

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