Deep Probabilistic Models (1)

Piyush Rai

Probabilistic Machine Learning (CS772A)

Oct 31, 2017

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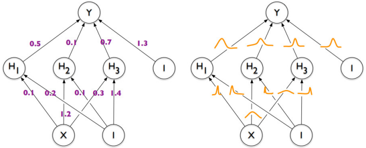

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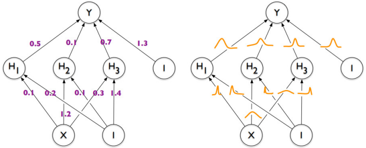

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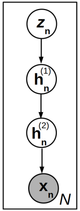

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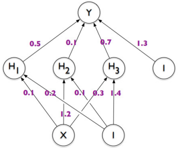

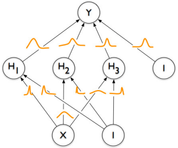

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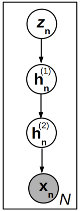

- Disclaimer: Very rapidly evolving area, deserves an entire course. Will only cover the basic principles underlying some of the representative models (from probabilistic/Bayesian perspective)

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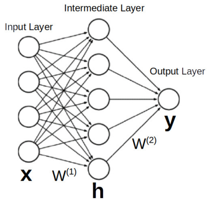
- Note: Such models are not limited to exp-family distributions only

Neural Network

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



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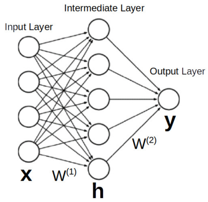

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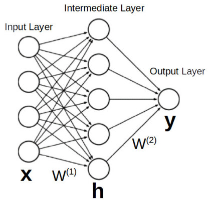

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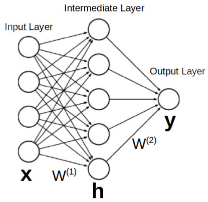

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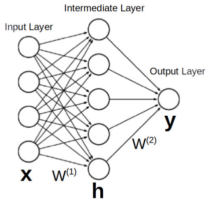

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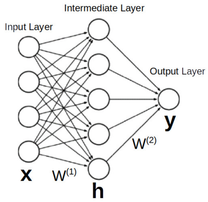

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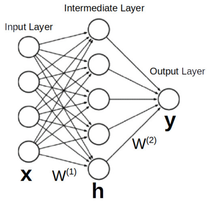

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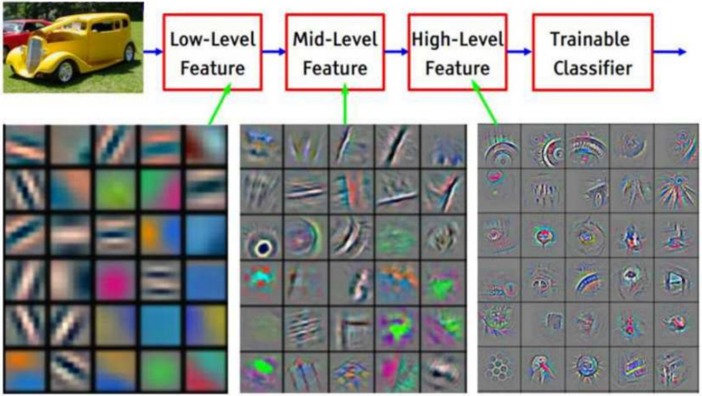
† Priors for Infinite Networks (Neal, 1995)

Deep Models as Feature Extractors

Deep models can learn features at different levels of abstraction



Example: Lowest layer learns edges, higher layers learns (parts of) objects

Deep Probabilistic Models for Supervised Learning

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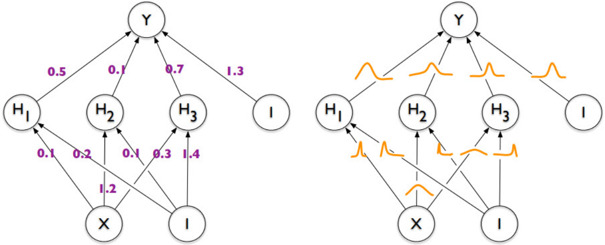

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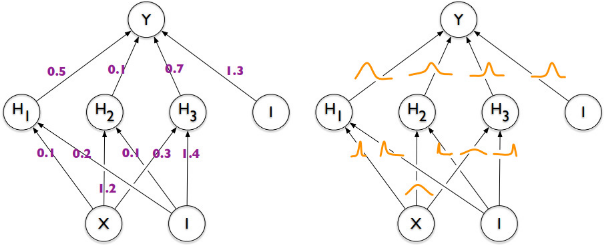

- Fully Bayesian treatment for such neural nets also has other benefits (e.g., Active Learning)

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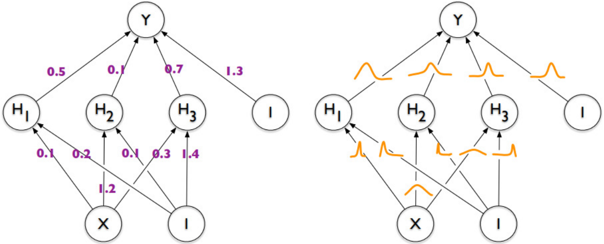
Learning Bayesian Neural Networks



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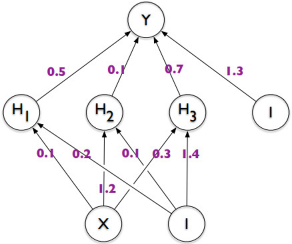

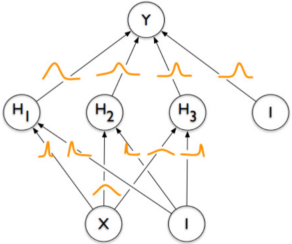

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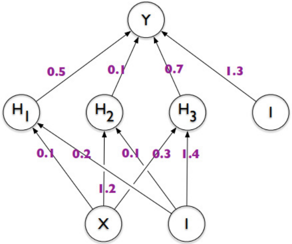

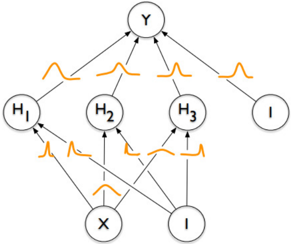

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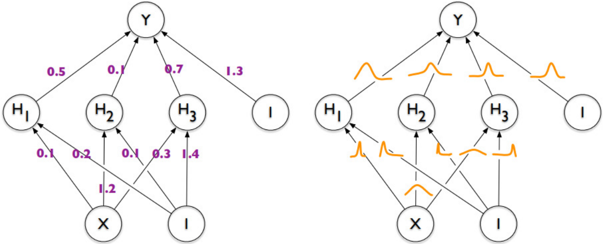

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- Variational inference is another popular alternative to MCMC for such models

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- Black-box VI can be another alternative (again based on Monte Carlo approximation)

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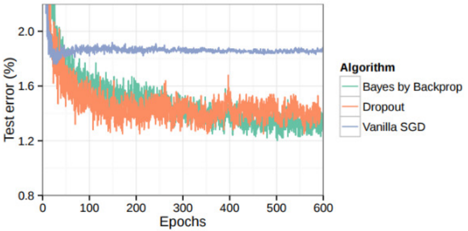
Bayesian Neural Networks on MNIST

- Some results on MNIST† (using standard feedforward network as the model; no convolution etc.)

Method	# Units/Layer	# Weights	Test Error
SGD, no regularisation (Simard et al., 2003)	800	1.3m	1.6%
SGD, dropout (Hinton et al., 2012)			≈ 1.3%
SGD, dropconnect (Wan et al., 2013)	800	1.3m	**1.2%***
SGD	400	500k	1.83%
	800	1.3m	1.84%
	1200	2.4m	1.88%
SGD, dropout	400	500k	1.51%
	800	1.3m	1.33%
	1200	2.4m	1.36%
Bayes by Backprop, Gaussian	400	500k	1.82%
	800	1.3m	1.99%
	1200	2.4m	2.04%
Bayes by Backprop, Scale mixture	400	500k	1.36%
	800	1.3m	1.34%
	1200	2.4m	**1.32%**



- Note: The scale mixture prior is a sparsity inducing prior of the form

$$p(\boldsymbol{w}) = \prod_j \pi \mathcal{N}(w_j|0,\sigma_1^2) + (1-\pi)\mathcal{N}(w_j|0,\sigma_2^2) \qquad (\sigma_1^2 \gg \sigma_2^2)$$

† "Weight Uncertainty in Neural Networks" (Blundell et al, 2015)

Bayesian Neural Networks: Summary

- Only scratched the surface. Many advanced variants exist
- Bayesian convolutional neural network[†] (CNN) for image data
- Since we get uncertainty in model and its predictions, can be extended to active learning[‡]
- Can also be extended to do semi-supervised learning when combined with deep generative models (we will look at DGMs)
- A lot of recent work on scalable Bayesian inference for Bayesian neural networks
  - Both MCMC and variational inference

[†] Bayesian convolutional neural networks with Bernoulli approximate variational inference (Gal and Ghahramani, 2016)
[‡] Deep Bayesian Active Learning with Image Data (Gal and Ghahramani, 2017)

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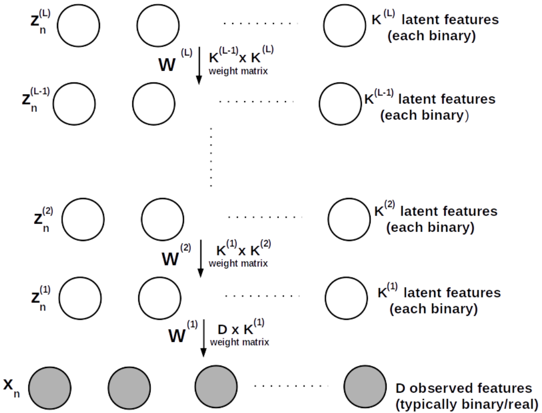
- Most of these models contain latent variable but some do not (some examples in next lecture)

Some Early Architectures: Sigmoid Belief Network (Neal 1992)

- Assumes data generated by successive nonlinear transformations of multiple layers of latent features



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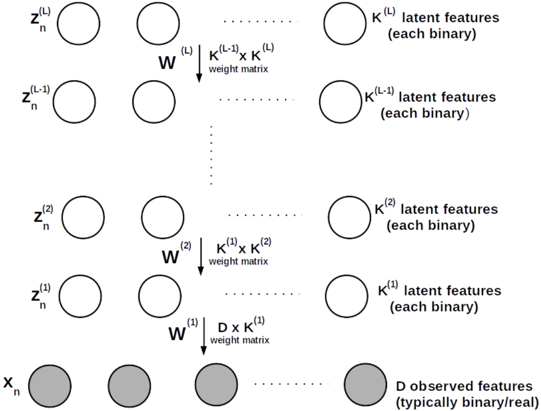
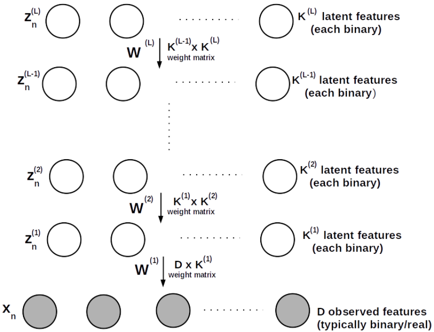


- in SBN, the latent features in each hidden layer are assumed to be binary-valued
- Unlike a Bayesian NN, this is a generative model for the data (which here are the only inputs $\boldsymbol{x}_n$'s)

Some Early Architectures: Sigmoid Belief Network (Neal 1992)

- The SBN generative model is

$$\begin{aligned} p(x_{nd} = 1|\boldsymbol{z}_n^{(1)}) &= \text{sigmoid}(\boldsymbol{w}_{d,:}^{(1)\top}\boldsymbol{z}_n^{(1)} + b_d) \qquad \text{(if features are binary)} \\ p(z_{nk}^{(1)} = 1|\boldsymbol{z}_n^{(2)}) &= \text{sigmoid}(\boldsymbol{w}_{k,:}^{(2)\top}\boldsymbol{z}_n^{(2)} + c_k) \end{aligned}$$



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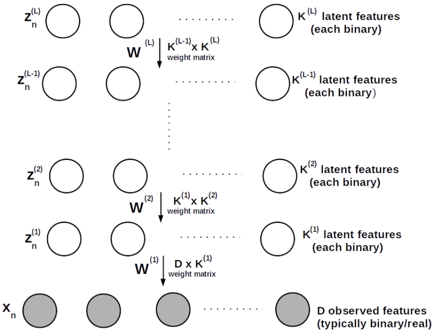

- Not a conjugate model. Inference using MCMC (Neal, 1992[†]; Gan et al, 2015[‡])

[†] Connectionist learning of belief networks (Neal, 1992)

[‡] Learning Deep Sigmoid Belief Networks with Data Augmentation (Gan et al, 2015)

Another Architecture: Latent Gaussian Models

- Observed data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$, with $\boldsymbol{x}_n \in \mathbb{R}^D$
- Assume each observation $\boldsymbol{x}_n$ to be generated by a Gaussian latent variable $\boldsymbol{z}_n \in \mathbb{R}^K$ as follows

$$p(\boldsymbol{z}_n) = \mathcal{N}(\boldsymbol{z}_n | 0, \mathbf{I}_K)$$

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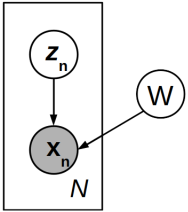

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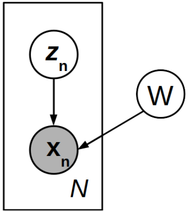

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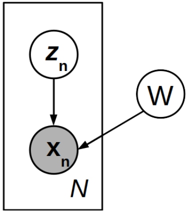

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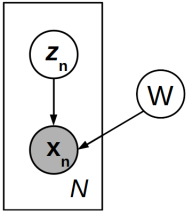

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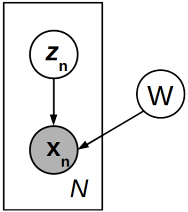

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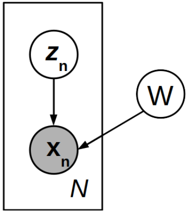

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Nonlinear Latent Gaussian Models

- Let's assume $\boldsymbol{z}_n$ goes through a nonlinear transformation f before it generates $\boldsymbol{x}_n$

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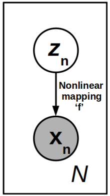

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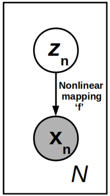

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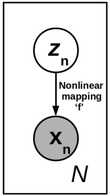

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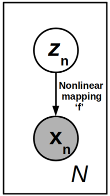

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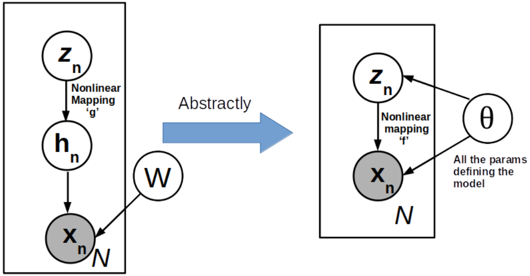

$$\begin{aligned}
\boldsymbol{z}_n &\sim \mathcal{N}(\boldsymbol{z}_n|0, \mathbf{I}_K) \\
\boldsymbol{h}_n &= g(\boldsymbol{z}_n) \quad \text{(deterministic nonlinear mapping)} \\
\boldsymbol{x}_n &\sim \text{ExpFam}(\boldsymbol{x}_n|\mathbf{W}\boldsymbol{h}_n) \\
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\end{aligned}$$

Inference for Deep Latent Gaussian Models

- Assume a prior $p_\theta(\boldsymbol{z})$ and likelihood $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ for this DLGM
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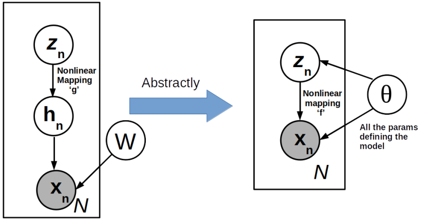

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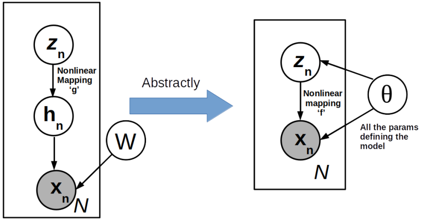

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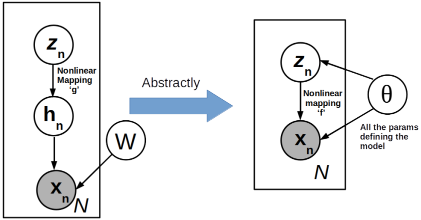

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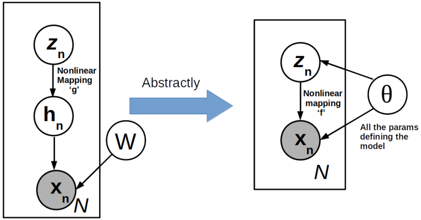

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- Given N observations $\mathbf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, the goal will be to infer $\mathbf{Z} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N\}$ and θ. In general, this will be an intractable problem (just like other Bayesian models).

Inference for Deep Latent Gaussian Models

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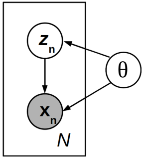

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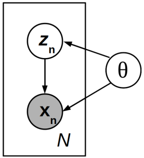

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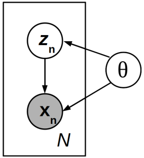

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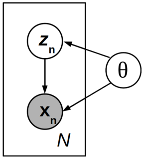

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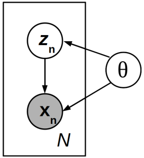

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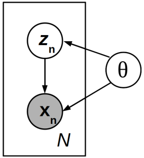

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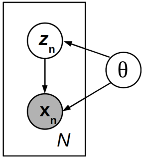

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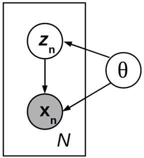

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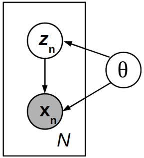

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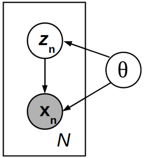

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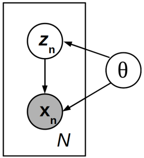

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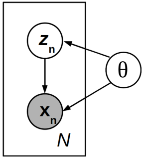

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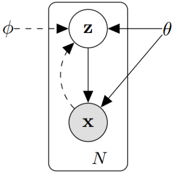

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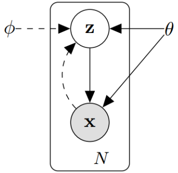

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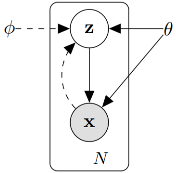

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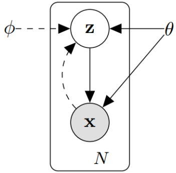

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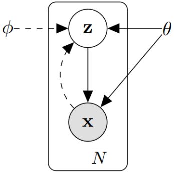

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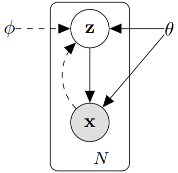

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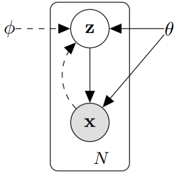

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