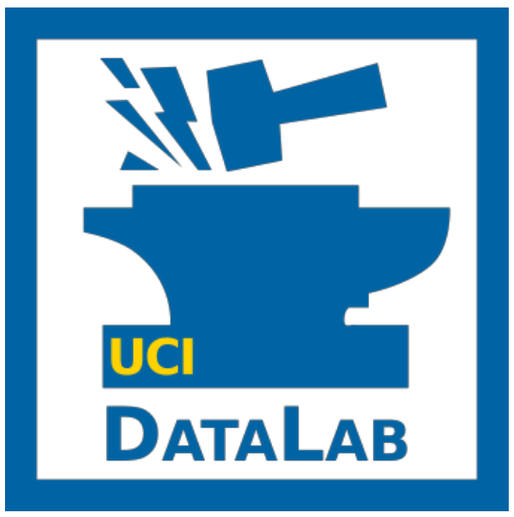
On Priors for Bayesian Neural Networks

Eric Nalisnick

PhD Defense
University of California, Irvine



First-Author Publications and Preprints

WORKING PAPERS / PREPRINTS

E. Nalisnick, D. Tran, D. Blei, and P. Smyth. ***Deep Learning: A Synthesis from Probabilistic Foundations.*** 2018.

E. Nalisnick and P. Smyth. ***Averaging and Combining Variational Models with Stein Particle Descent.*** 2018.

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PRE-UCI

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Outline

1 **Motivation**

2 **Bayesian Neural Networks and Their Priors**

3 **Approximating Objective Priors**

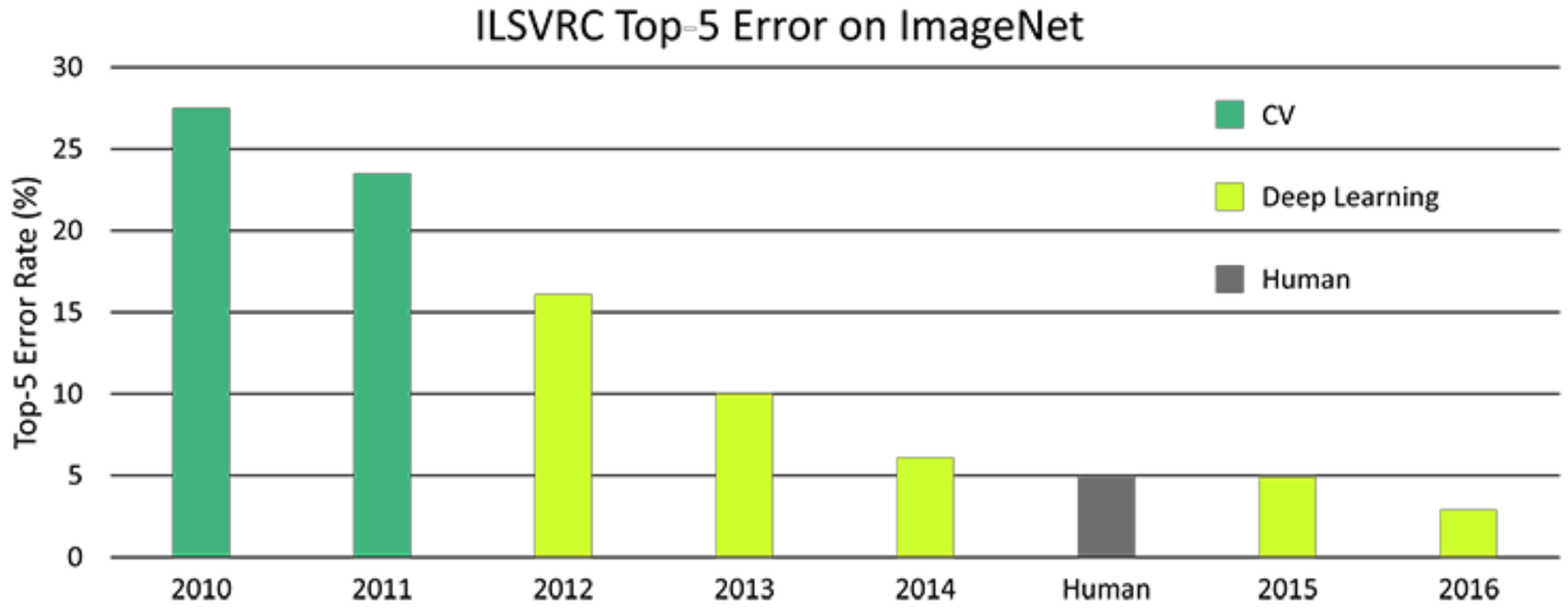
4 **Nonparametric Density Networks**

5 **Future Directions and Conclusions**

Motivation for Bayesian Deep Learning

Deep Learning Results

Computer Vision: Results on ImageNet object classification dataset.



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Deep Learning Results

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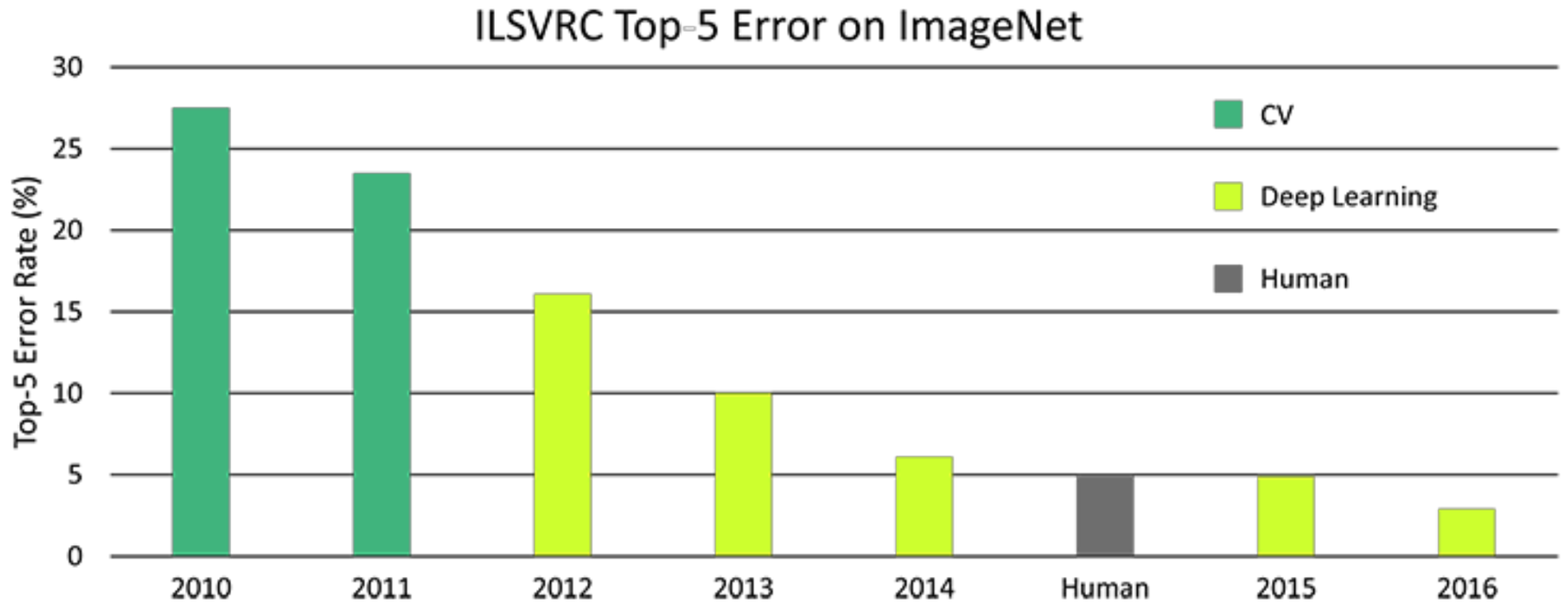

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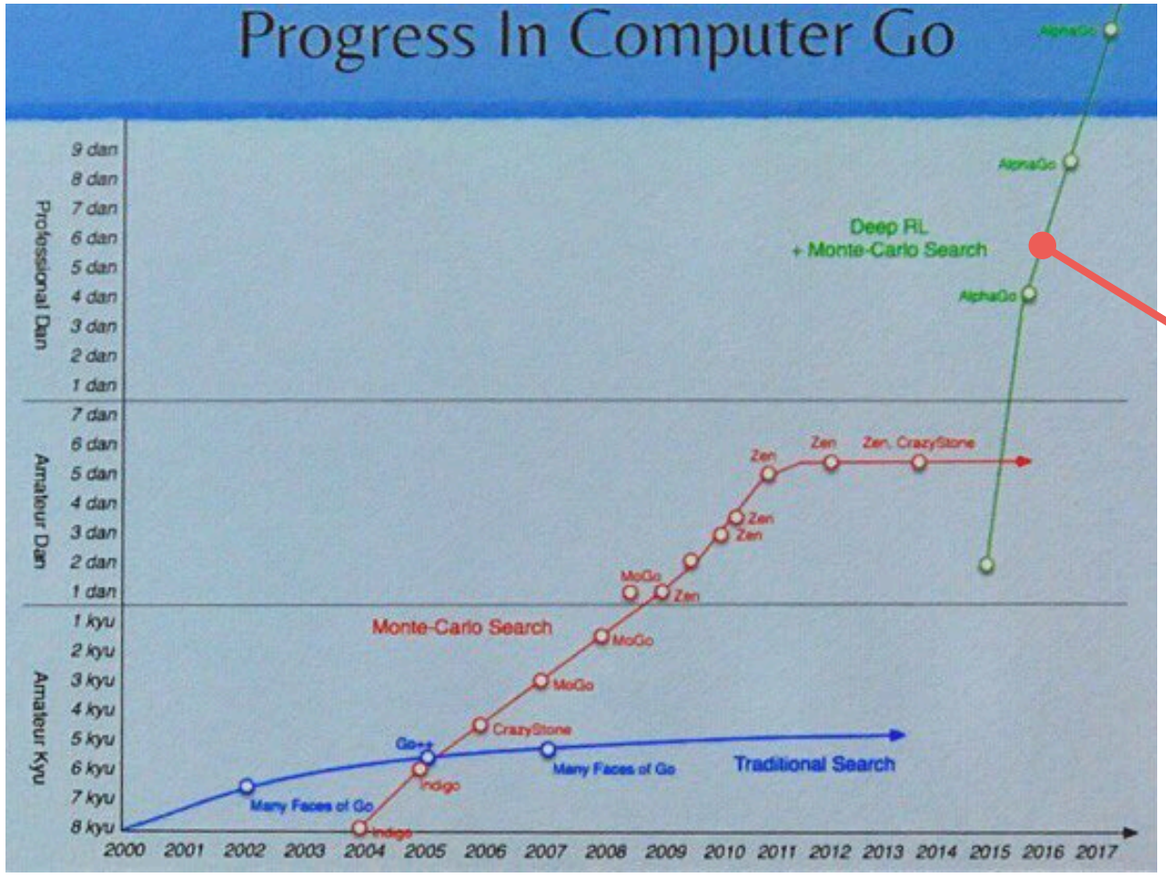
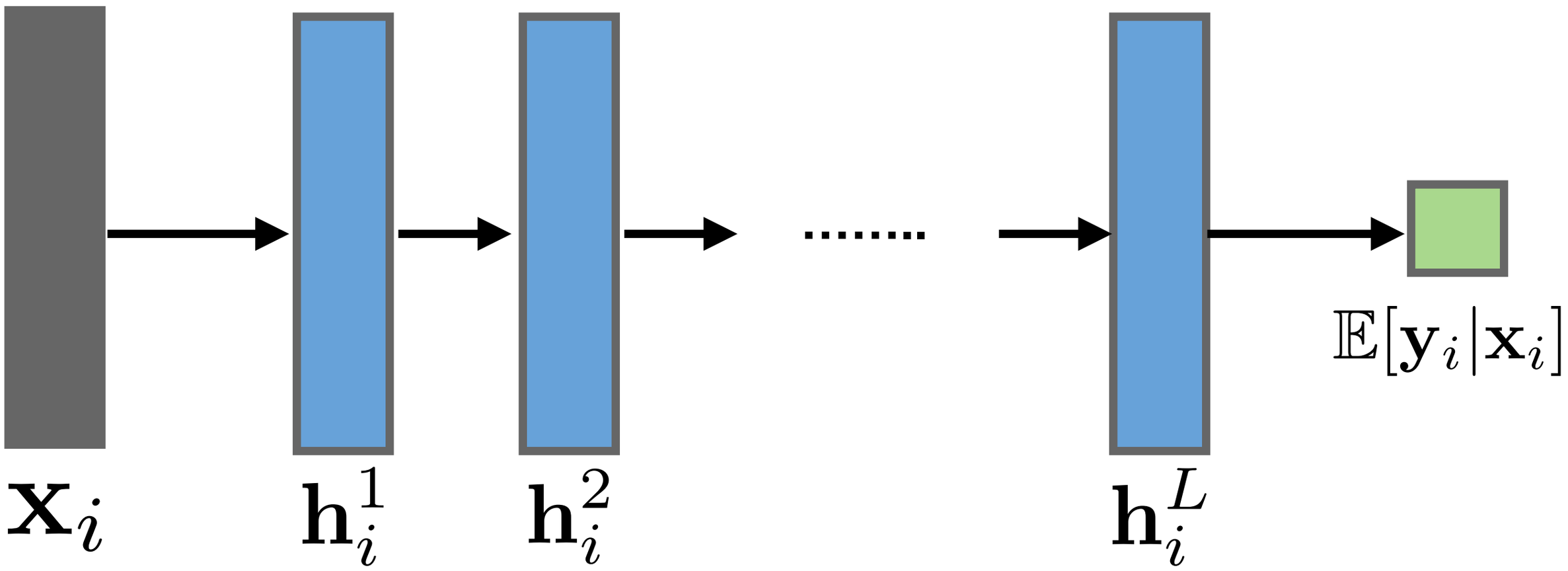


Reinforcement Learning: Results in playing Go.

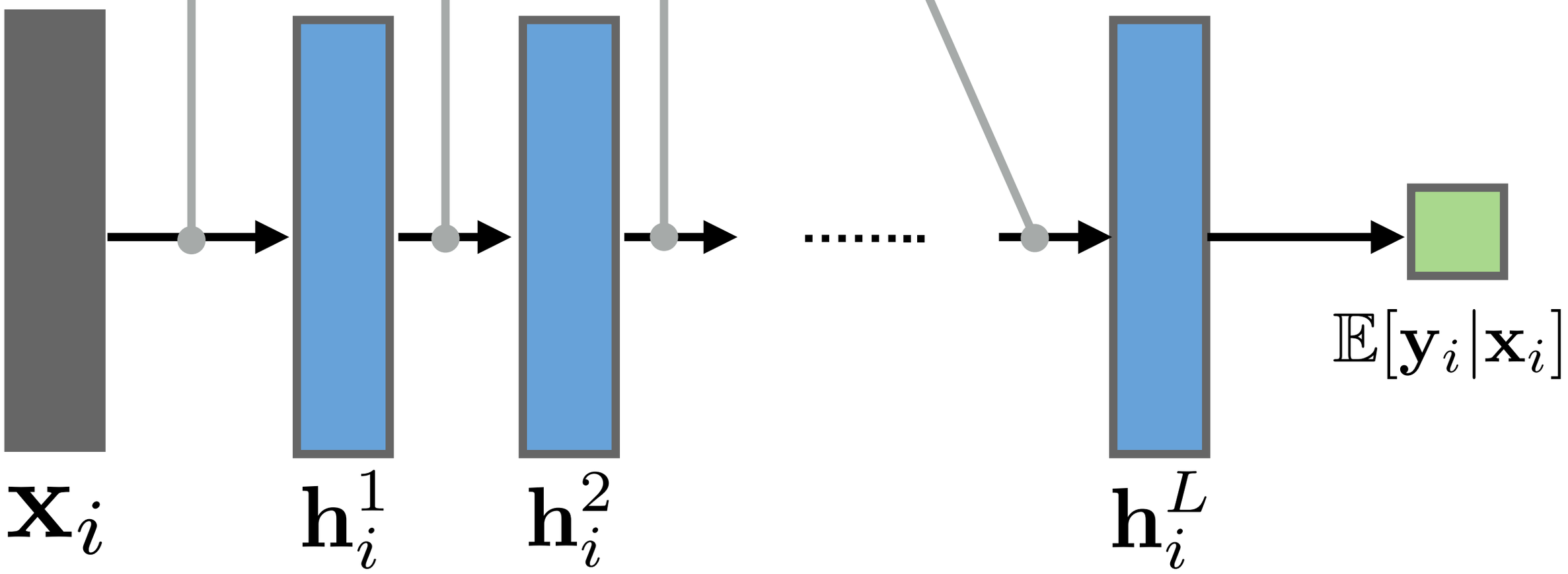
DEEP NEURAL NETWORKS

Neural Networks



Neural Networks

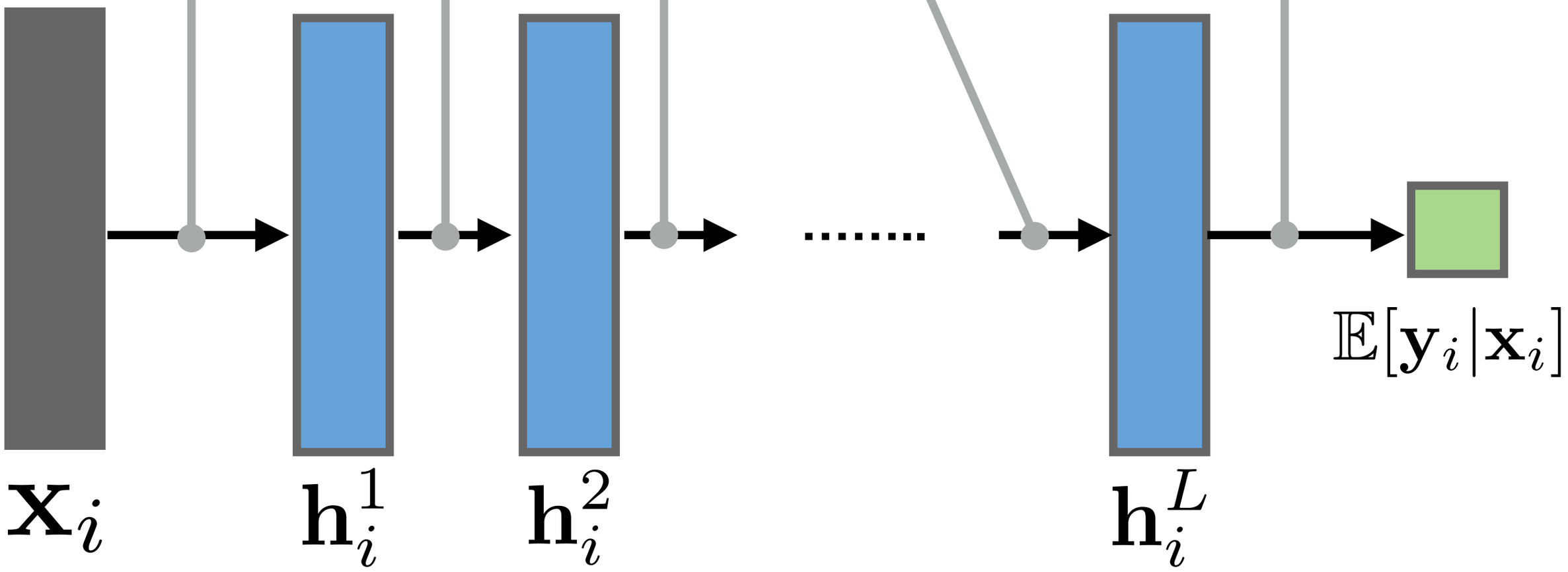
$$\mathbf{h}_i^l = f_l(\mathbf{h}_i^{l-1}\mathbf{W}_l + \mathbf{b}_l), \quad \mathbf{h}_i^0 = \mathbf{x}_i$$



Neural Networks

$$\mathbf{h}_i^l = f_l(\mathbf{h}_i^{l-1}\mathbf{W}_l + \mathbf{b}_l), \quad \mathbf{h}_i^0 = \mathbf{x}_i$$

$$\mathbb{E}[y_i|\mathbf{x}_i] = g^{-1}(\mathbf{h}_i^L \mathbf{w}_{L+1} + b_{L+1})$$



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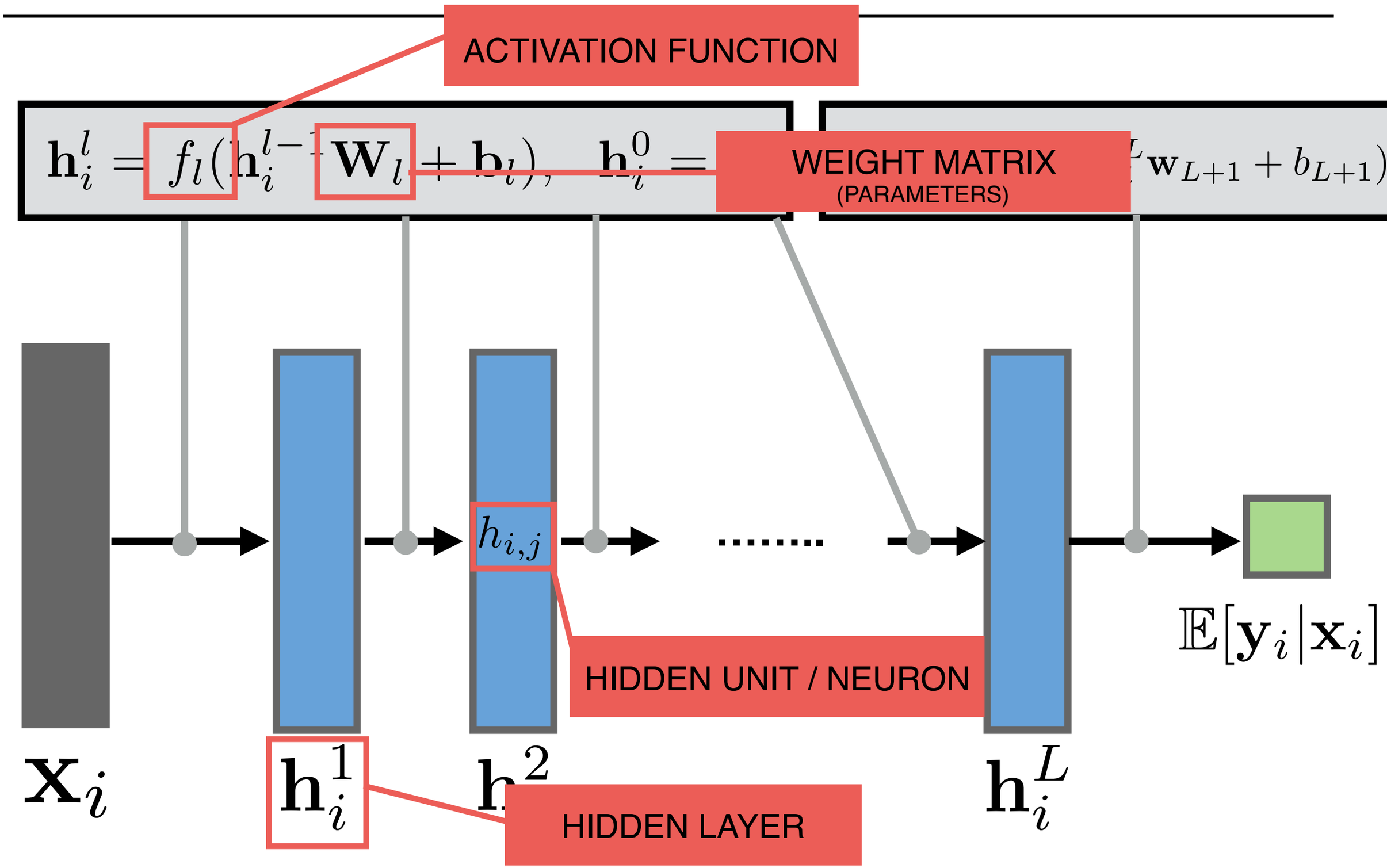

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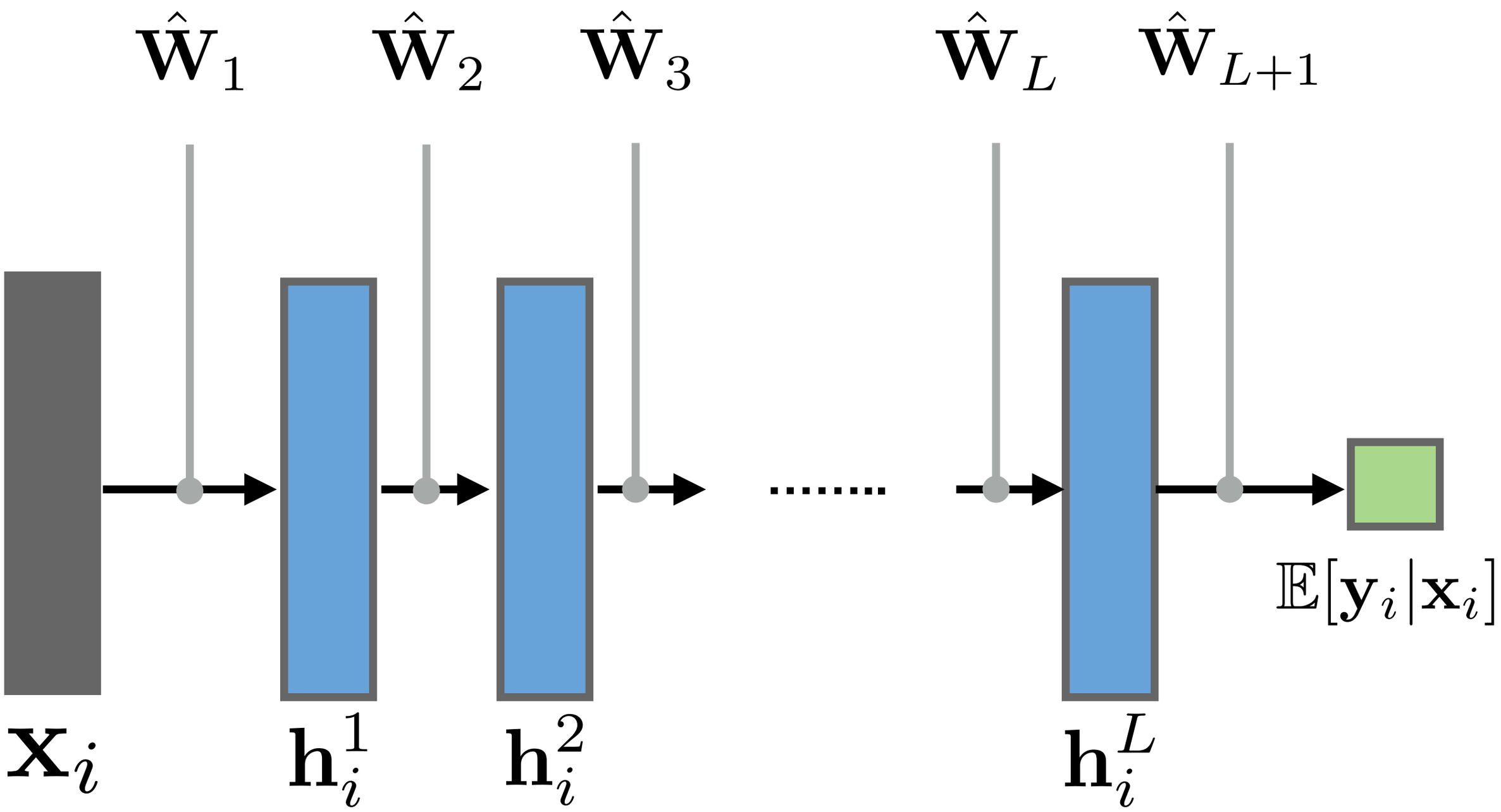

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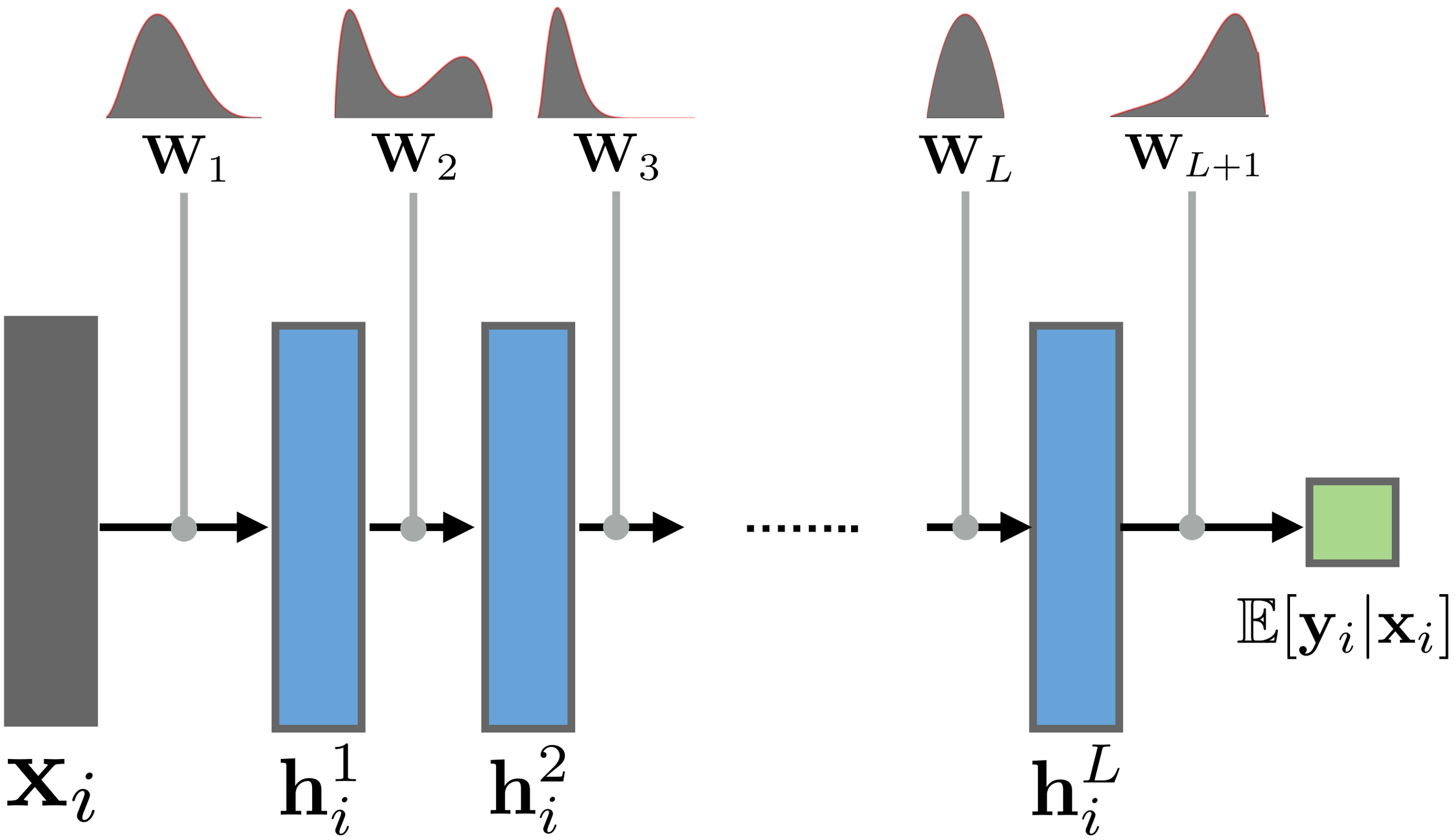
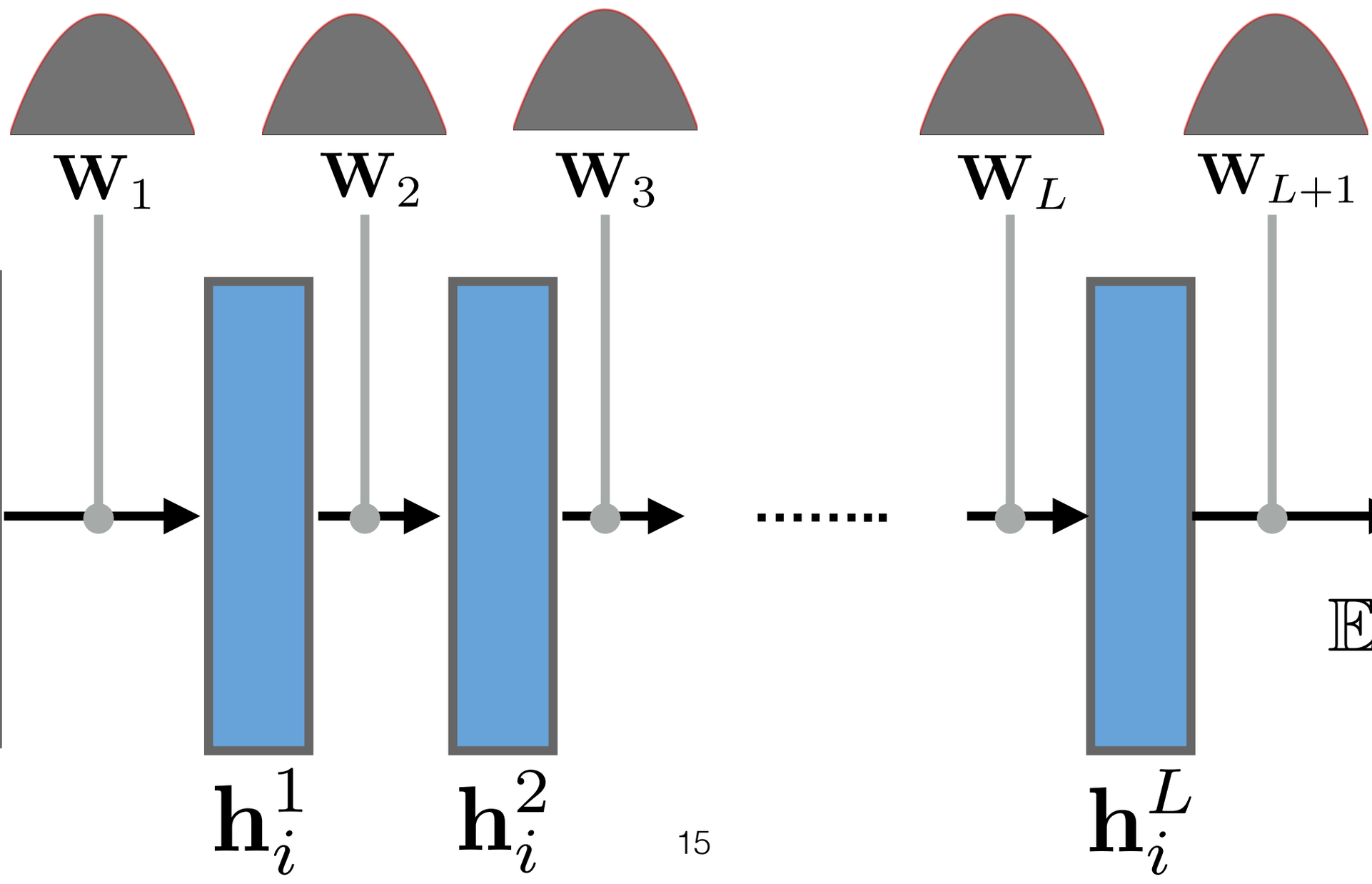


Bayesian Neural Networks

STEP #1: $p(\{\mathbf{W}_l\}_{l=1}^{L+1}) = \prod_{l=1}^{L+1} p(\mathbf{W}_l)$

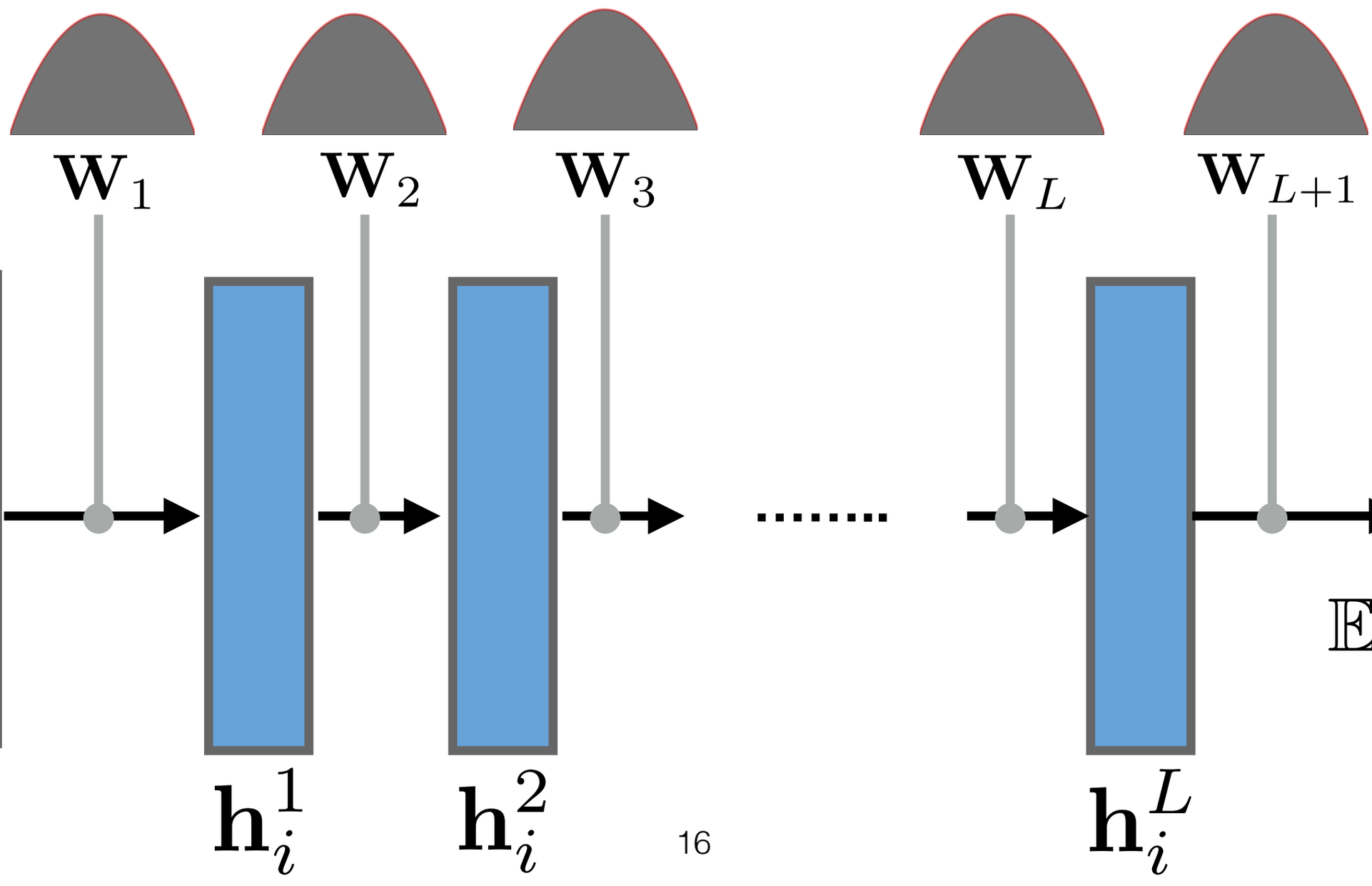
PRIOR



Bayesian Neural Networks

STEP #2: $p(\mathbf{y}|\mathbf{X}, \{\mathbf{W}_l\}_{l=1}^{L+1}) \prod_{l=1}^{L+1} p(\mathbf{W}_l)$

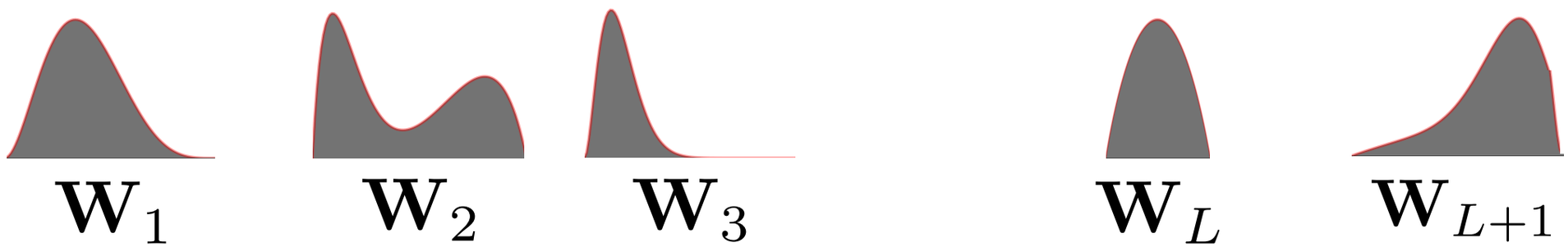
LIKELIHOOD

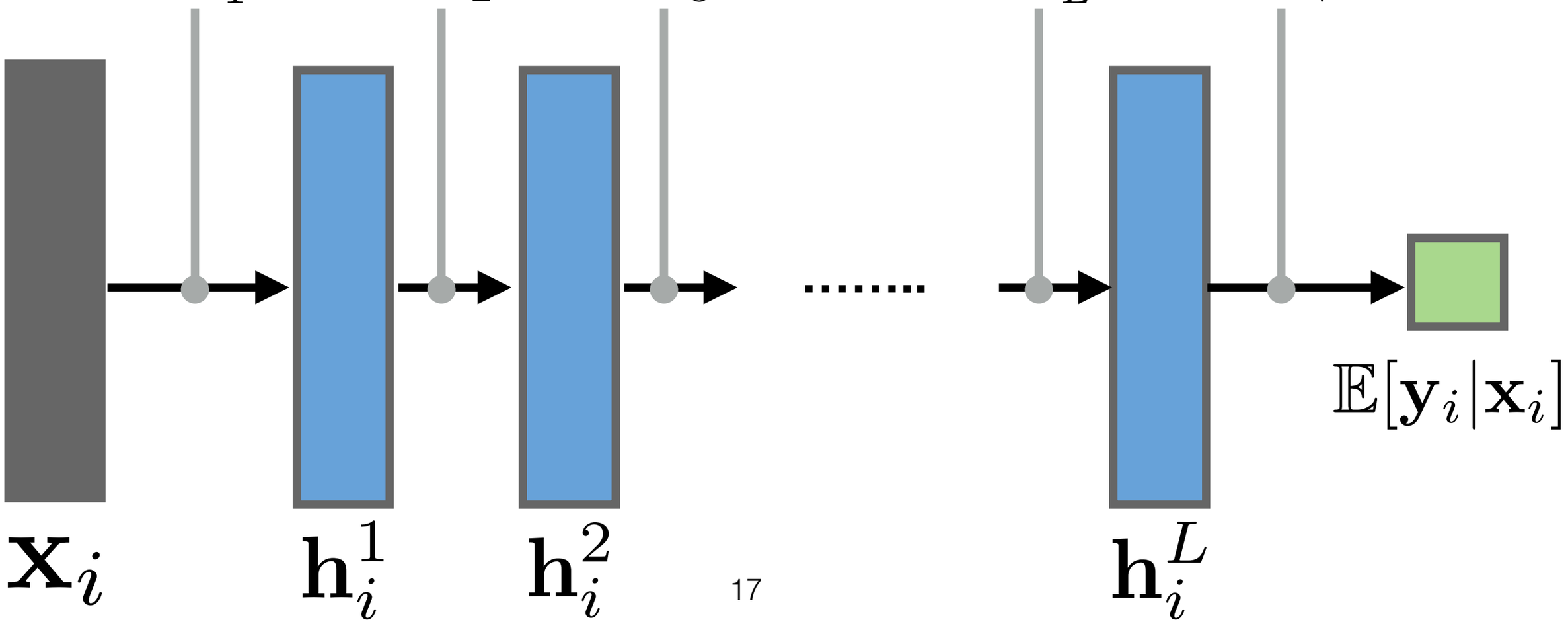


Bayesian Neural Networks

STEP #3: $p(\{\mathbf{W}_l\}_{l=1}^{L+1}|\mathbf{y},\mathbf{X})$

POSTERIOR





Benefits of Bayesian Neural Networks

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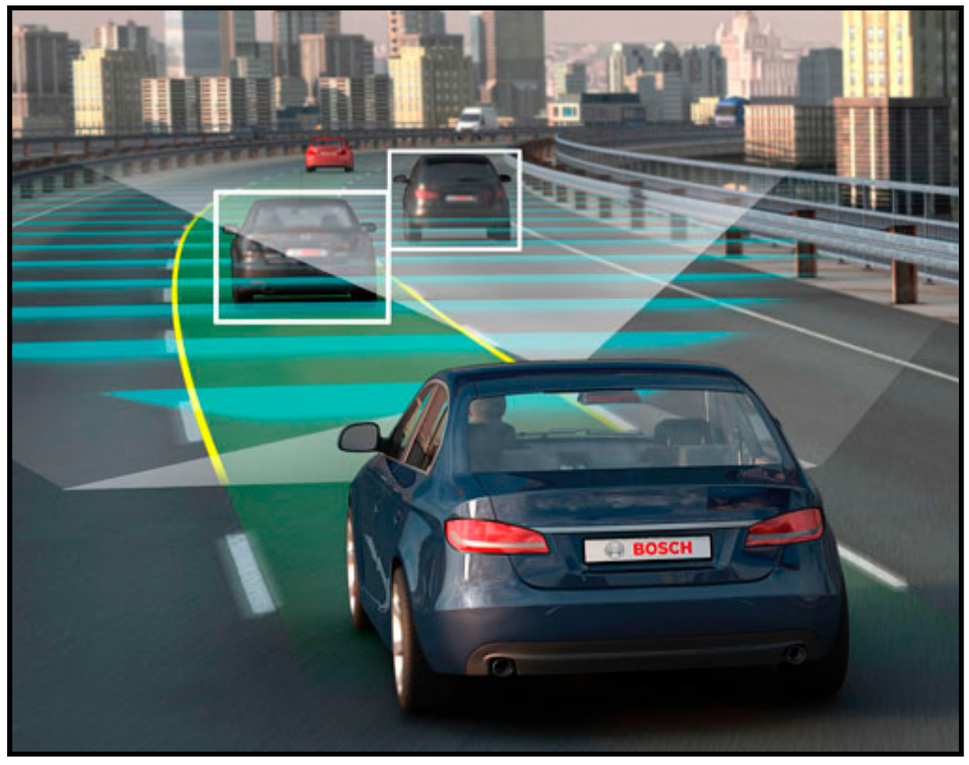
Model Uncertainty for Safe Automation.



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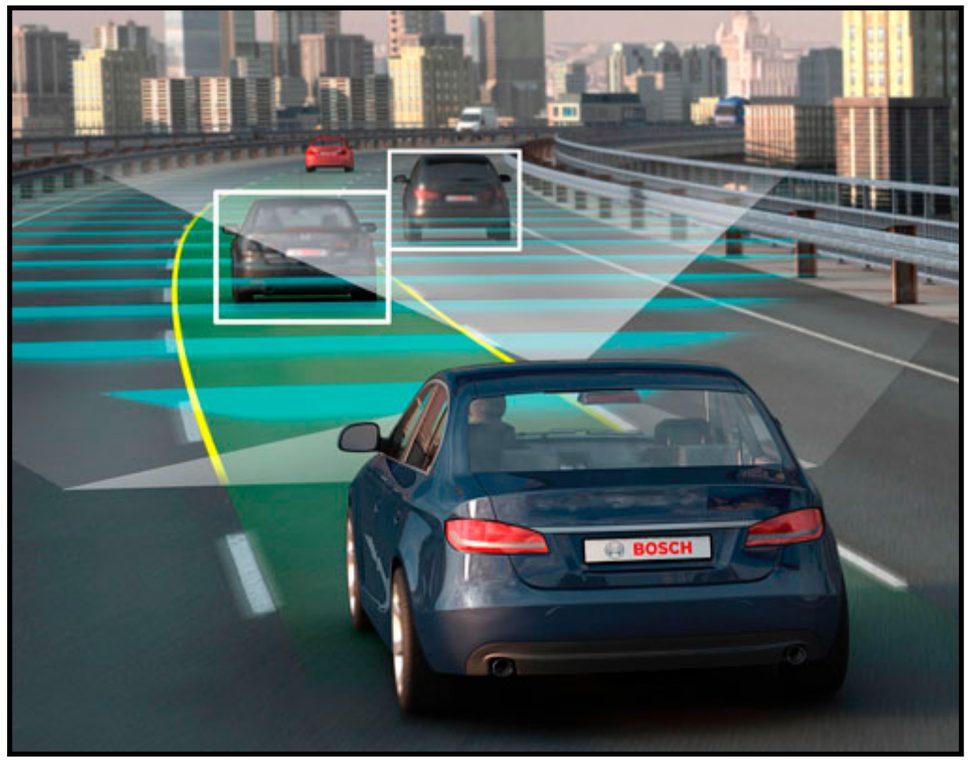

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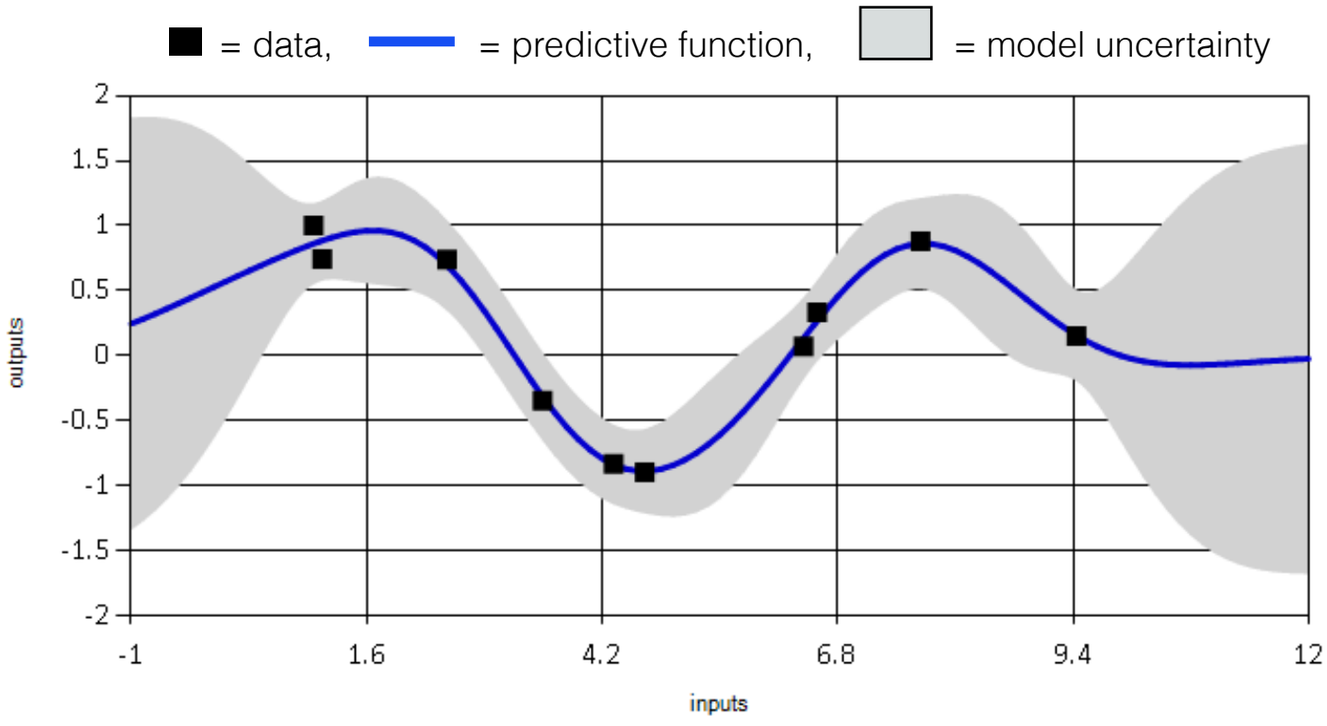

Posterior Predictive Distribution

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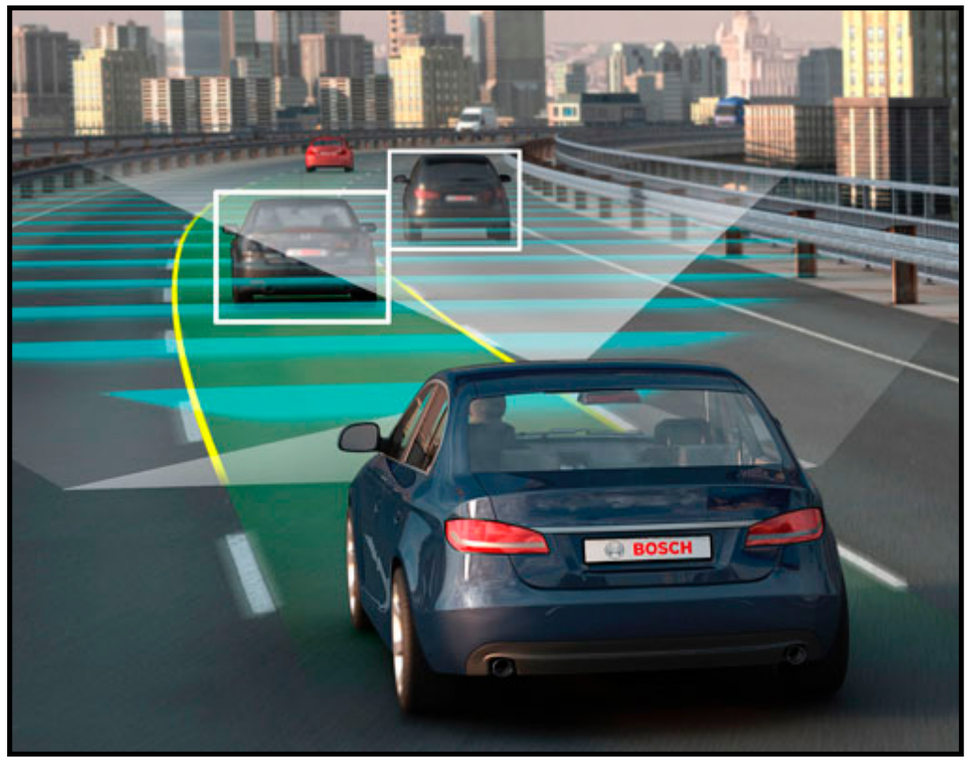

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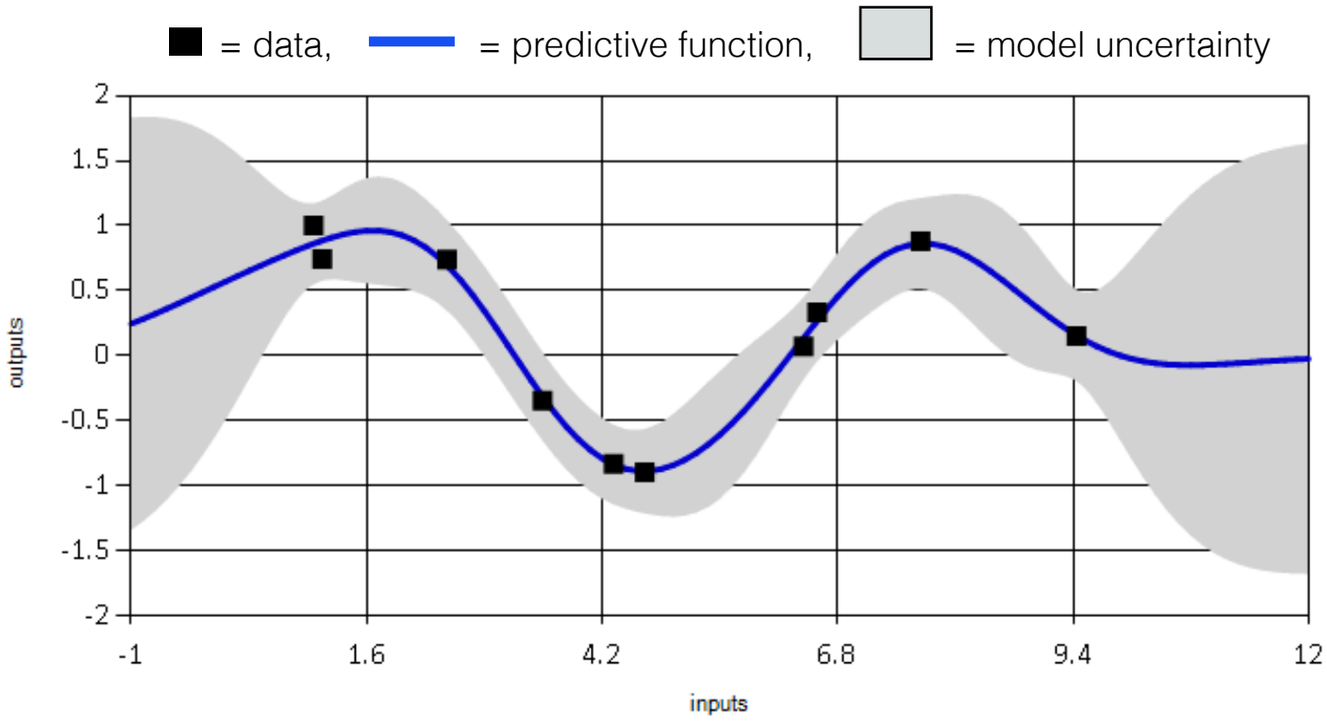

Posterior Predictive Distribution

$$p(y^*|\mathbf{x}^*, \mathbf{y}, \mathbf{X}) = \int_{\mathbf{W}} p(y^*|\mathbf{x}^*, \mathbf{W}) p(\mathbf{W}|\mathbf{y}, \mathbf{X}) \, d\mathbf{W}$$

LIKELIHOOD OF NEW DATA

POSTERIOR FOR TRAINING DATA

Benefits of Bayesian Neural Networks

Coherent Framework for Online / Sequential Learning.

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BAYESIAN UPDATING

$$p\left(\mathbf{W}|\{\mathbf{y}_t, \mathbf{y}_{t+1}\}, \{\mathbf{X}_t, \mathbf{X}_{t+1}\}\right)$$

$$\propto p(\mathbf{y}_{t+1}|\mathbf{X}_{t+1}, \mathbf{W}) p(\mathbf{W}|\mathbf{y}_t, \mathbf{X}_t)$$

LIKELIHOOD OF NEW DATA

POSTERIOR
SERVES AS PRIOR

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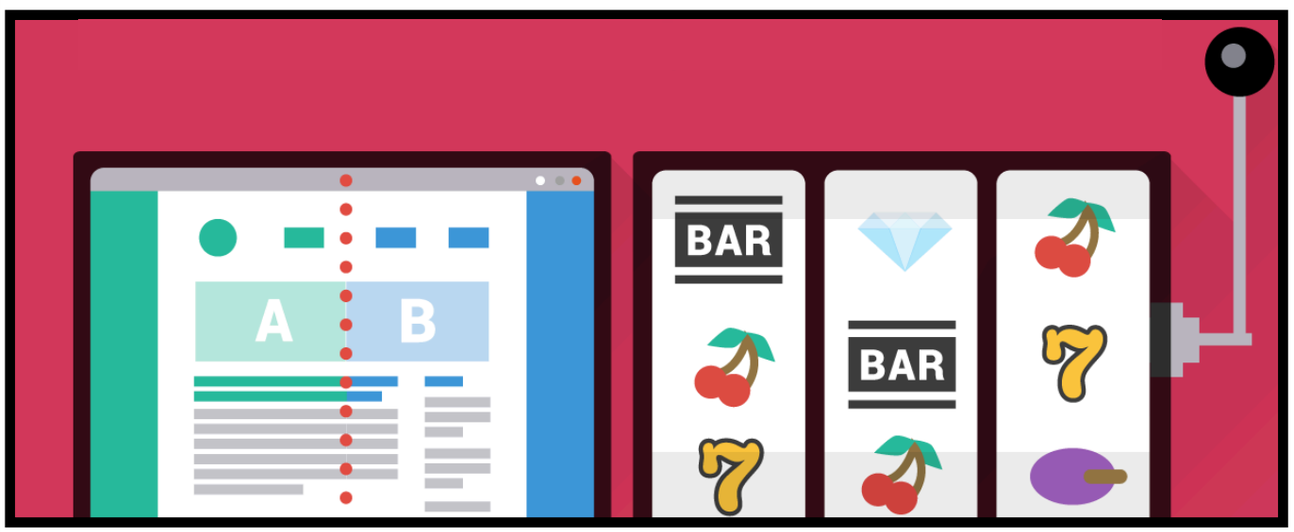
LIKELIHOOD OF NEW DATA

POSTERIOR SERVES AS PRIOR

THOMPSON SAMPLING FOR EXPLORE/EXPLOIT

$$\underset{\text{action}}{\text{argmax}} \; \mathbb{E}[\text{reward}_{T+1}|\text{action}_{T+1}, \hat{\mathbf{W}}]$$

$$\hat{\mathbf{W}} \sim p(\mathbf{W}|\{(\text{reward}_t, \text{action}_t)\}_{t=0}^{T})$$



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Benefits of Bayesian Neural Networks

Regularization and Model Selection to Ease NN's Data Hunger.

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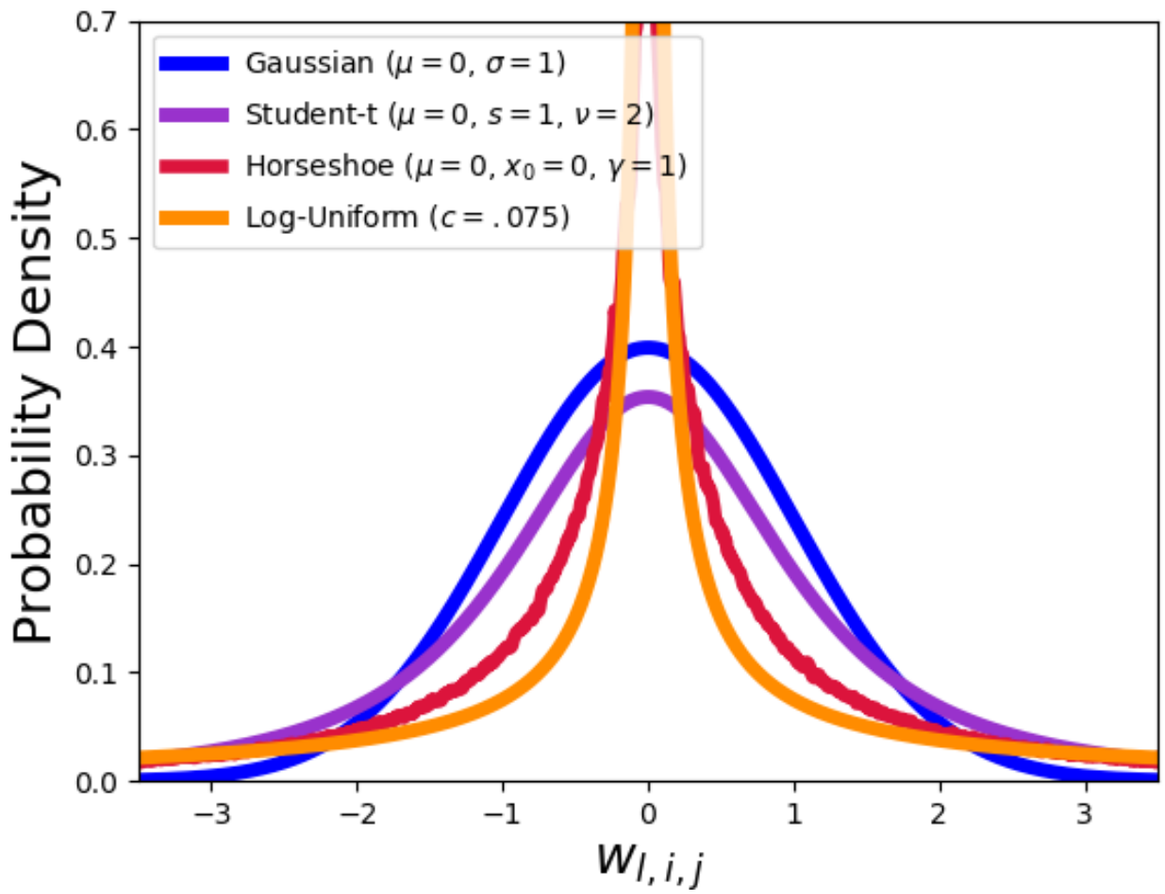
SPARSITY-INDUCING PRIORS



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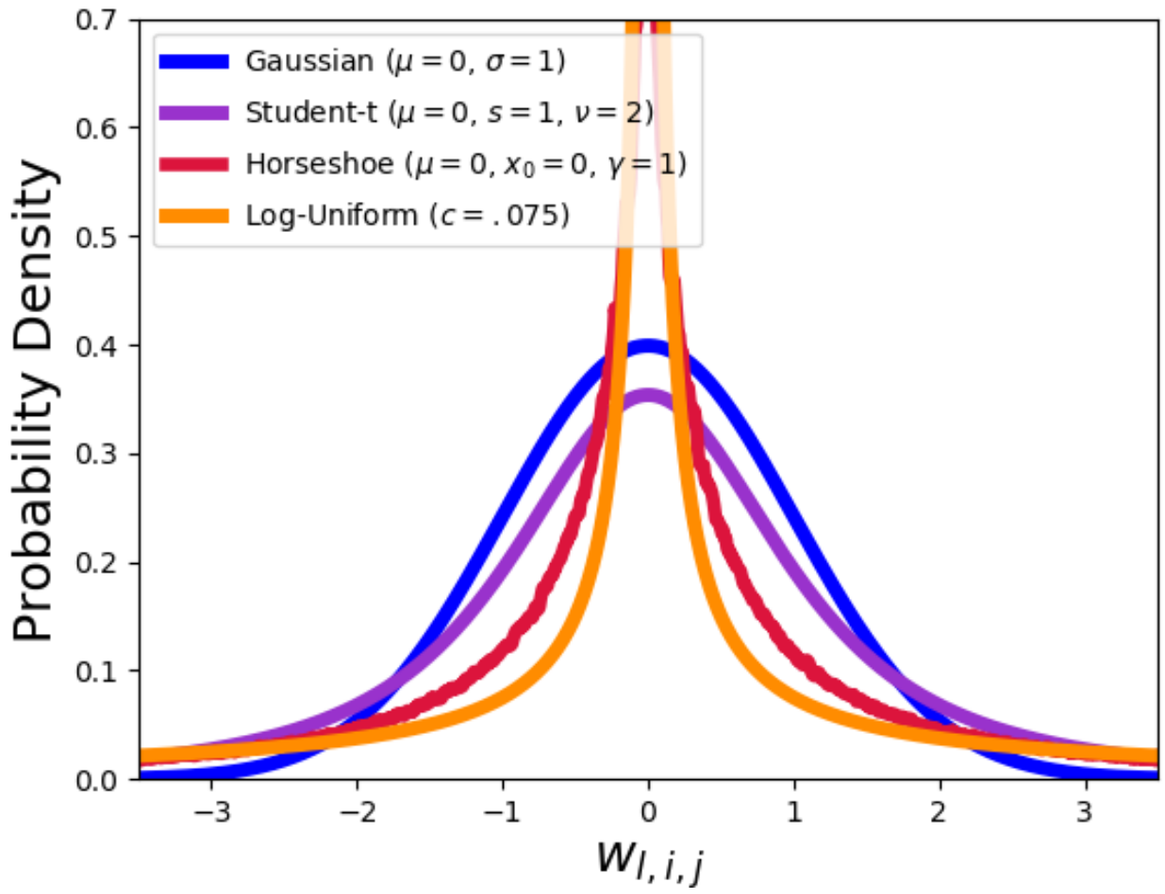
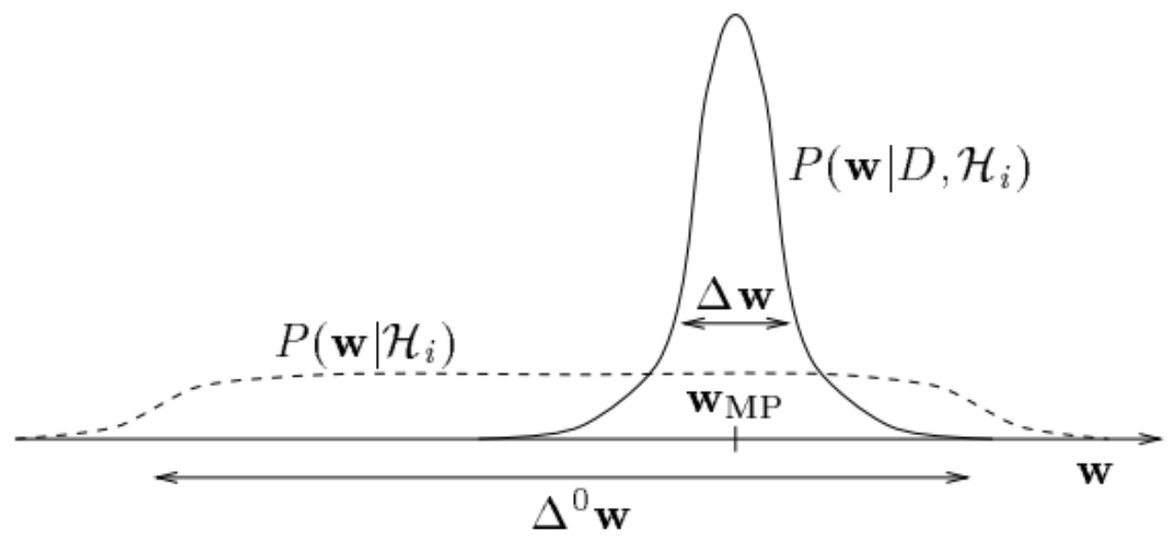


BAYESIAN EVIDENCE FRAMEWORK

$$P(D|\mathcal{H}_i) \simeq \underbrace{P(D|\mathbf{w}_{\mathrm{MP}}, \mathcal{H}_i)}_{\text{Best fit likelihood}} \underbrace{P(\mathbf{w}_{\mathrm{MP}}|\mathcal{H}_i)\,\Delta\mathbf{w}}_{\text{Occam factor}}$$

$$\text{Evidence} \simeq \text{Best fit likelihood} \quad \text{Occam factor}$$



[MacKay, 1991]

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- **Computational and Memory Cost:** Obtaining distributions instead of point estimates is intrinsically more costly.
  - **Computation**: A fully Bayesian treatment requires solving high-dimensional integration problems, which are especially intractable to neural networks.
  - **Memory**: Even coarse posterior approximations (e.g. fully-factorized Gaussian) usually require at least 2x the number of parameters.

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- [ ] **Computational and Memory Cost:** Obtaining distributions instead of point estimates is intrinsically more costly.

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  - ↳ **Aggressive Factorization**: For the sake of tractability, need to factorize the posterior across layers (and usually further).

$$p(\{\mathbf{W}_l\}_{l=1}^{L+1}|\mathbf{y},\mathbf{X}) \approx \prod_{l=1}^{L+1} q(\mathbf{W}_l)$$

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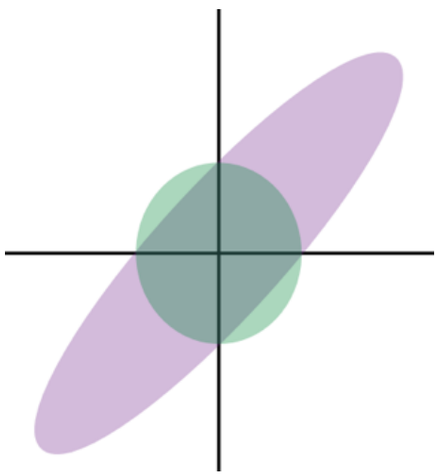
$$\approx \prod_{l=1}^{L+1}\prod_{j=1}^{R_l}\prod_{k=1}^{C_l} q(w_{l,j,k})$$



Exact Posterior

Mean-field Approximation [Blei et al., 2017]

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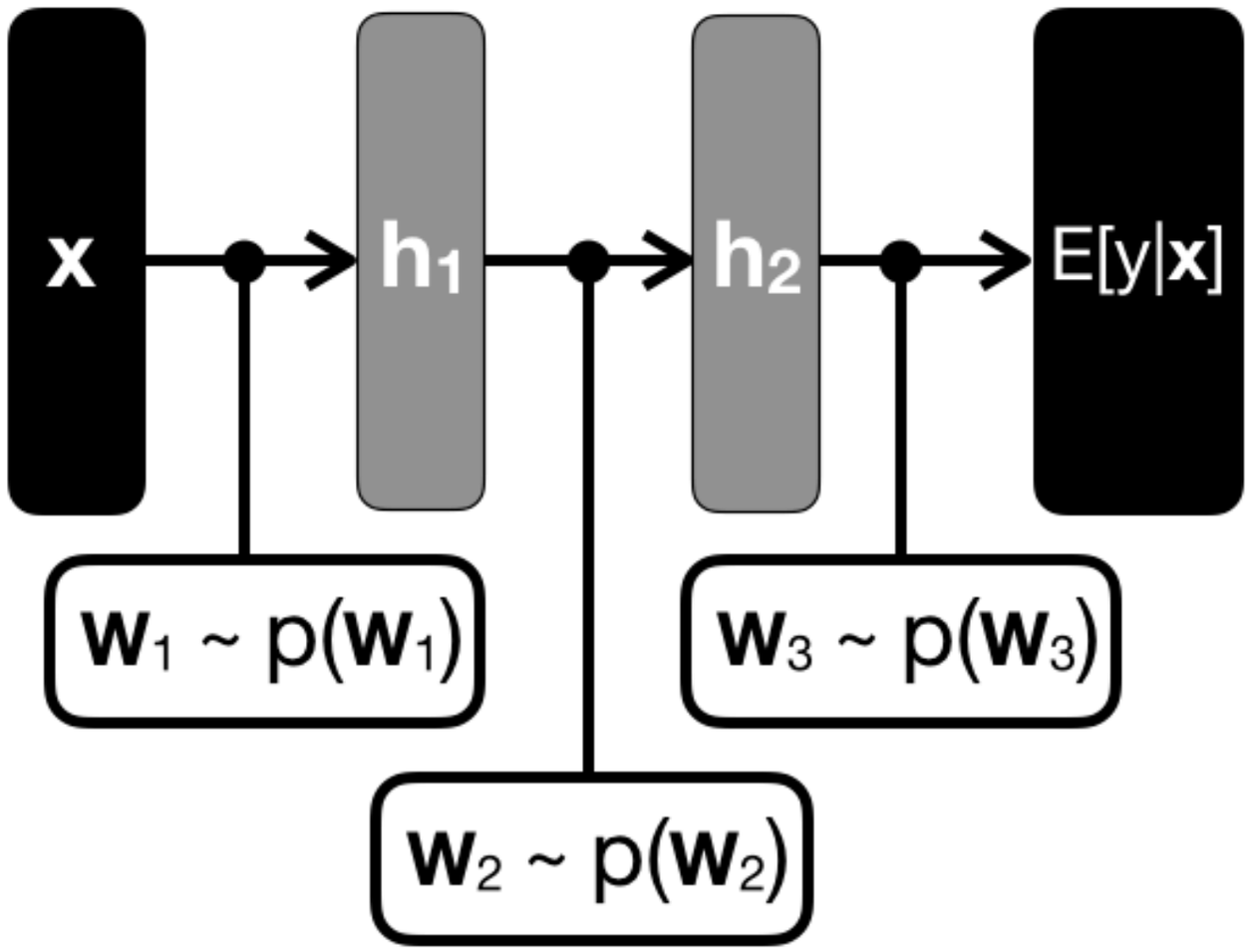
Bayesian Neural Networks and Their Priors

Bayesian Neural Networks

CONDITIONAL MODEL (SUPERVISED)

[Buntine & Weigend, 1991; MacKay, 1991; Seung et al., 1991]



Bayesian Neural Networks

CONDITIONAL MODEL (SUPERVISED)

[Buntine & Weigend, 1991; MacKay, 1991; Seung et al., 1991]

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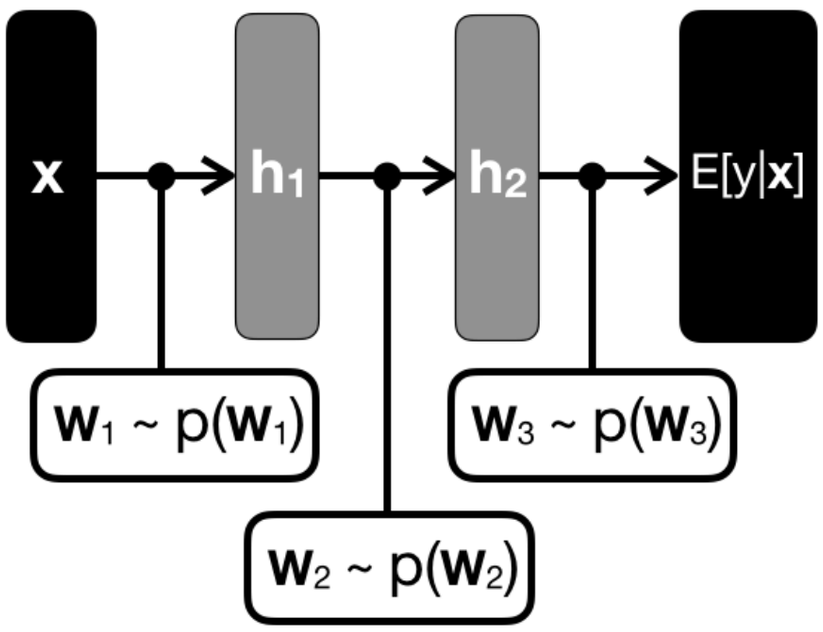

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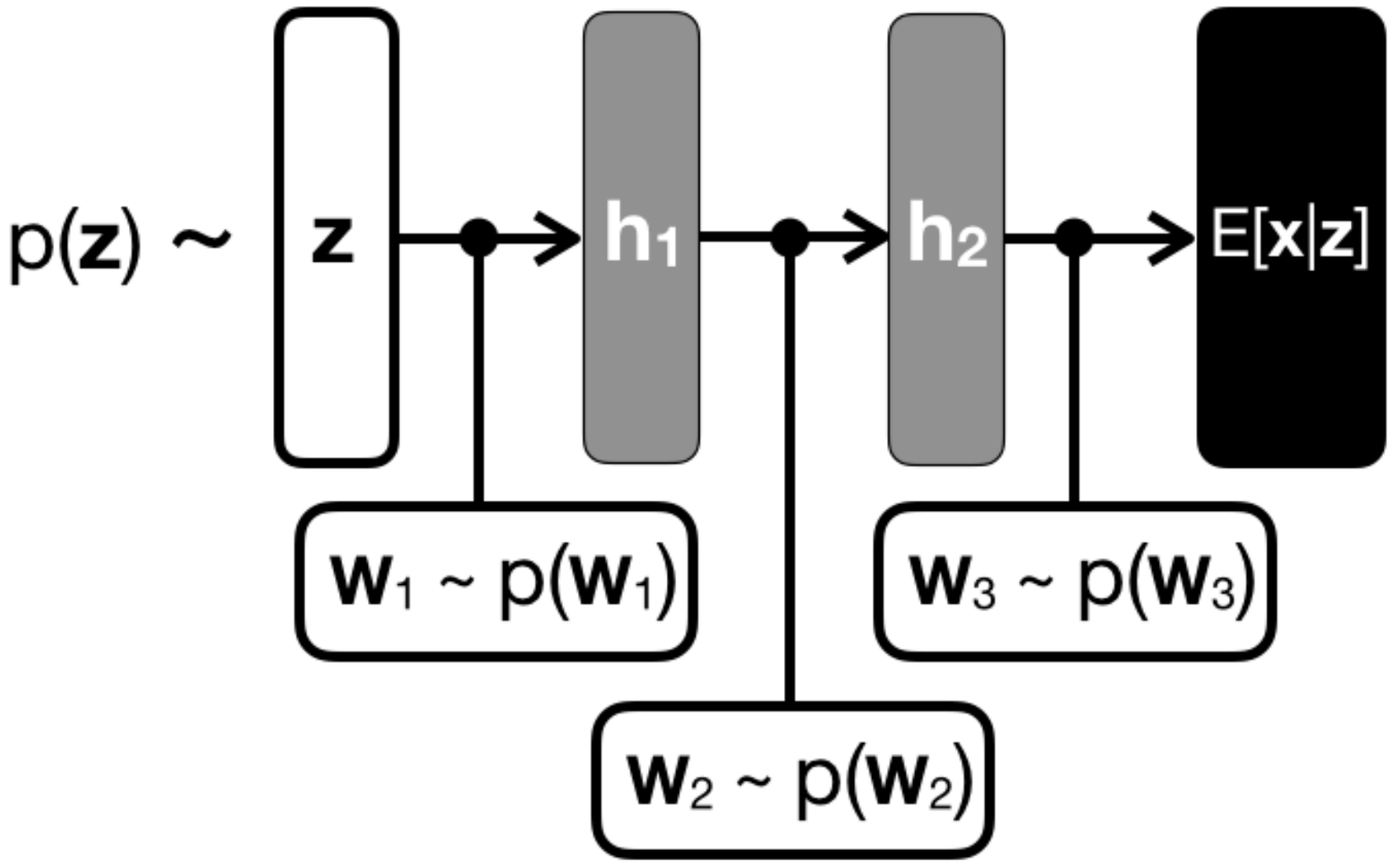
Bayesian Neural Networks

DENSITY NETWORK (UNSUPERVISED)

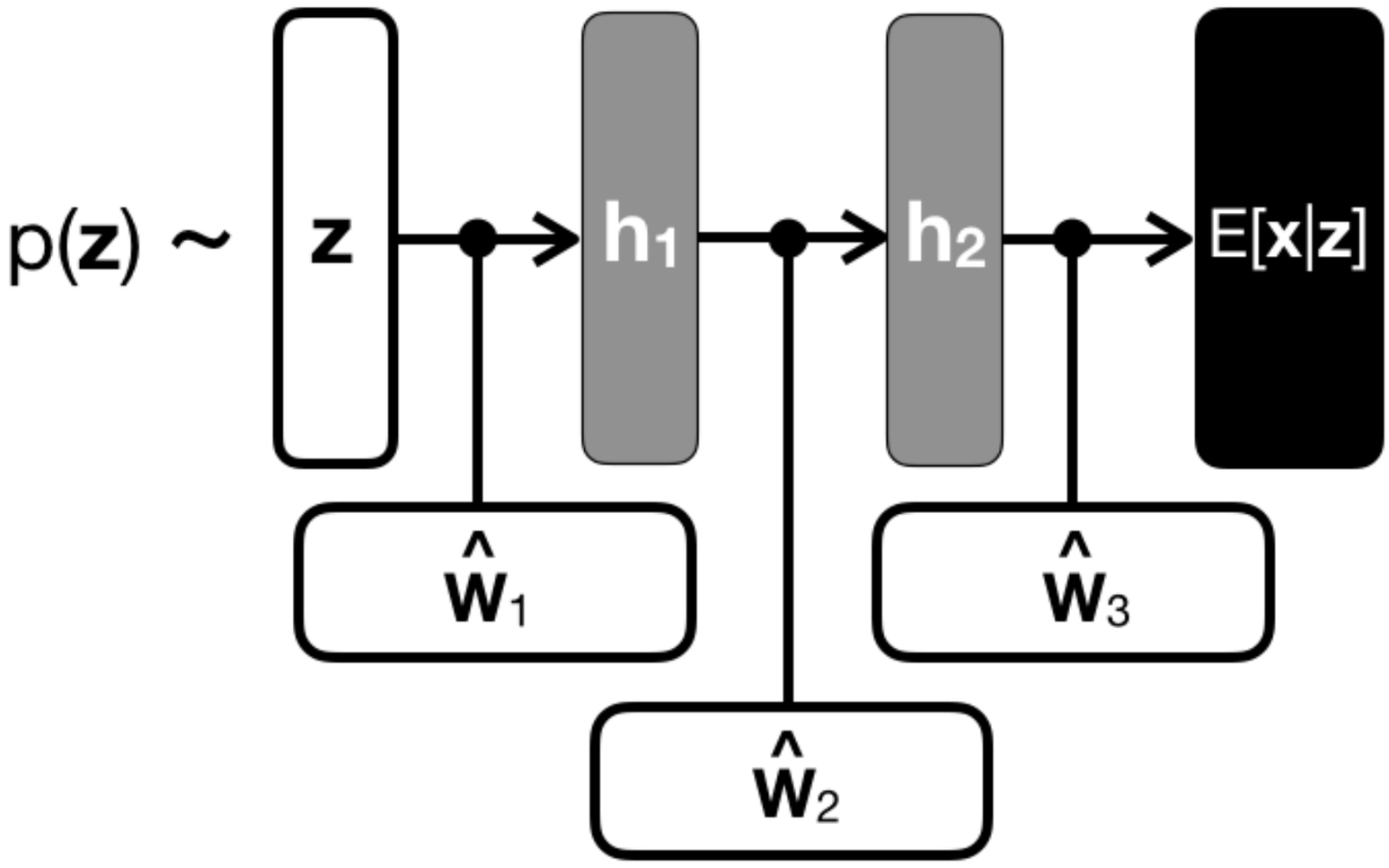
[Amemiya, 1993; MacKay, 1999]



Bayesian Neural Networks

DENSITY NETWORK (UNSUPERVISED)

[Amemiya, 1993; MacKay, 1999]



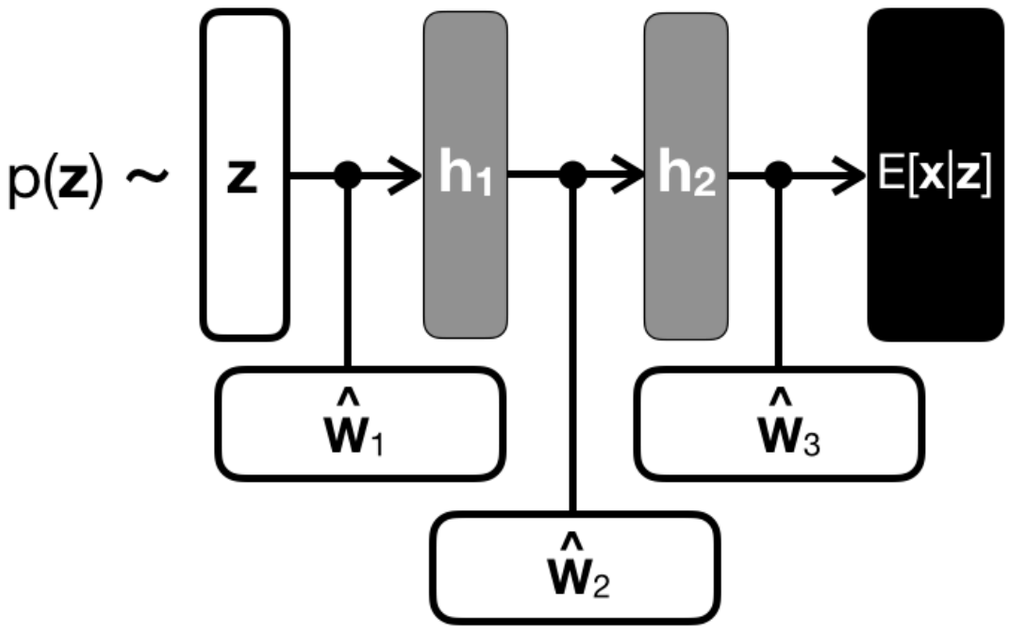
Bayesian Neural Networks

DENSITY NETWORK (UNSUPERVISED)

[Amemiya, 1993; MacKay, 1999]

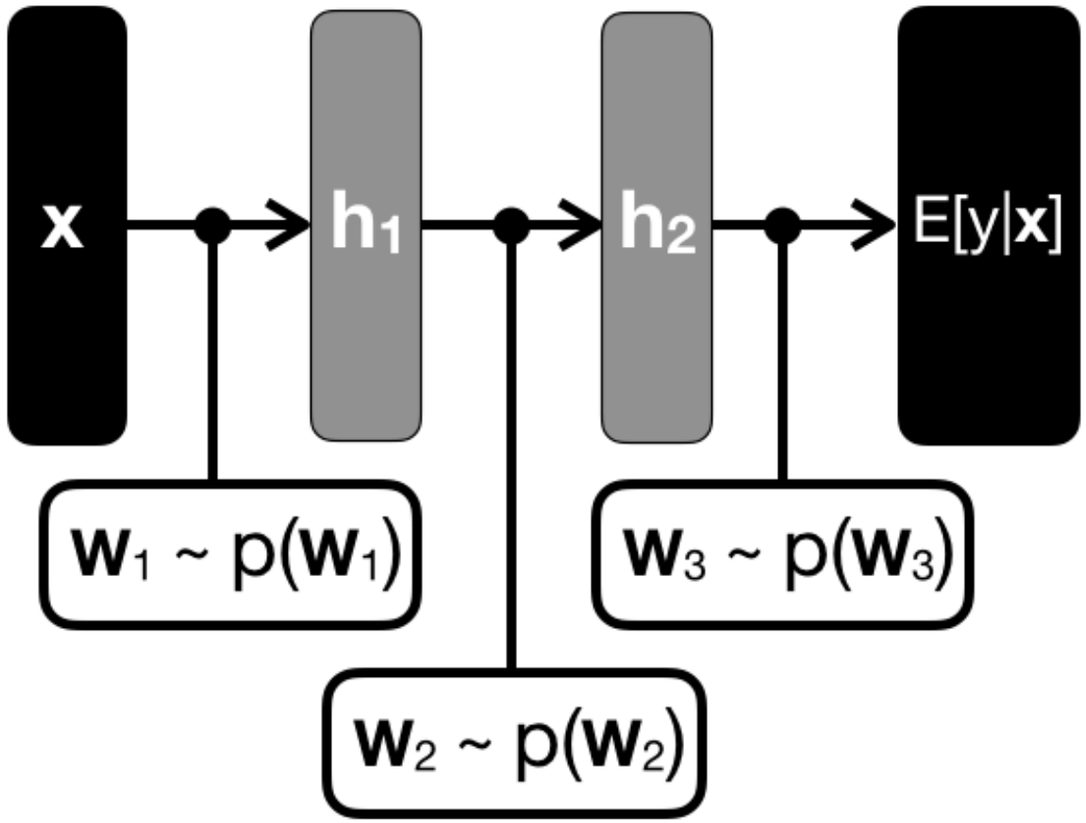
$$p(\{\mathbf{z}_i\}_{i=1}^N|\mathbf{X};\{\mathbf{W}_l\}_{l=1}^{L+1}) = \frac{\prod_{i=1}^N p(\mathbf{x}_i|\mathbf{z}_i;\{\mathbf{W}_l\}_{l=1}^{L+1})p(\mathbf{z}_i)}{p(\mathbf{X};\{\mathbf{W}_l\}_{l=1}^{L+1})}$$

$$p(\mathbf{X};\{\mathbf{W}_l\}_{l=1}^{L+1}) = \prod_{i=1}^N \int_{\mathbf{z}_i} p(\mathbf{x}_i|\mathbf{z}_i;\{\mathbf{W}_l\}_{l=1}^{L+1})p(\mathbf{z}_i)\ d\mathbf{z}_i$$



Bayesian Neural Networks

CONDITIONAL MODEL



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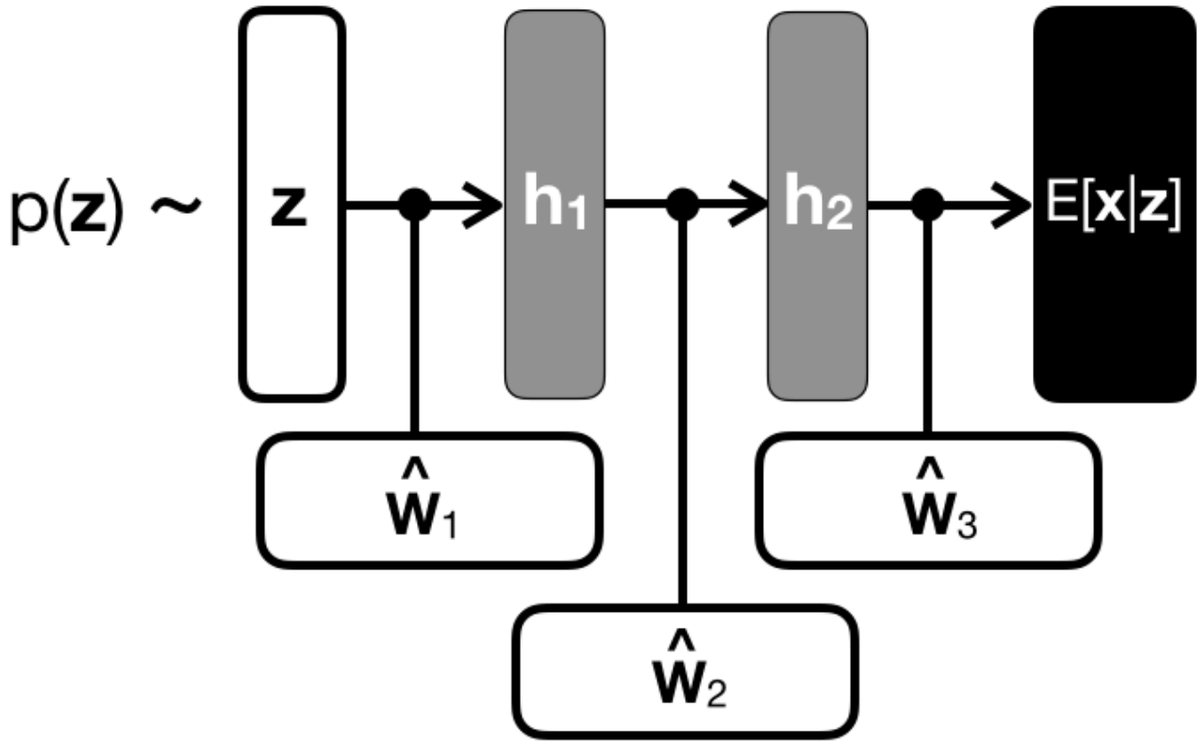

Bayesian Neural Networks

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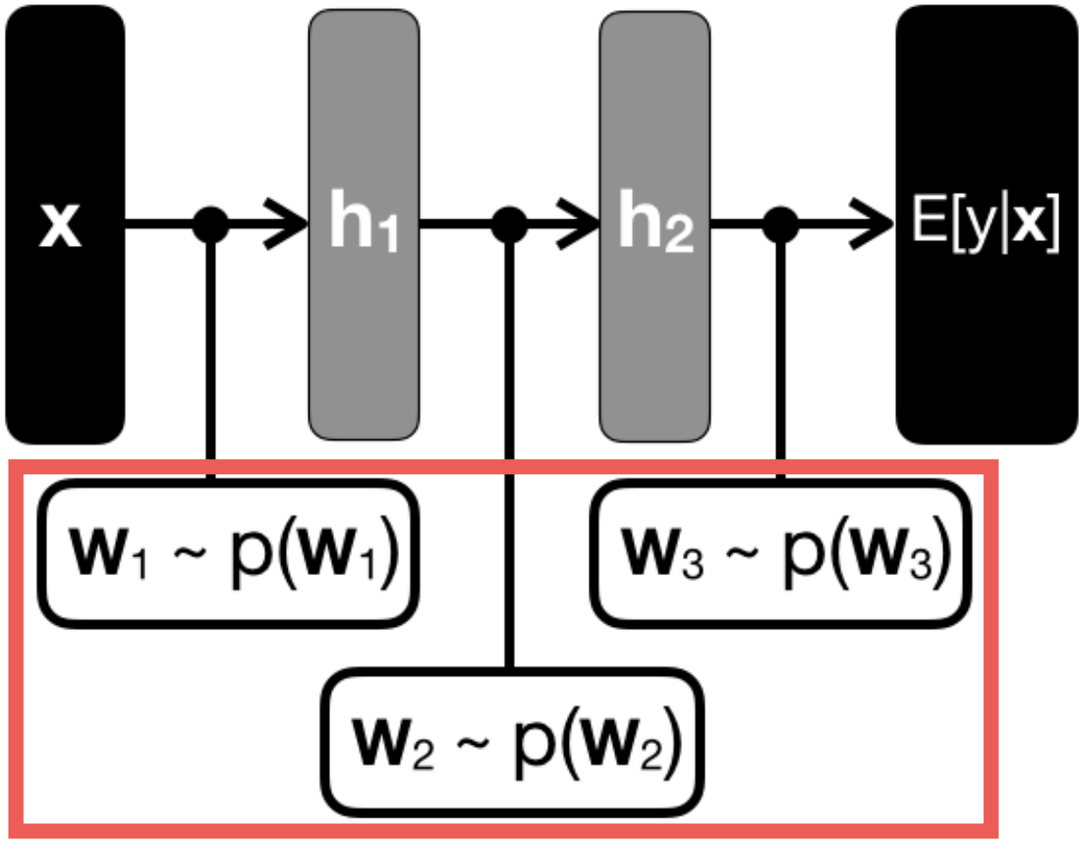

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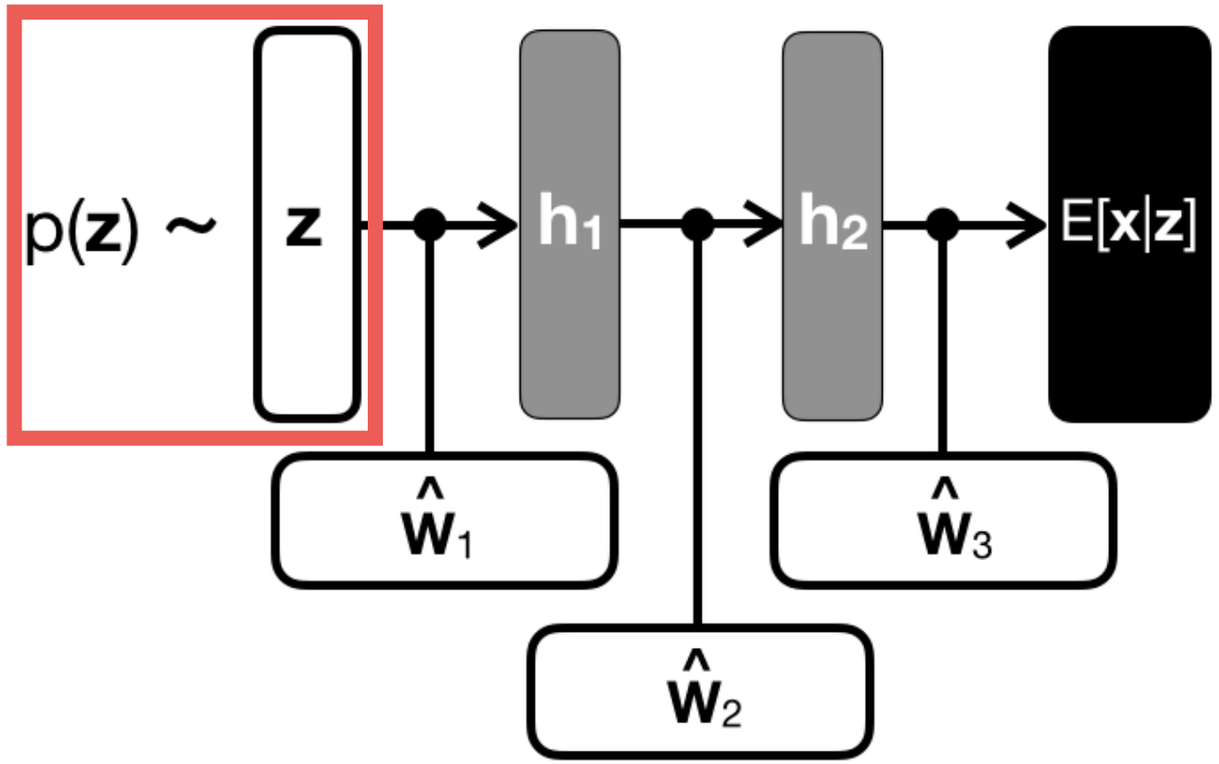


Priors for Neural Networks

A SPECTRUM OF PRIORS

NONPARAMETRIC

Infinite dimensional priors that give the model adaptive capacity. Examples: Dirichlet process, Indian Buffet process.

INDUCTIVE BIAS

Priors that give the model some inductive bias that improves performance. Example: sparsity.

OBJECTIVE

SUBJECTIVE

OBJECTIVE

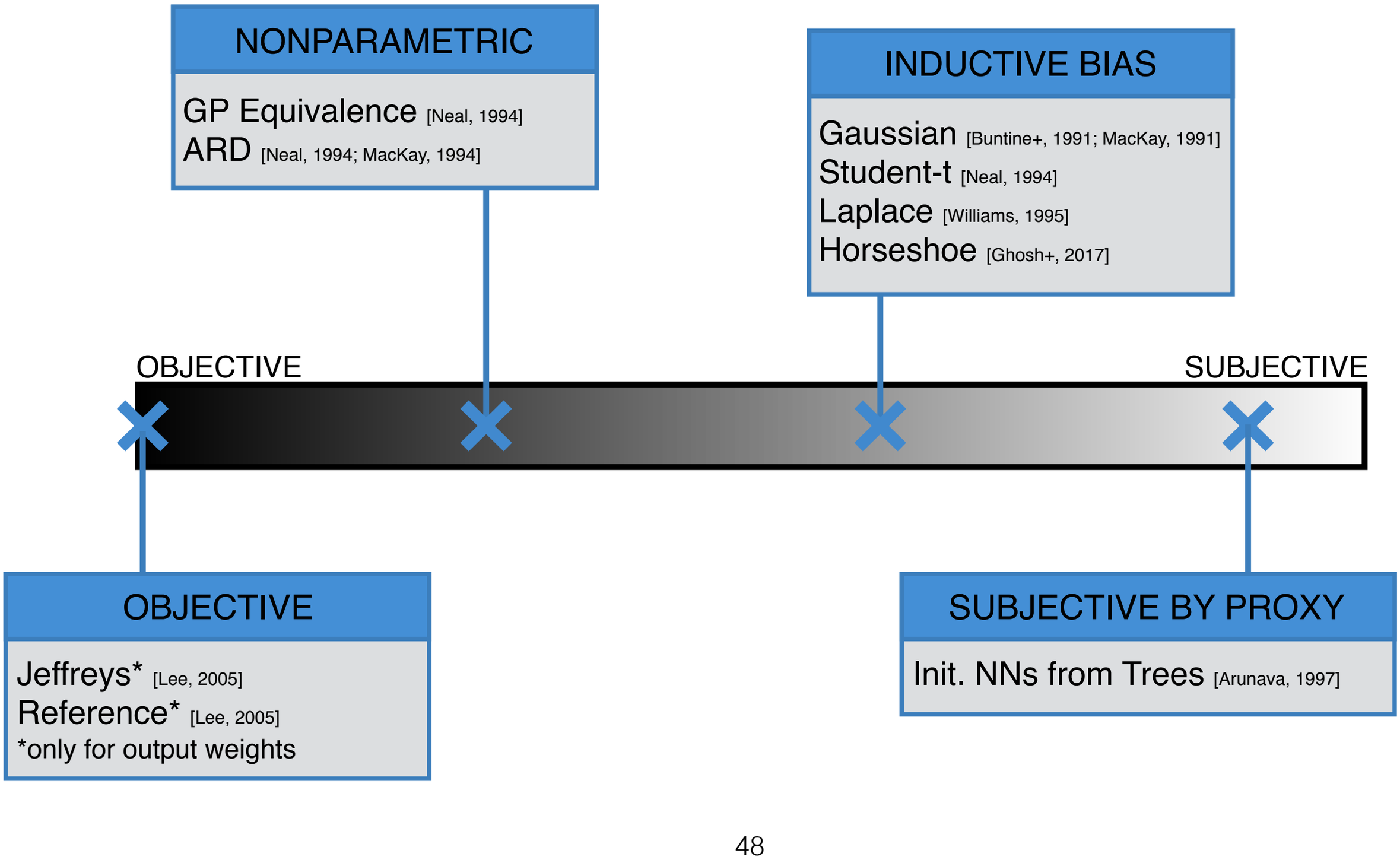
Priors that 'follow the data,' perhaps having frequentist properties. Examples: diffuse, Jeffreys, reference, empirical Bayes.

SUBJECTIVE

Priors determined by previous experiments or expert knowledge.

Priors for Neural Networks

CONDITIONAL MODEL: p(**W**)



Priors for Neural Networks

DENSITY NETWORK: p(**z**)

NONPARAMETRIC

?

INDUCTIVE BIAS

Gaussian [MacKay, 1999; Kingma+, 2014; Rezende+, 2014]
Laplace [Kingma, unpublished]
Scale Mixture [Kingma, unpublished]
Discrete [Neal, 1992]
Structured [Johnson+, 2016]

OBJECTIVE ← → SUBJECTIVE

OBJECTIVE

Parametrized [Chen+, 2017; Makhzani+, 2015]
Empirical/Parametrized [Tomczak+, 2018; Higgins+, 2017]

SUBJECTIVE

Context Free Grammar [Kushner+, 2017]

Priors for Neural Networks

CONDITIONAL MODEL: p(**W**)

NONPARAMETRIC

GP Equivalence [Neal, 1994]
ARD [Neal, 1994; MacKay, 1994]

OBJECTIVE

Jeffreys* [Lee, 2005]
Reference* [Lee, 2005]
*only for output weights

INDUCTIVE BIAS

Gaussian [Buntine+, 1991; MacKay, 1991]
Student-t [Neal, 1994]
Laplace [Williams, 1995]
Horseshoe [Ghosh+, 2017]

SUBJECTIVE BY PROXY

Init. NNs from Trees [Arunava, 1997]

OBJECTIVE

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DENSITY NETWORK: p(**z**)

CONTRIBUTION

Approximating Objective Priors

CHAPTER #5 [Nalisnick & Smyth, UAI 2017]

OBJECTIVE

Priors that ‘follow the data,’ perhaps having frequentist properties. Examples: diffuse, Jeffreys, **reference**, empirical Bayes.

Objective Priors

Reference Priors [Bernardo, 1979] are objective priors defined as:

$$p^*(\boldsymbol{\theta}) = \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}}\ \mathbb{I}[\boldsymbol{\theta}, \mathbf{X}]$$

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\begin{aligned}
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&= \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}} \int_{\mathbf{X}} p(\mathbf{X})\ \mathrm{KLD}[p(\boldsymbol{\theta}|\mathbf{X})||p(\boldsymbol{\theta})]\ d\mathbf{X}
\end{aligned}
$$

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- **Independent** of any dataset for generative models.
- Need posterior in closed-form and therefore difficult to derive.
- Termed *reference* since they serve as a reference against which to compare other priors.

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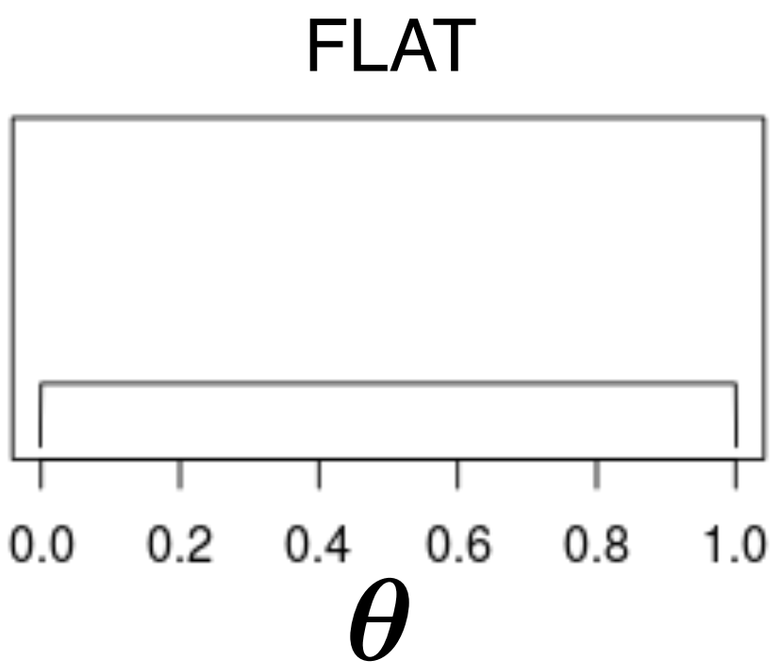
Bernoulli Priors:



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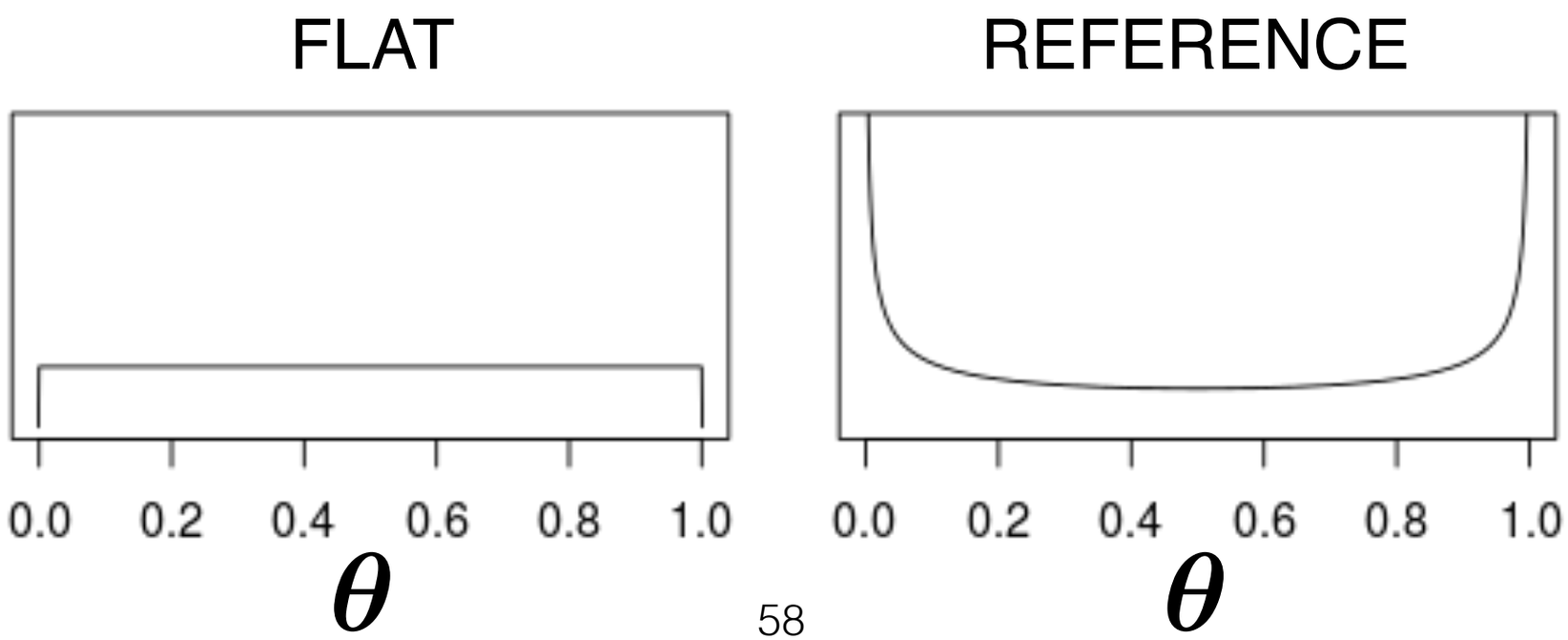

Previous Work

- **Markov Chain Monte Carlo** [Lafferty & Wasserman, 2001]**:** Given a likelihood function, use MCMC to draw samples from the reference prior.

$$\{p(\mathbf{x}|\boldsymbol{\theta})\} \longrightarrow \{\hat{\boldsymbol{\theta}}_1, \ldots, \hat{\boldsymbol{\theta}}_S\}$$

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- **Numerical Algorithm** [Berger et al., 2009]**:** Given a user-specified parameter value and likelihood function, it can compute the reference prior density at that point.

$$\{p(\mathbf{x}|\boldsymbol{\theta}), \boldsymbol{\theta}_0\} \longrightarrow p^*(\boldsymbol{\theta}_0)$$

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- **Numerical Algorithm** [Berger et al., 2009]**:** Given a user-specified parameter value and likelihood function, it can compute the reference prior density at that point.

  ↳ **Drawback**: Have to choose the evaluation points yourself, which is very hard to do in high dimensions.

$$\{p(\mathbf{x}|\boldsymbol{\theta}), \boldsymbol{\theta}_0\} \longrightarrow p^*(\boldsymbol{\theta}_0)$$

Proposed Method

- **Parametric Approximation:** Posit a parametric family and optimize the parameters to find an approximation.

$$p^*(\boldsymbol{\theta}) \approx p(\boldsymbol{\theta}; \boldsymbol{\lambda}^*)$$

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$$\mathbb{I}[\boldsymbol{\theta}, \mathbf{X}] \geq \mathbb{E}_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}, \mathbf{x}} \left[\log p(\mathbf{X}|\boldsymbol{\theta}) - \frac{1}{1+\alpha} \log \mathbb{E}_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}} \left[p(\mathbf{X}|\boldsymbol{\theta})^{1+\alpha} \right] \right]$$

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$$\approx \mathbb{E}_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}, \mathbf{X}} \left[\log p(\mathbf{X}|\boldsymbol{\theta}) - \max_s \log p(\mathbf{X}|\hat{\boldsymbol{\theta}}_s) \right]$$

[Li & Turner, 2016]

Proposed Method

Lower Bound Optimization: We derive a lower bound on the mutual information and optimize it w.r.t. $\boldsymbol{\lambda}$.

$$\{p(\mathbf{x}|\boldsymbol{\theta}), p(\boldsymbol{\theta};\boldsymbol{\lambda})\} \longrightarrow p(\boldsymbol{\theta};\boldsymbol{\lambda}^*)$$

BENEFITS

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Gaussian mean: $p^*(\boldsymbol{\mu}) \propto 1$

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Gaussian mean: $p^*(\boldsymbol{\mu}) \propto 1$

- **Conjugate Reference Priors**: Can pick a prior family that is conjugate and then find the member that is nearest to a reference prior.

Proposed Method

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BENEFITS

Gaussian mean: $p^*(\boldsymbol{\mu}) \propto 1$

- **Conjugate Reference Priors**: Can pick a prior family that is conjugate and then find the member that is nearest to a reference prior.
- **Proper Reference Priors**: If concerned b/c a reference prior is improper, can use an approximation that is proper.

Proposed Method

Lower Bound Optimization: We derive a lower bound on the mutual information and optimize it w.r.t. $\boldsymbol{\lambda}$.

$$\{p(\mathbf{x}|\boldsymbol{\theta}), p(\boldsymbol{\theta};\boldsymbol{\lambda})\} \longrightarrow p(\boldsymbol{\theta};\boldsymbol{\lambda}^*)$$

BENEFITS

- **Comparison to Lafferty & Wasserman's [2001] MCMC**: No need to perform a second modeling step to evaluate the prior.

- **Comparison to Berger et al.'s [2009] Algorithm**: No need to specify evaluation points.

Proposed Method

Drawback?: Need to specify the variational family.

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Notice that the objective doesn't require evaluation of the prior, only expectations / samples:

$$\mathbb{I}[\boldsymbol{\theta}, \mathbf{X}] \geq \mathbb{E}_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}, \mathbf{x}} \left[\log p(\mathbf{X}|\boldsymbol{\theta}) - \frac{1}{1+\alpha} \log \mathbb{E}_{\boldsymbol{\theta}_{\boldsymbol{\lambda}}} \left[p(\mathbf{X}|\boldsymbol{\theta})^{1+\alpha} \right] \right]$$

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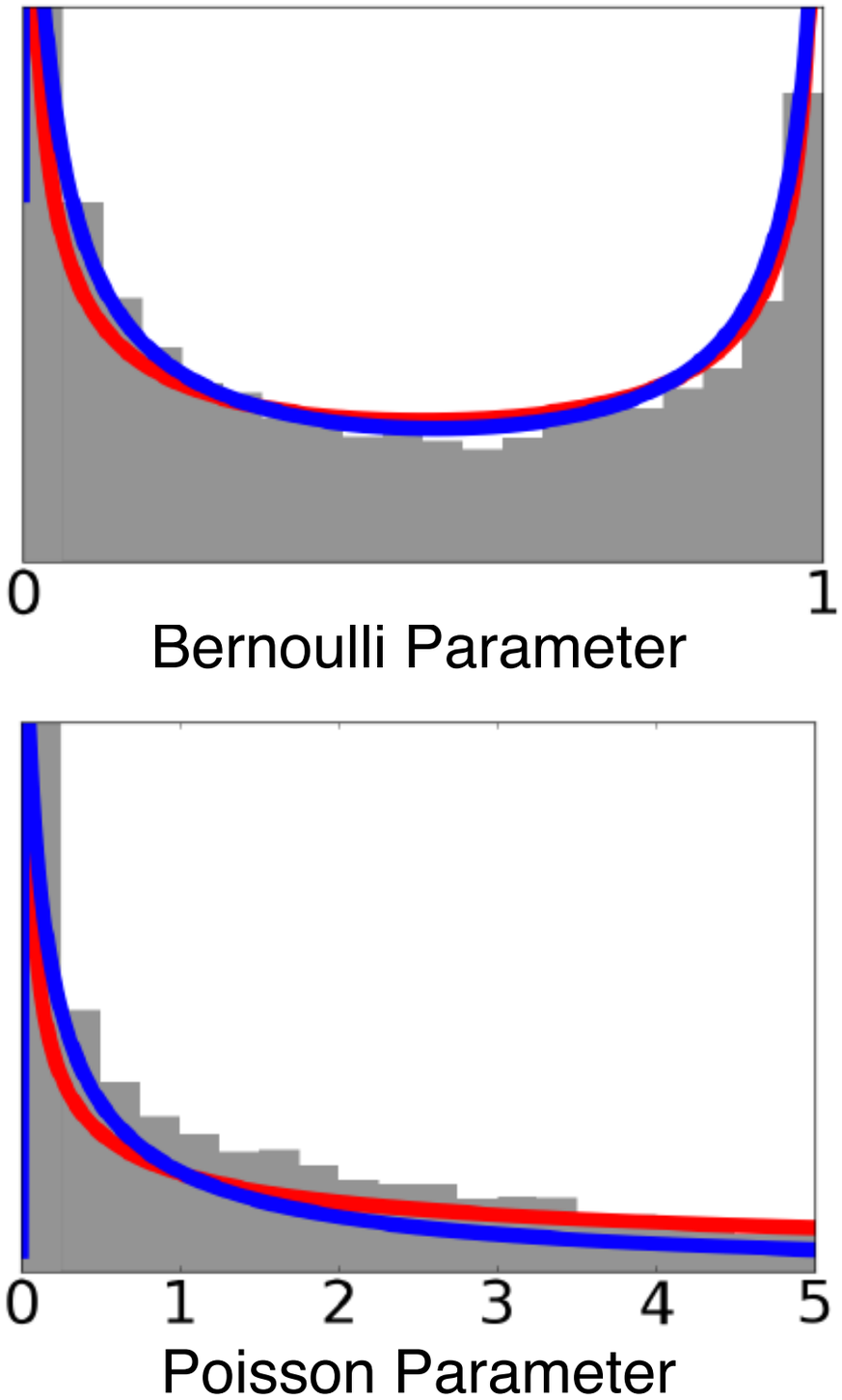
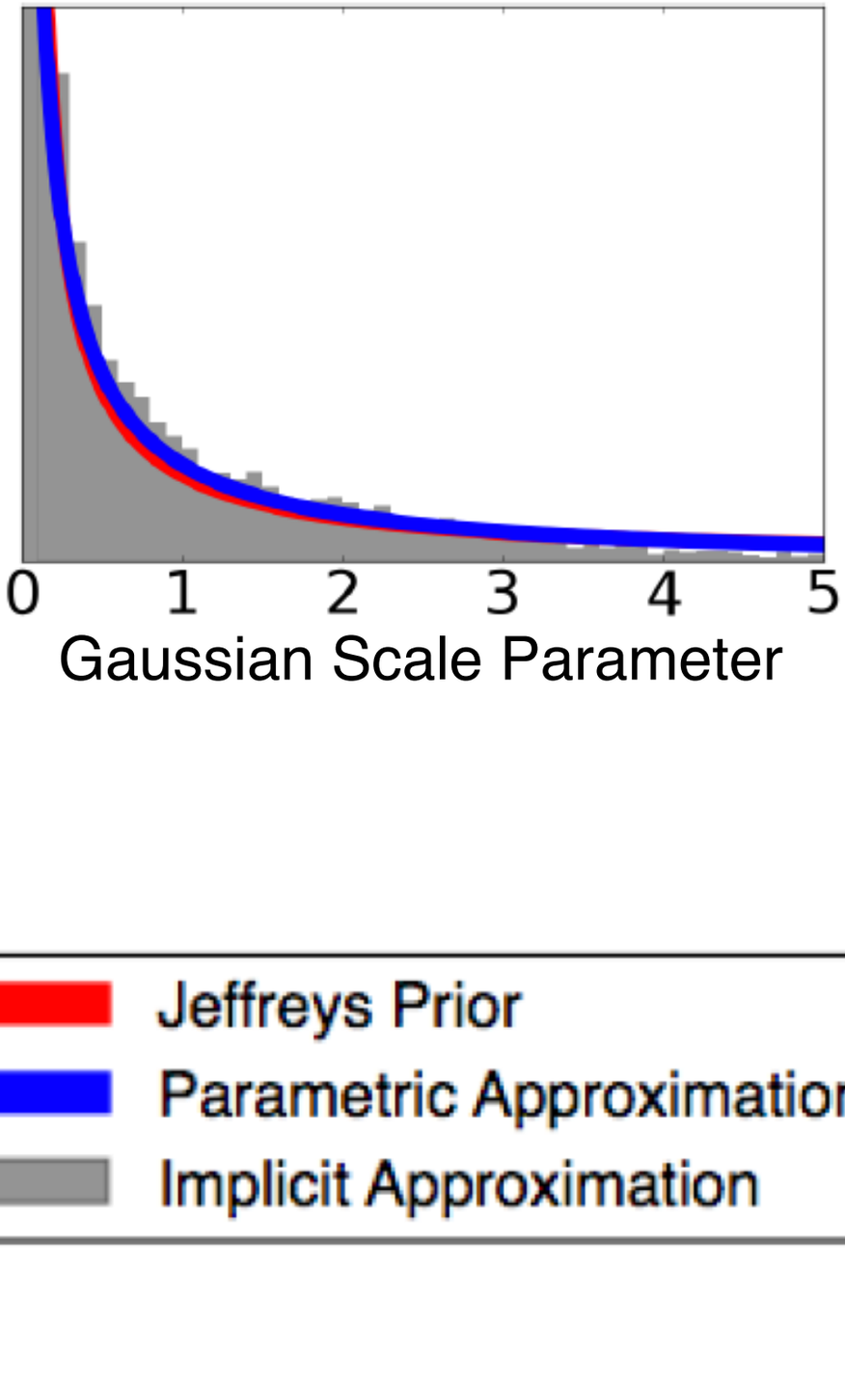
Thus, we can use an **implicit prior**:

$$\hat{\boldsymbol{\theta}} = f(\hat{\boldsymbol{\epsilon}}; \boldsymbol{\lambda}), \quad \hat{\boldsymbol{\epsilon}} \sim p_0(\boldsymbol{\epsilon})$$

This results in *f* being a functional sampler, similar to the MCMC approach.

Recovering Jeffreys Priors





See paper / dissertation for two-sample tests comparing approximation methods.

Finding the Density Net's Reference Prior

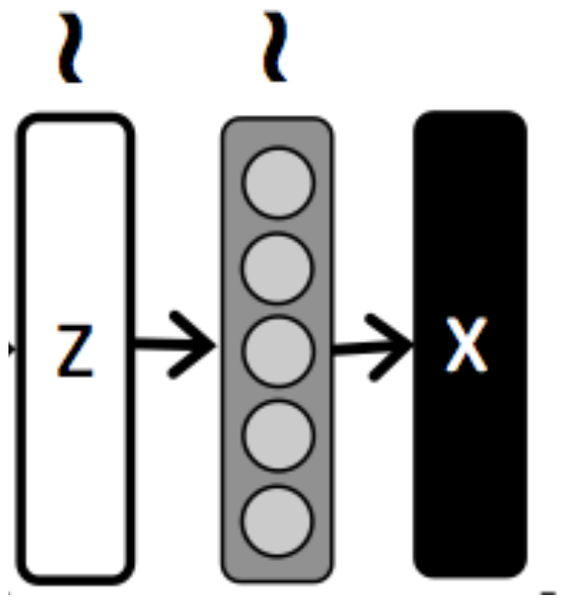
"…to improve our variational bounds we should improve our priors and not just the encoder and decoder….perhaps we should investigate multimodal priors…"

M. Hoffman & M. Johnson. "ELBO Surgery". NIPS 2016 Workshop on *Advances in Approx. Bayesian Inference*.

Finding the Density Net's Reference Prior

ALGORITHM

$p(\mathbf{z};\boldsymbol{\lambda})$ $p(\mathbf{W})$



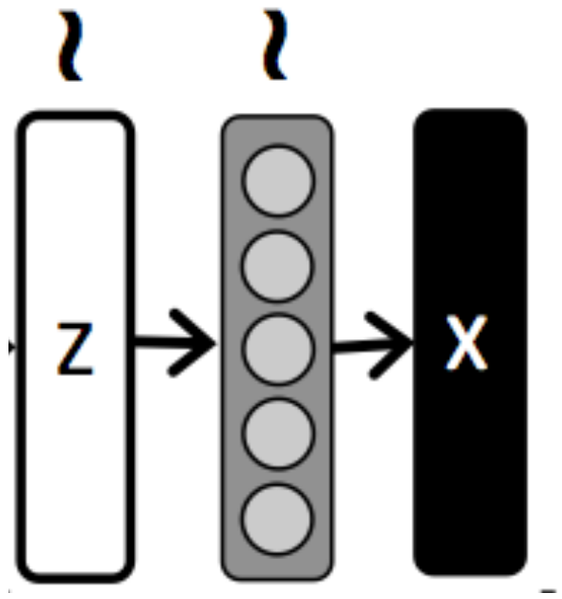
DENSITY NET

Finding the Density Net's Reference Prior

ALGORITHM

STEP #1: sample $\hat{\mathbf{z}}_0 \sim p(\mathbf{z}; \boldsymbol{\lambda})$

$p(\mathbf{z}; \boldsymbol{\lambda})$ $p(\mathbf{W})$



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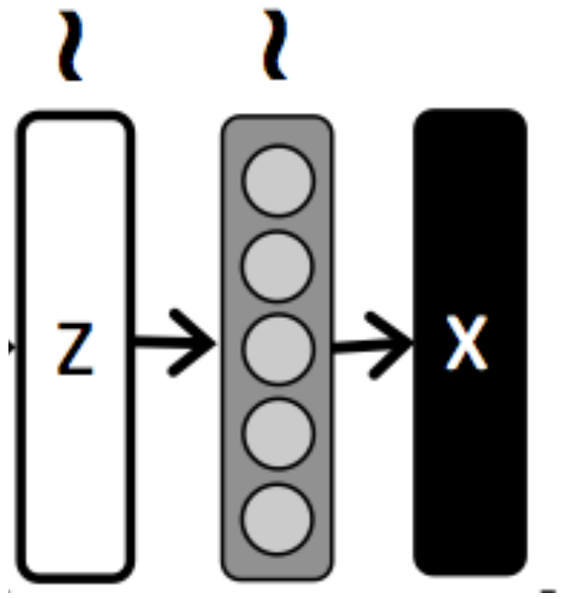
$p(\mathbf{z}; \boldsymbol{\lambda})$ $p(\mathbf{W})$



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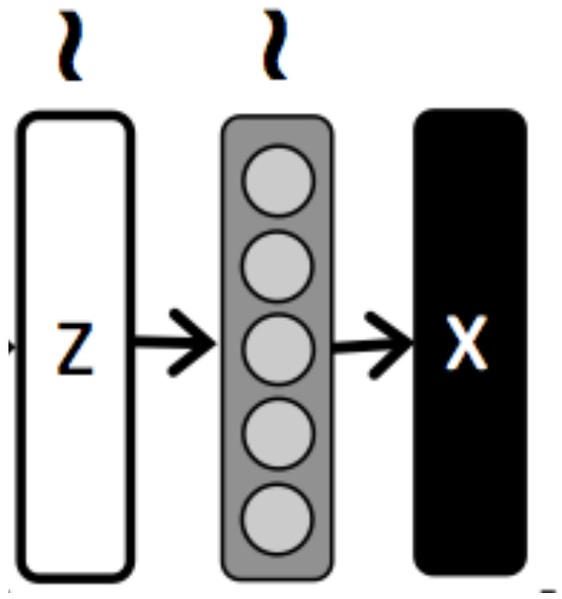
$p(\mathbf{z}; \boldsymbol{\lambda})$ $p(\mathbf{W})$



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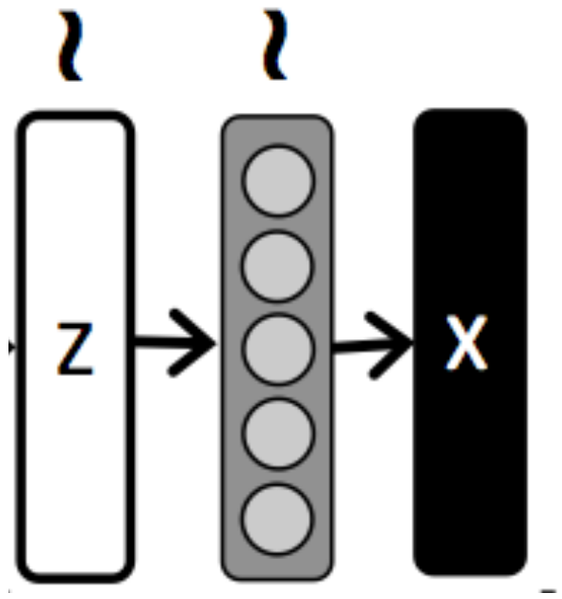

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STEP #5: maximize w.r.t. $\boldsymbol{\lambda}$

$$\mathcal{J}(\boldsymbol{\lambda}) = \log p(\hat{\mathbf{X}}|\hat{\mathbf{z}}_0, \hat{\mathbf{W}}) - \max_s \log p(\hat{\mathbf{X}}|\hat{\mathbf{z}}_s, \hat{\mathbf{W}})$$

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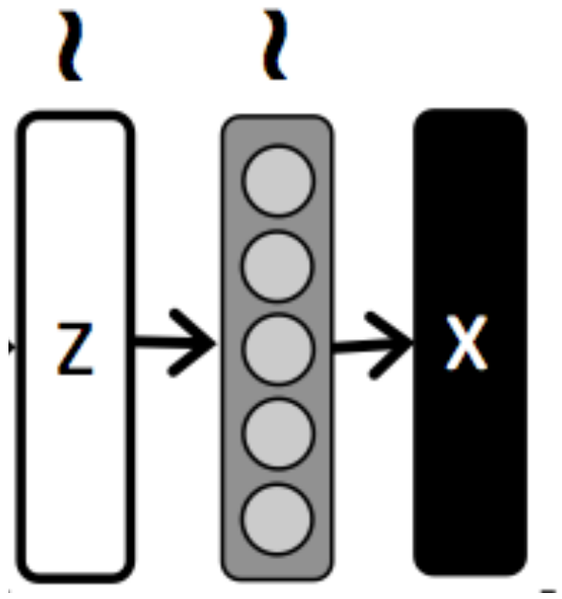

DENSITY NET

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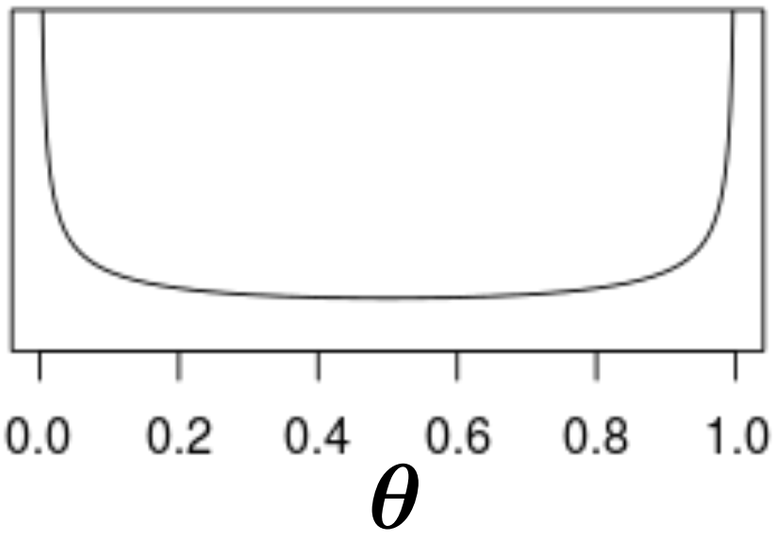

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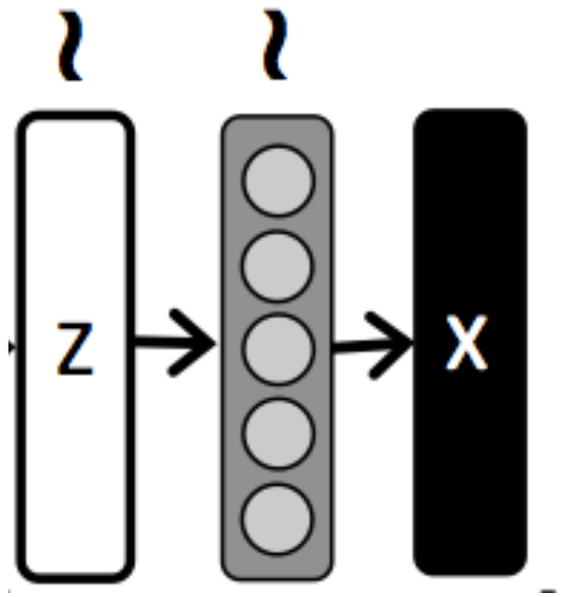
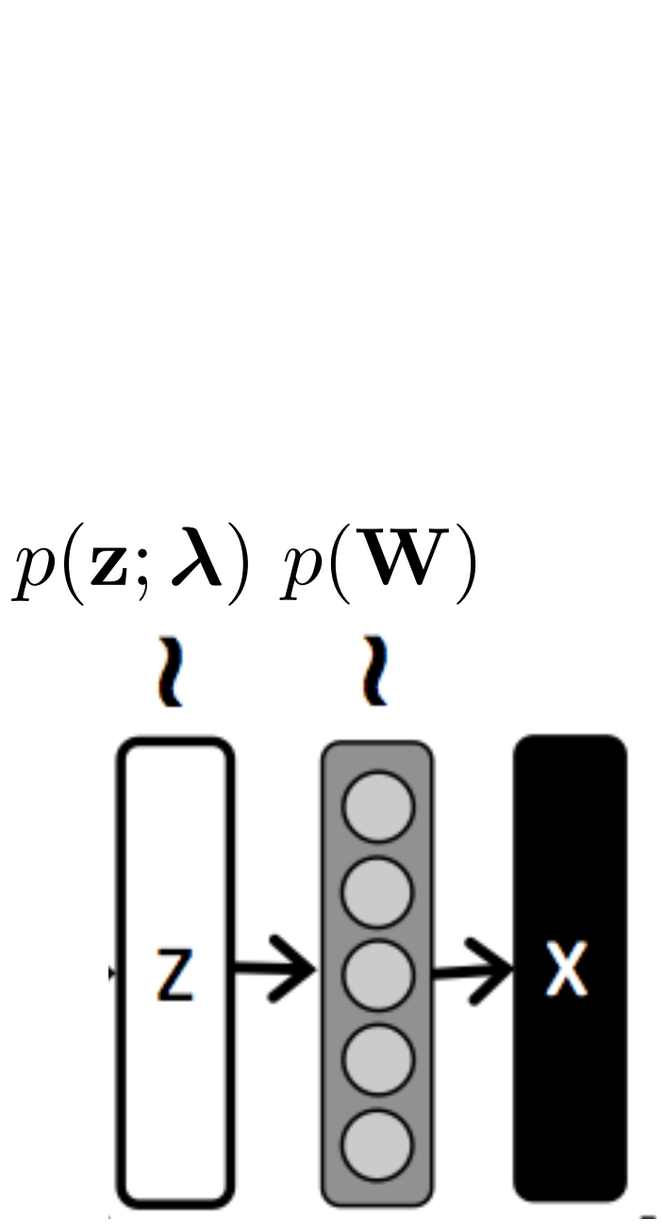
$p(\mathbf{z}; \boldsymbol{\lambda})$ $p(\mathbf{W})$



DENSITY NET

Finding the Density Net's Reference Prior



DENSITY NET

ALGORITHM

STEP #1: sample $\hat{\mathbf{z}}_0 \sim p(\mathbf{z};\boldsymbol{\lambda})$

STEP #2: sample $\hat{\mathbf{W}} \sim p(\mathbf{W})$

STEP #3: sample $\hat{\mathbf{X}} = \{\hat{\mathbf{x}}_1, \ldots, \hat{\mathbf{x}}_N\} \sim p(\mathbf{x}|\hat{\mathbf{z}}_0, \hat{\mathbf{W}})$

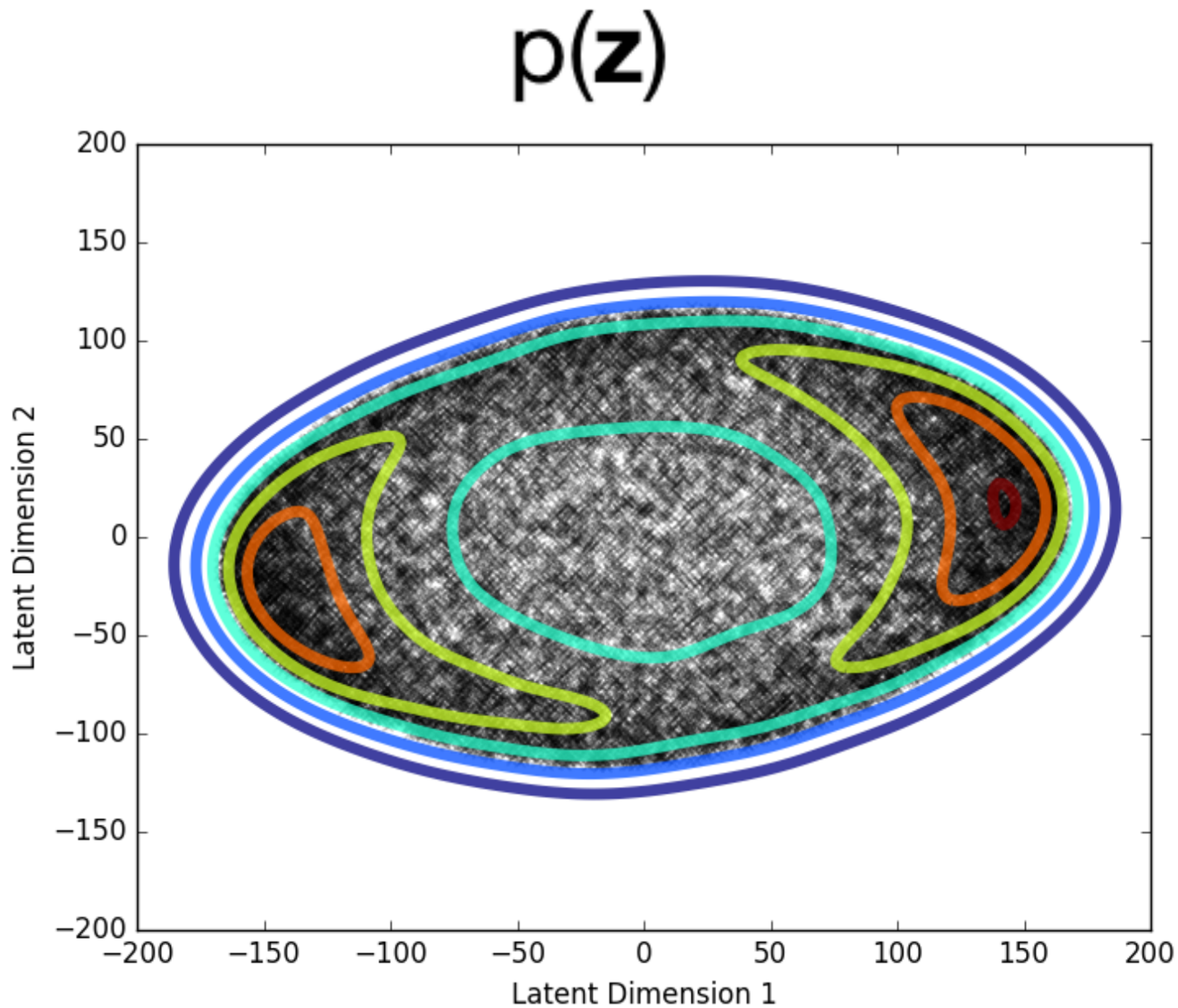
STEP #4: sample $\{\hat{\mathbf{z}}_1, \ldots, \hat{\mathbf{z}}_S\} \sim p(\mathbf{z};\boldsymbol{\lambda})$

STEP #5: maximize w.r.t. $\boldsymbol{\lambda}$

$$\mathcal{J}(\boldsymbol{\lambda}) = \log p(\hat{\mathbf{X}}|\hat{\mathbf{z}}_0, \hat{\mathbf{W}}) - \max_s \log p(\hat{\mathbf{X}}|\hat{\mathbf{z}}_s, \hat{\mathbf{W}})$$

STEP #6: repeat

Finding the Density Net's Reference Prior



Improves performance in low dimensions but no gains in high dimensions (25+).

Priors for Neural Networks

CONDITIONAL MODEL: p(**W**)

NONPARAMETRIC

OBJECTIVE

Jeffreys* [Lee, 2005]
Reference* [Lee, 2005]
Reference Approx.

INDUCTIVE BIAS

SUBJECTIVE BY PROXY

OBJECTIVE

SUBJECTIVE

OBJECTIVE

Parametrized [Chen+, 2017; Makhzani+, 2015]
Empirical/Parametrized [Tomczak+, 2018; Higgins+, 2017]
Reference Approx. **[Nalisnick & Smyth, 2017]**

INDUCTIVE BIAS

SUBJECTIVE

NONPARAMETRIC

DENSITY NETWORK: p(**z**)

CONTRIBUTION

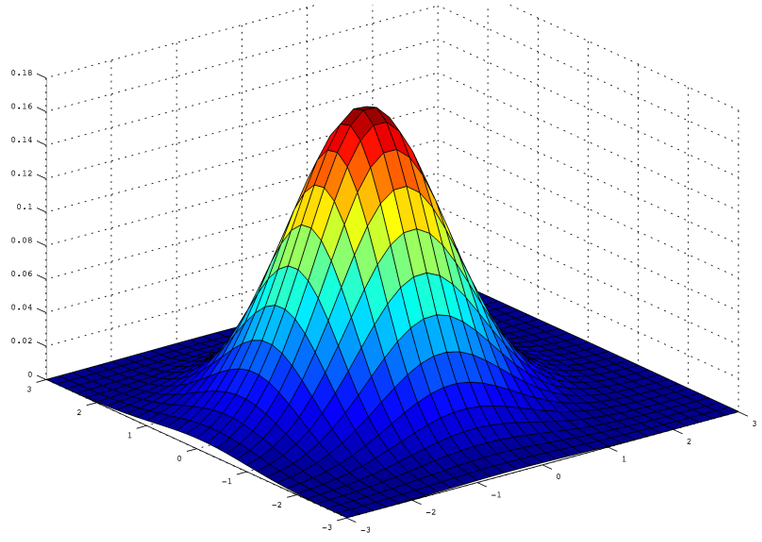
Nonparametric Priors

CHAPTER #7 [Nalisnick & Smyth, ICLR 2017]

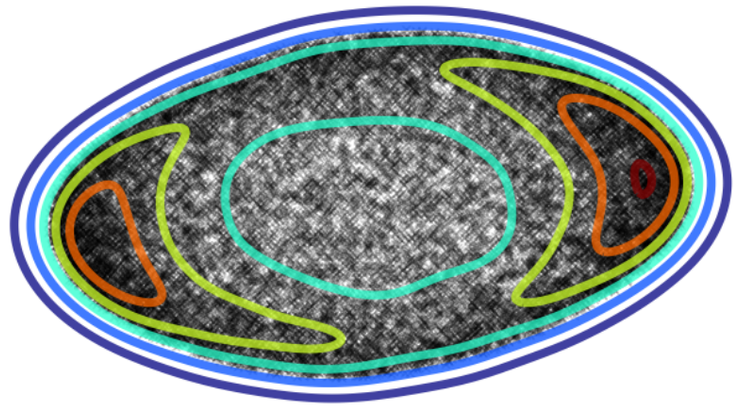
NONPARAMETRIC

Infinite dimensional priors that give the model adaptive capacity. Examples: **Dirichlet process,** Indian Buffet process.

Nonparametric Priors for Density Nets



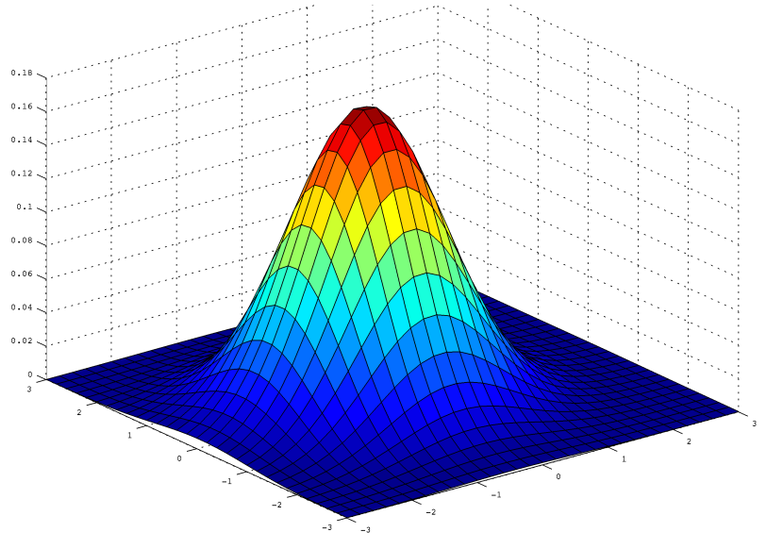
GAUSSIAN PRIOR



REFERENCE PRIOR

FINITE DIMENSIONAL

Nonparametric Priors for Density Nets



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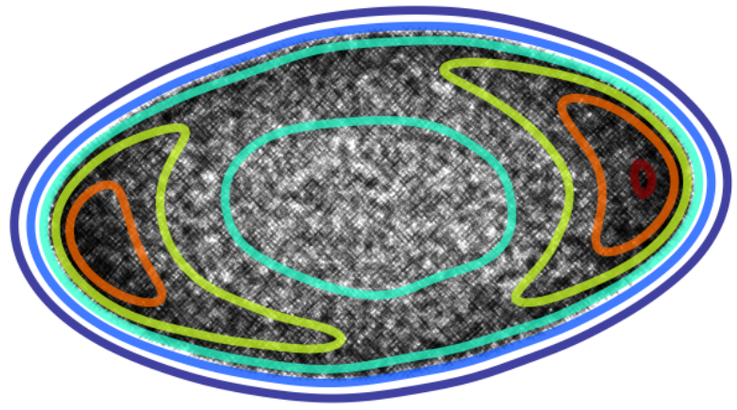
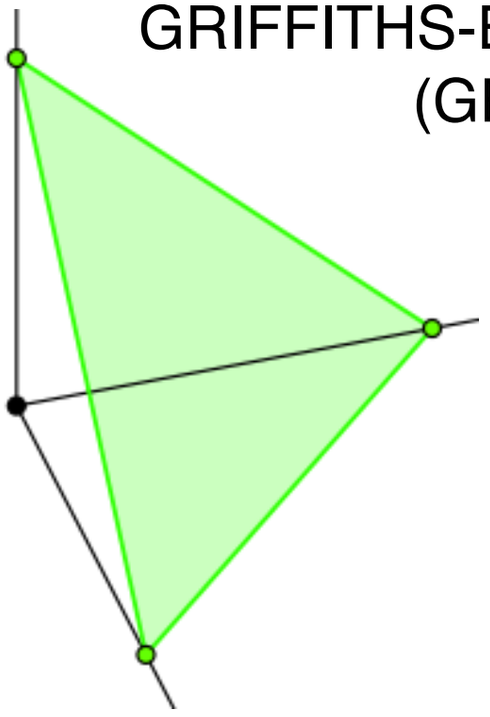


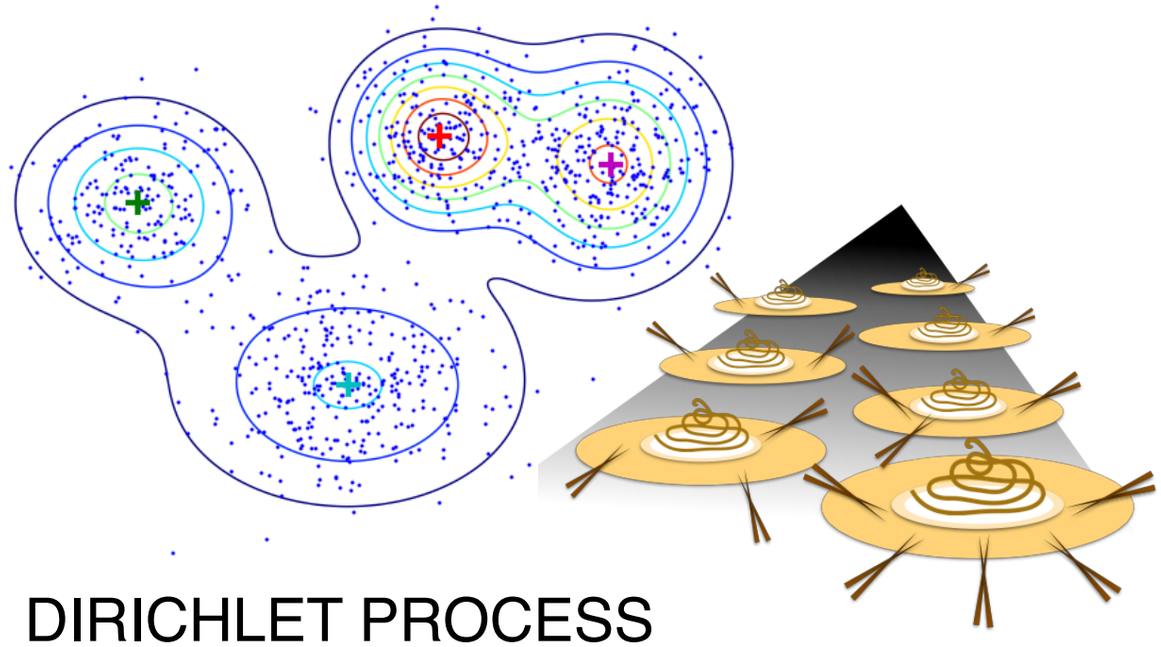
REFERENCE PRIOR

FINITE DIMENSIONAL

INFINITE DIMENSIONAL

GRIFFITHS-ENGEN-McCLOSKEY
(GEM) PRIOR

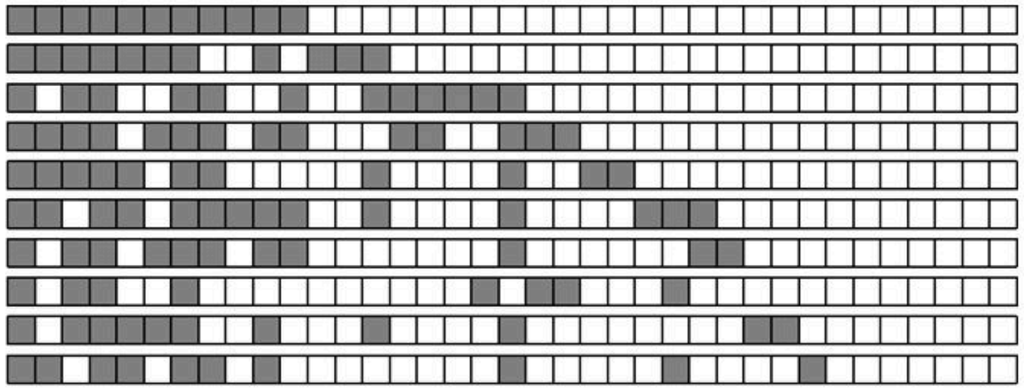




DIRICHLET PROCESS
MIXTURE PRIOR

Nonparametric Priors for Density Nets

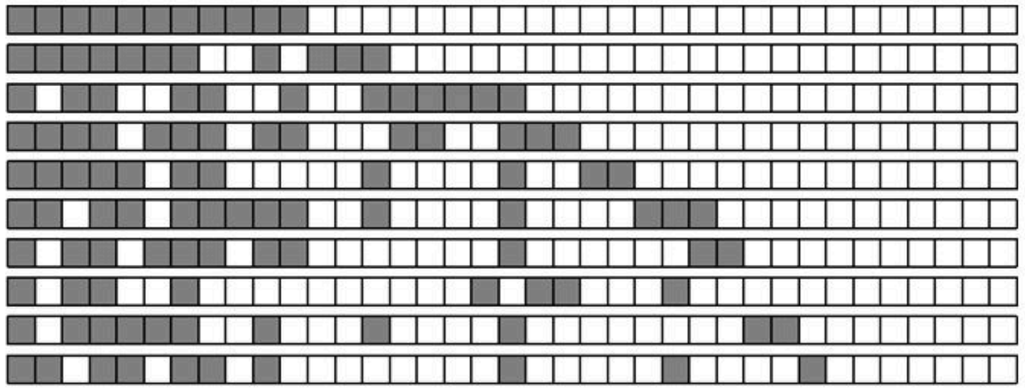
What about the IBP, the natural nonparametric prior for latent feature models?



INDIAN BUFFET PROCESS

Nonparametric Priors for Density Nets

What about the IBP, the natural nonparametric prior for latent feature models?



INDIAN BUFFET PROCESS

Structured Variational Autoencoders for the Beta-Bernoulli Process

Rachit Singh* **Jeffrey Ling*** **Finale Doshi-Velez**
Harvard University
{rachitsingh@college,jling@college,finale@seas}.harvard.edu

Abstract

Beta-Bernoulli processes, also known as Indian buffet processes, are nonparametric priors that allow generative models to automatically infer the number of features in datasets. However, inference for these models proves to be challenging, often relying on specific forms of the likelihood for computational tractability.

We propose to amortize inference using a variational autoencoder trained via gradient descent, allowing for arbitrary likelihood models. Our model extends previously considered mean field variational methods with a structured posterior and new developments in the training of discrete variable VAEs. We experimentally demonstrate a Beta-Bernoulli process VAE that learns decomposable latent features and allows for scalable inference of arbitrary likelihoods on large datasets.

Training

Two methods to compute backpropagation gradients:

- Black box variational inference (BBVI): directly backpropagate with score estimator
- Replace non-reparameterizable variables in variational approximation:
  - Bernoulli $\rightarrow$ Gumbel softmax (Maddison et al. 2017, Jang et al. 2017)
  - Beta $\rightarrow$ Kumaraswamy (Nalisnick & Smyth 2017)

The Dirichlet Process

$$G \sim \mathrm{DP}(\alpha, H)$$

CONCENTRATION

BASE MEASURE

The Dirichlet Process

$$G \sim \mathrm{DP}(\alpha, H)$$

CONCENTRATION

BASE MEASURE

BASE MEASURE

$$\boldsymbol{\mu}_k \sim H(\boldsymbol{\mu})$$

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BASE MEASURE

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$$\boldsymbol{\mu}_k \sim H(\boldsymbol{\mu})$$

WEIGHTS

$$\{\pi_1, \ldots, \pi_k, \ldots\} = \mathrm{GEM}(\alpha)$$

$$\pi_k = v_k \prod_{j=1}^{k} (1 - v_j)$$

$$v_k \sim \mathrm{Beta}(1, \alpha)$$

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DISTRIBUTION

$$G(\boldsymbol{\mu}) = \sum_{k=1}^{\infty} \pi_k \delta[\boldsymbol{\mu}_k]$$

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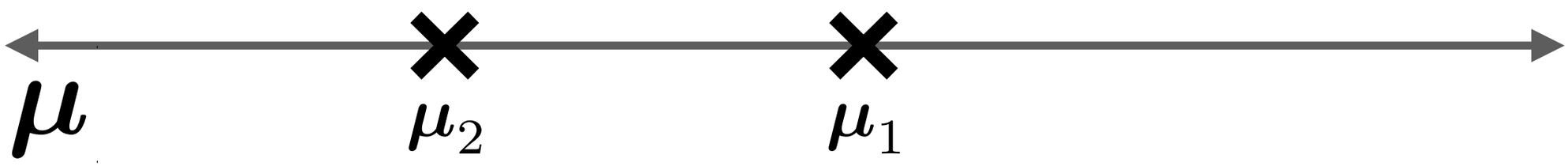

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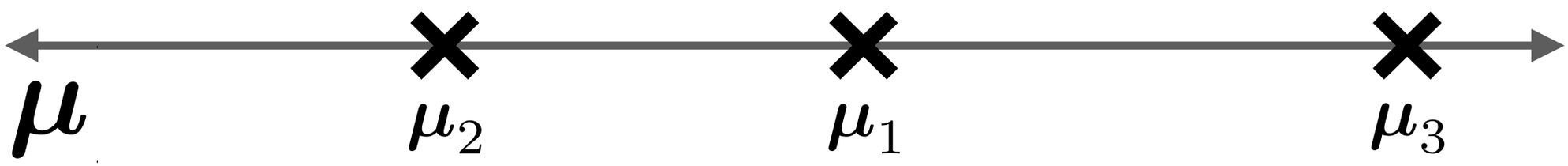

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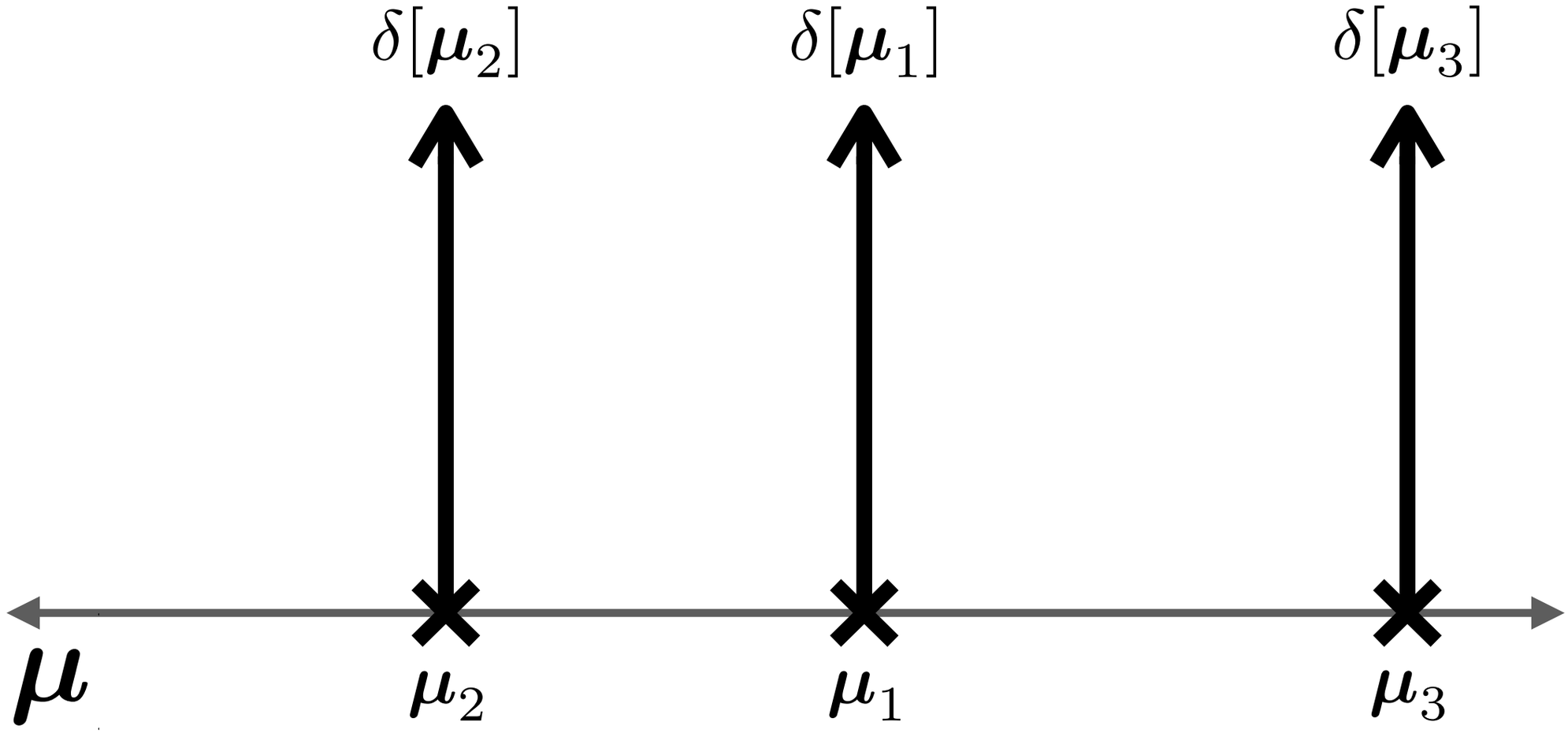

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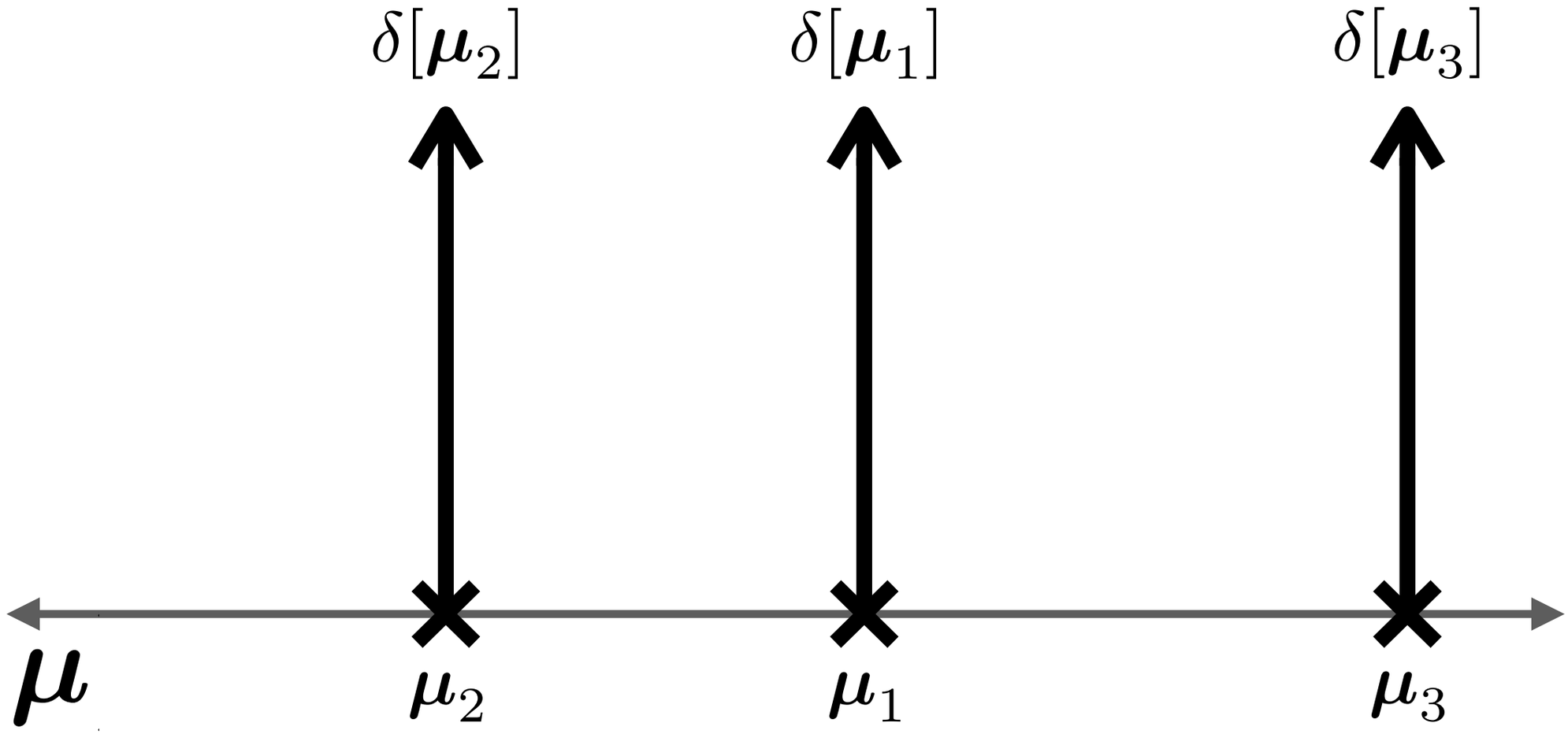

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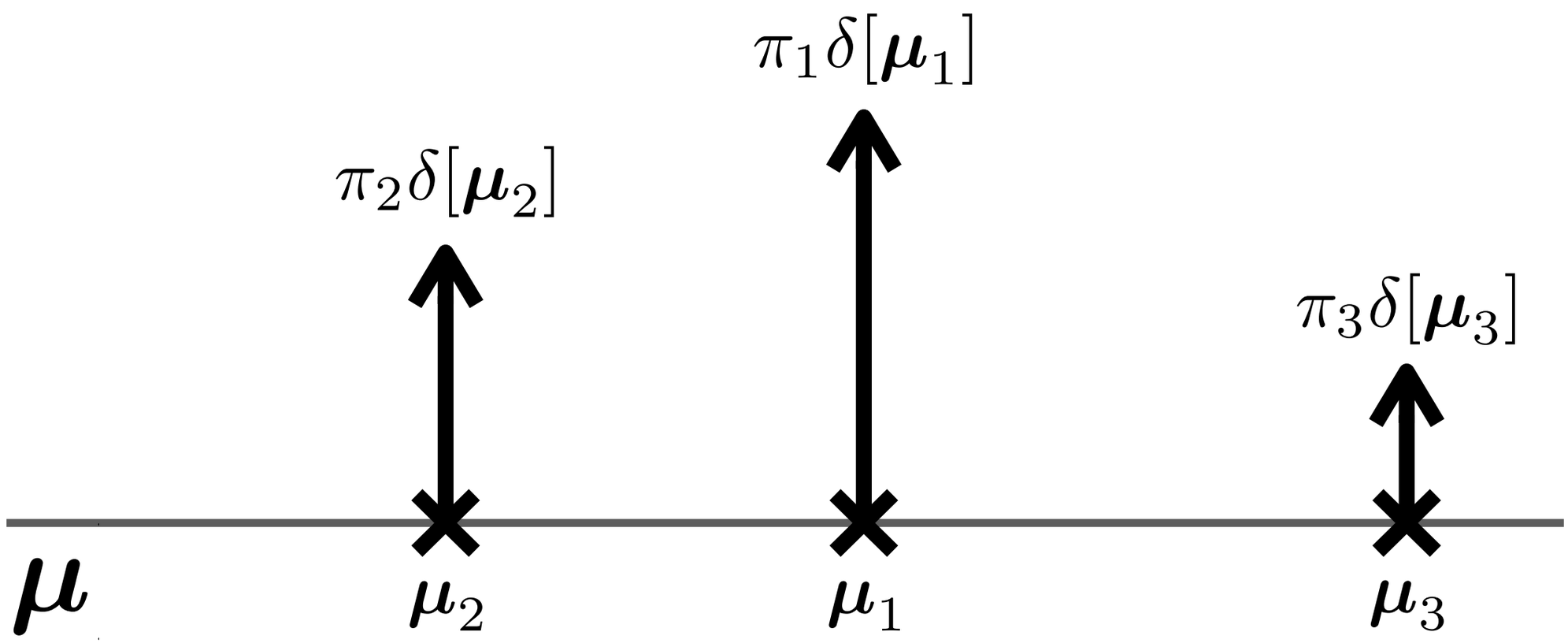

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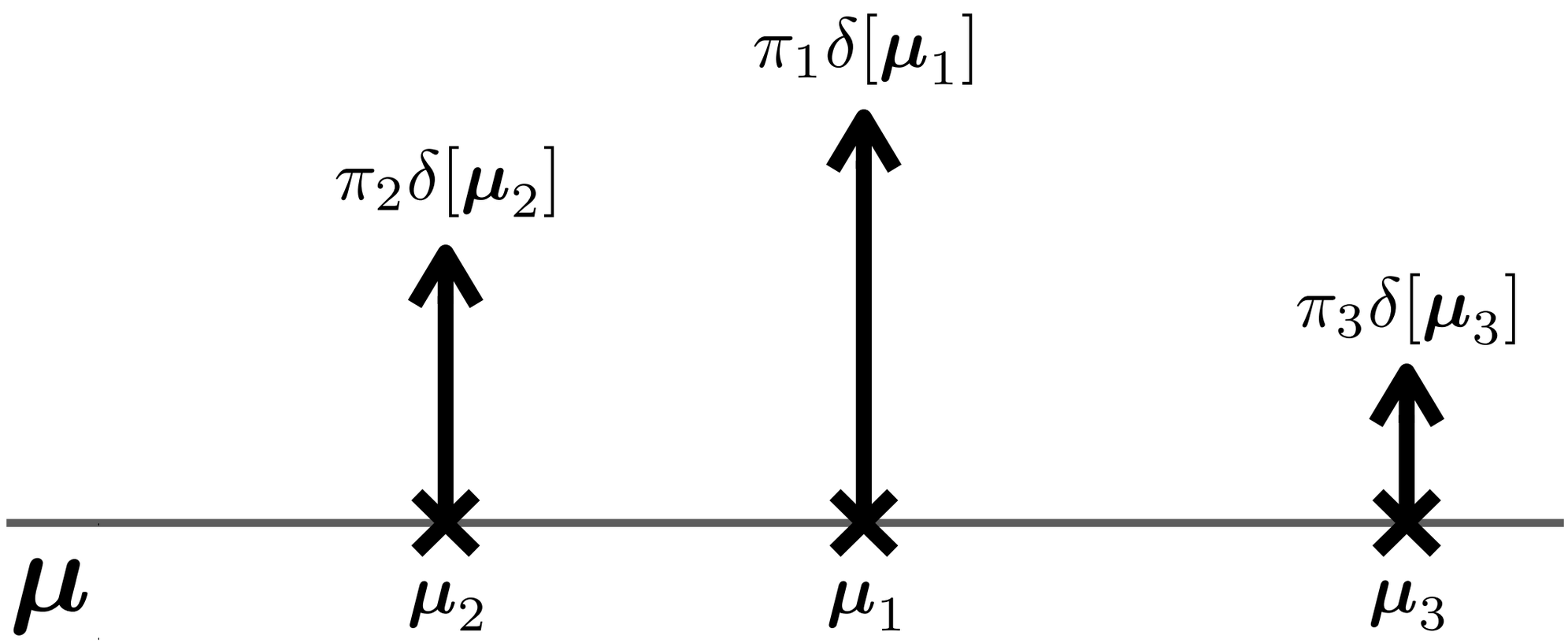

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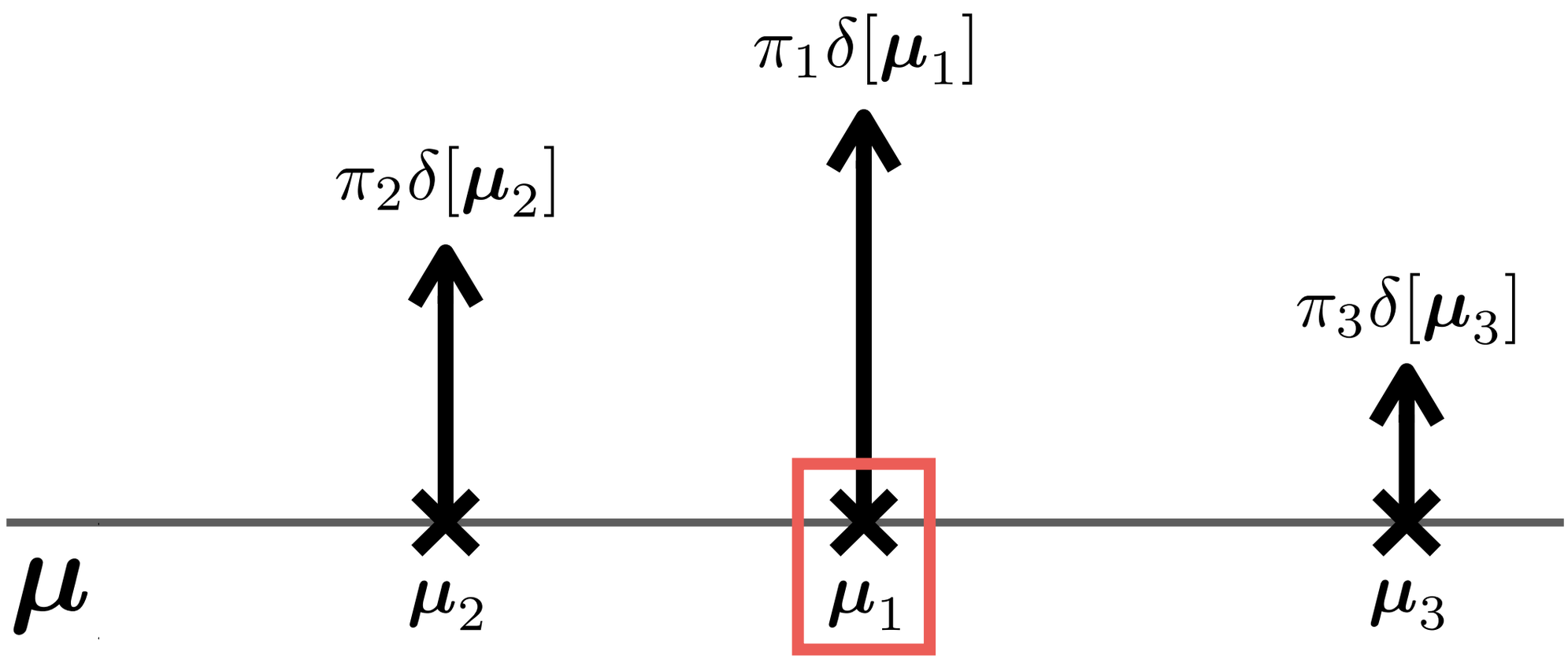

The Dirichlet Process Mixture Model

$$G \sim \mathrm{DP}(\alpha, H)$$

The Dirichlet Process Mixture Model

$$G \sim \mathrm{DP}(\alpha, H) \qquad \mathbf{z}|G \sim \int p(\mathbf{z}|\boldsymbol{\mu})G(\boldsymbol{\mu})$$

KERNEL
(EMISSION DISTRIBUTION)

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KERNEL
(EMISSION DISTRIBUTION)

COLLAPSING OUT G, WE HAVE…

$$\mathbf{z}|\{\boldsymbol{\mu}_k\}, \{\pi_k\} \sim \sum_{k=1}^{\infty} \pi_k p(\mathbf{z}|\boldsymbol{\mu}_k)$$

$$\{\pi_k\} \sim \mathrm{GEM}(\alpha)$$

$$\{\boldsymbol{\mu}_k\} \sim H(\boldsymbol{\mu})$$

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COLLAPSING OUT G, WE HAVE…

$$\mathbf{z} \sim \mathrm{DPMM}(p, \alpha, H) \Bigg| \begin{aligned} \mathbf{z}|\{\boldsymbol{\mu}_k\}, \{\pi_k\} &\sim \sum_{k=1}^{\infty} \pi_k p(\mathbf{z}|\boldsymbol{\mu}_k) \\ \{\pi_k\} &\sim \mathrm{GEM}(\alpha) \\ \{\boldsymbol{\mu}_k\} &\sim H(\boldsymbol{\mu}) \end{aligned}$$

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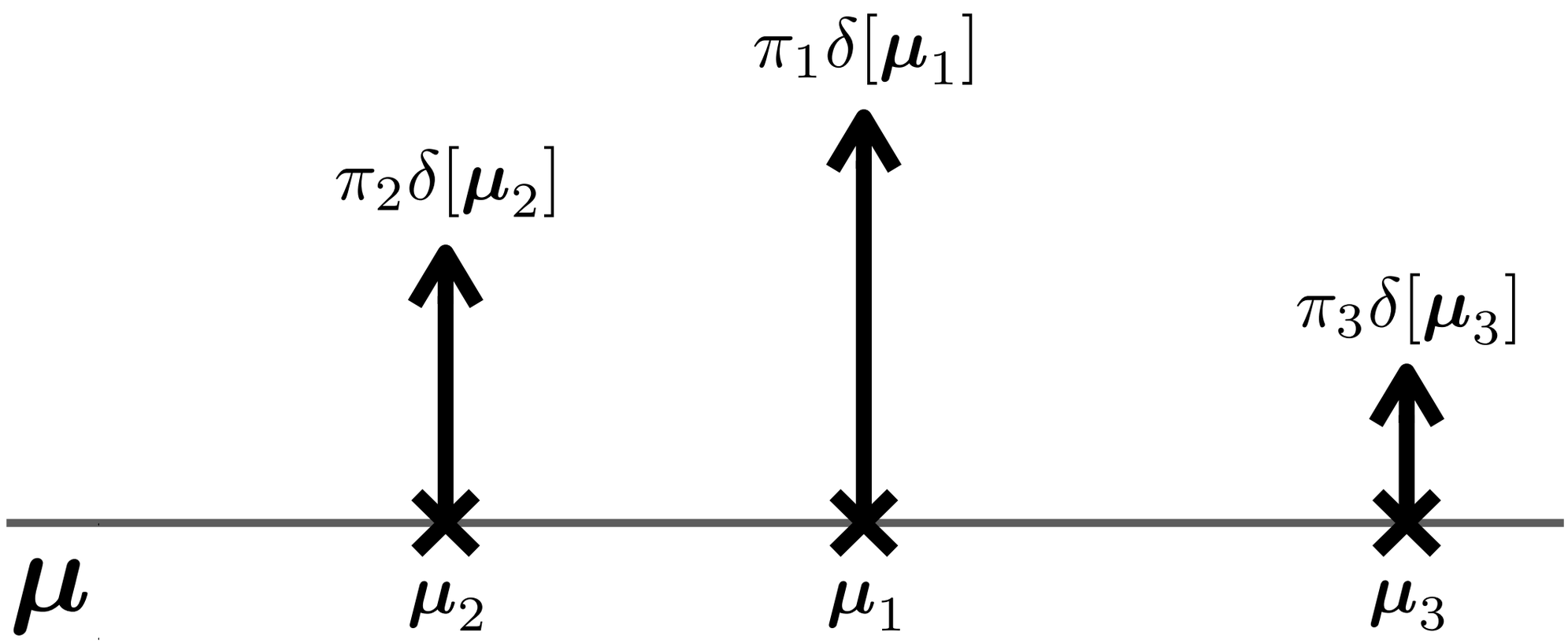

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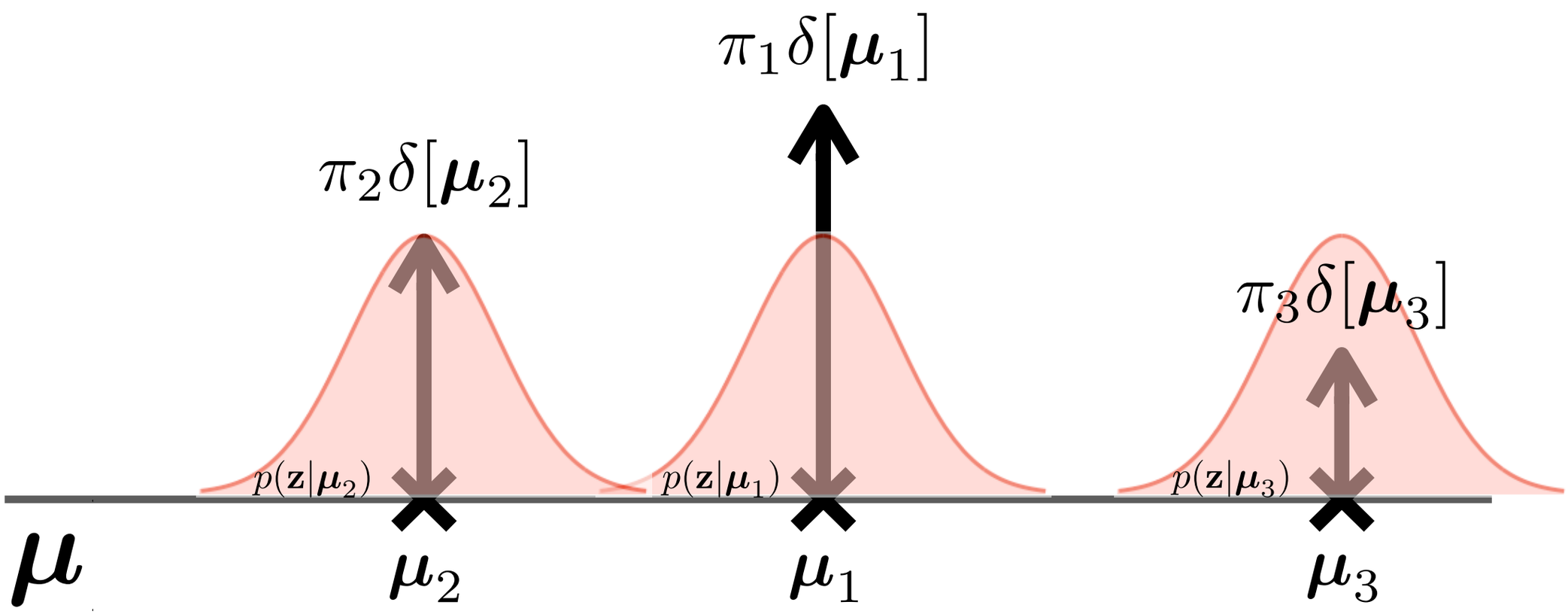

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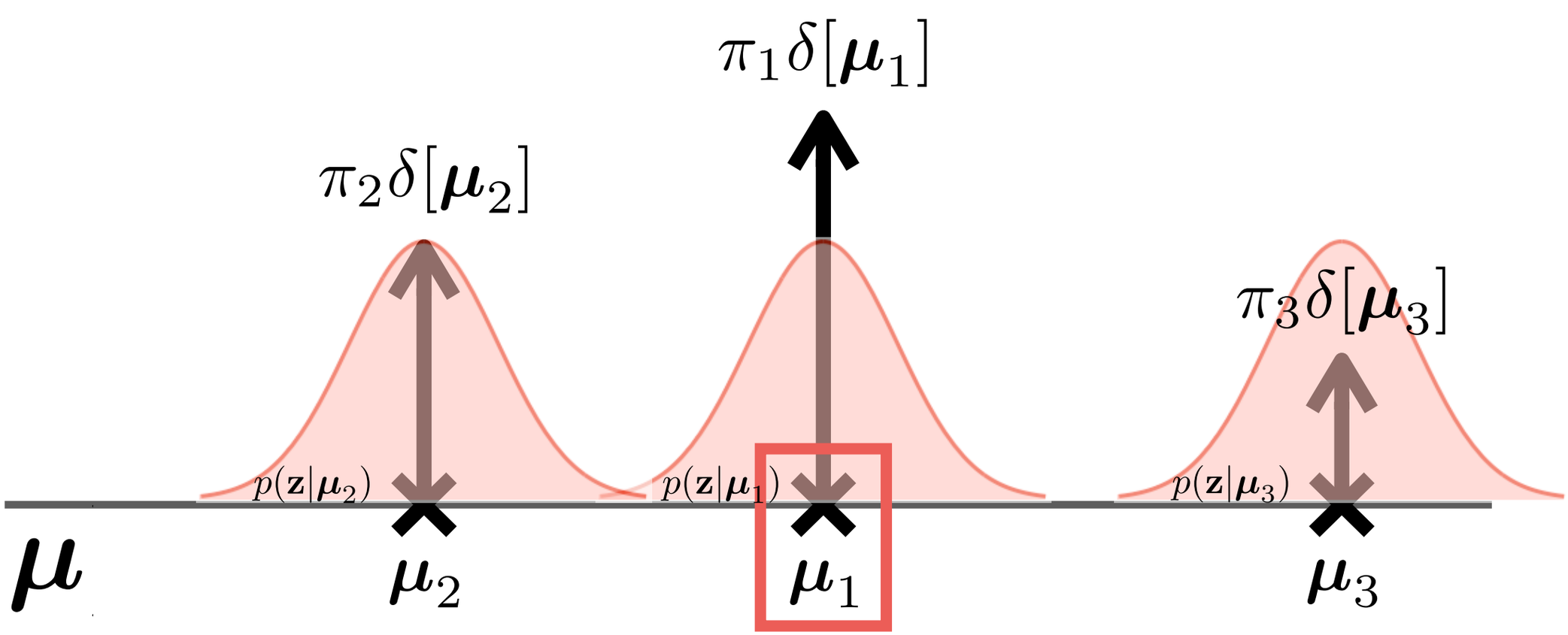

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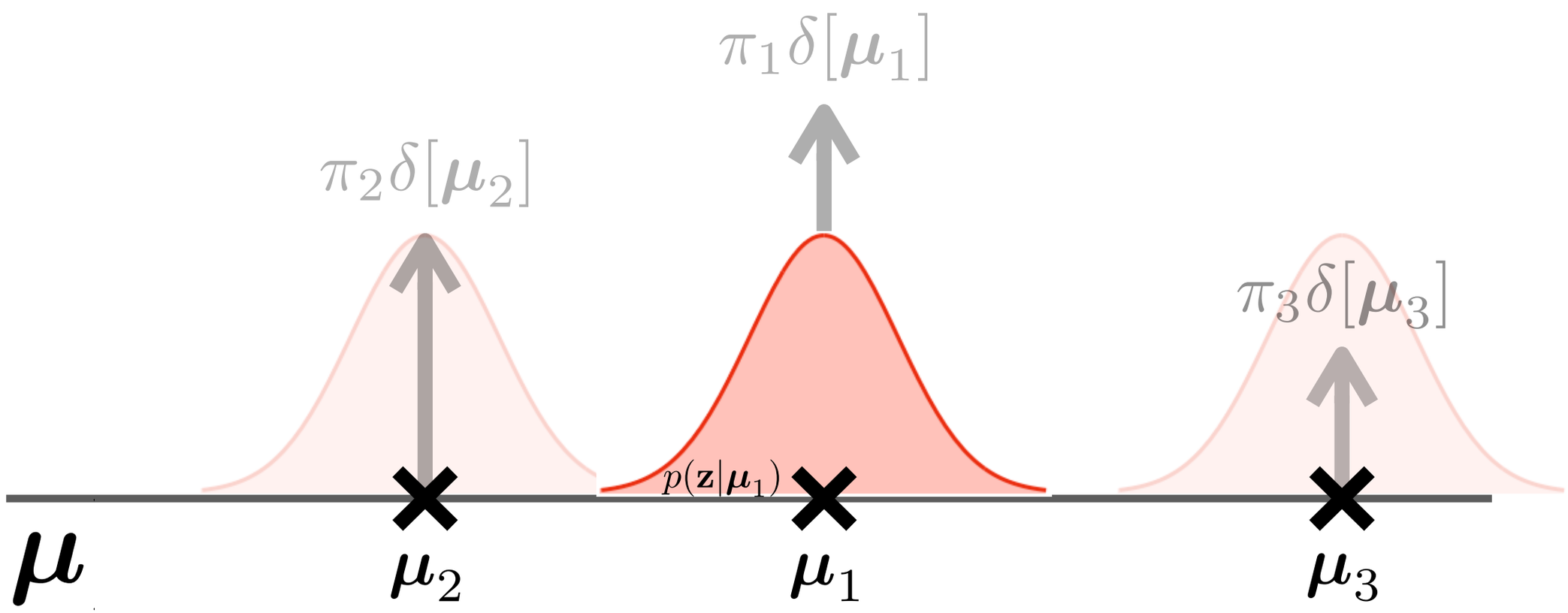

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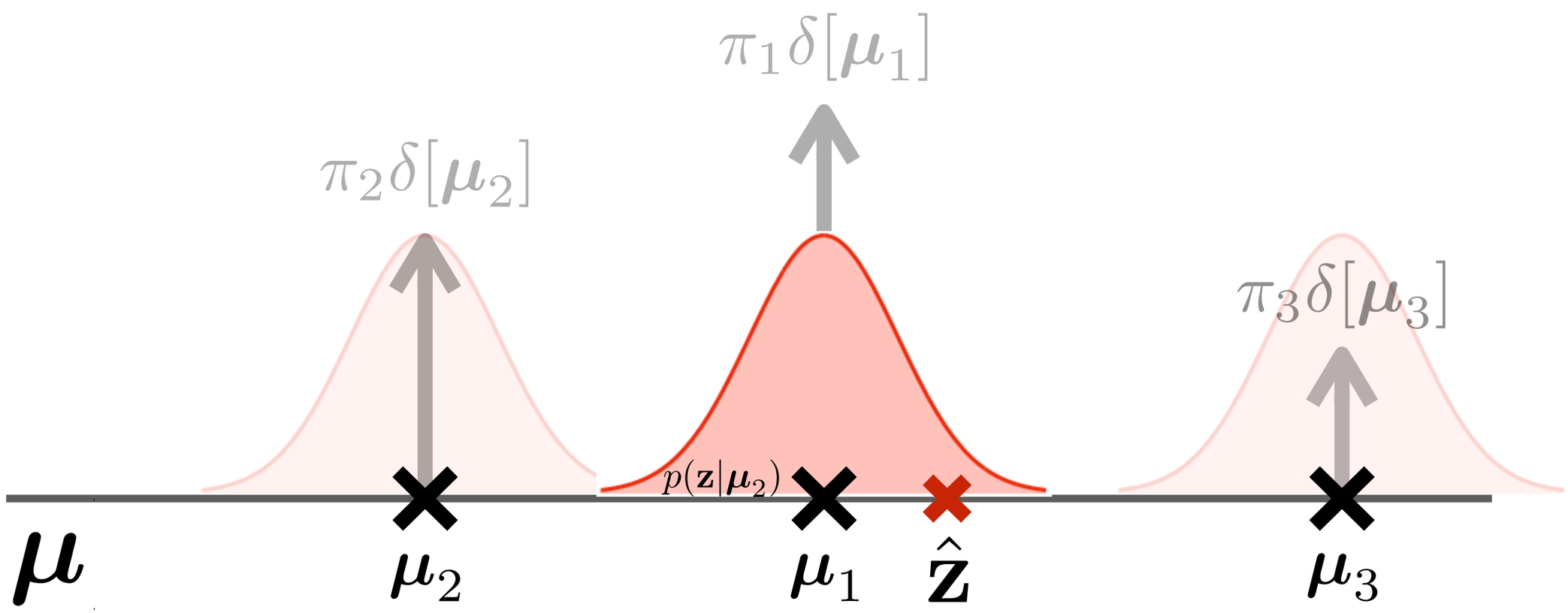

Nonparametric Density Networks

Nonparametric Density Networks

STICK-BREAKING
DENSITY NETWORK

$$\boldsymbol{\pi}_i \sim \mathrm{GEM}(\alpha)$$

$$\mathbf{x}_i \sim p\left(\mathbf{x}_i | \boldsymbol{\pi}_i; \{\mathbf{W}\}_{l=1}^{L+1}\right)$$

Adaptive Width: Due to order bias, can think of the network as having adaptive width, using enough latent variables as the data needs.

Nonparametric Density Networks

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Adaptive Width: Due to order bias, can think of the network as having adaptive width, using enough latent variables as the data needs.

LATENT DIRICHLET PROCESS DENSITY NETWORK

$$\mathbf{z}_i \sim \mathrm{DPMM}(N(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \alpha, N(\boldsymbol{\mu}))$$

$$\mathbf{x}_i \sim p(\mathbf{x}_i|\mathbf{z}_i; \{\mathbf{W}\}_{l=1}^{L+1})$$

Adaptive Complexity: Can draw the latent representation from as complex a distribution as needed.

Amortized Variational Inference

Poondi Kumaraswamy
(1930-1988)

Gradient-Based Inference: Want to use an **inference model** to predict the latent variables and thus need to take gradients through samples. The Beta distribution does not allow this so we use the Beta-like **Kumaraswamy distribution** as the posterior on stick segments

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STICK-BREAKING VAE

Truncated posterior;
not necessary but learns faster

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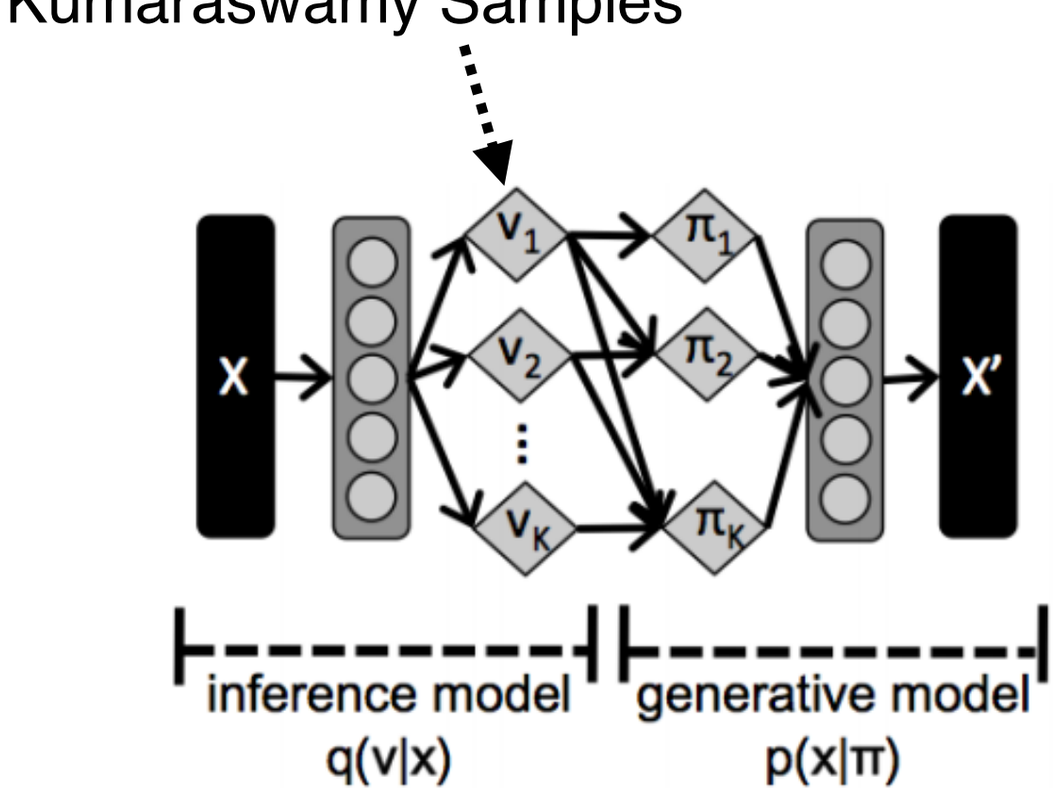

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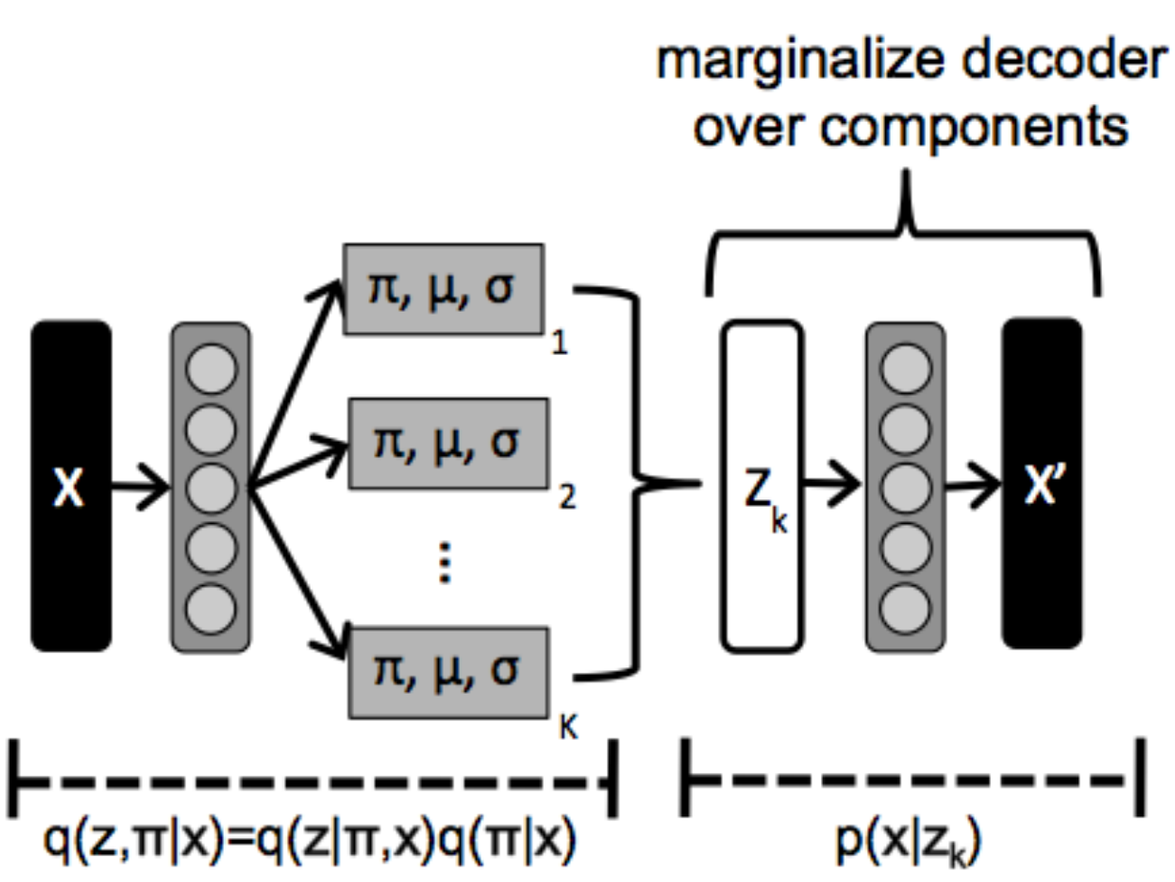
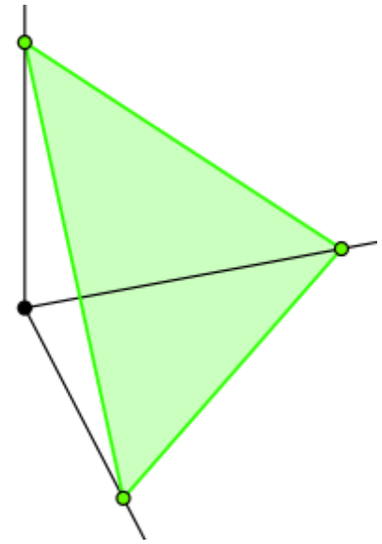
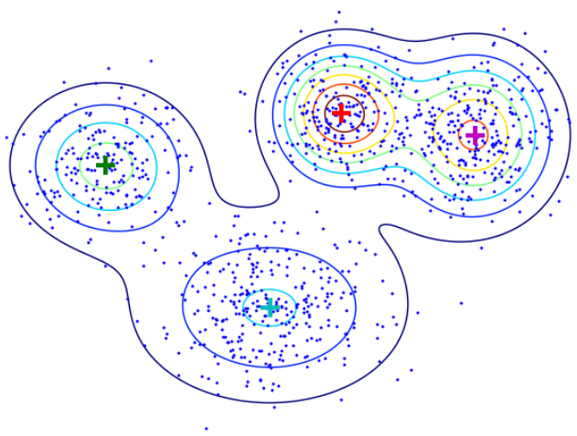


Results: MNIST Samples

STICK-BREAKING VAE

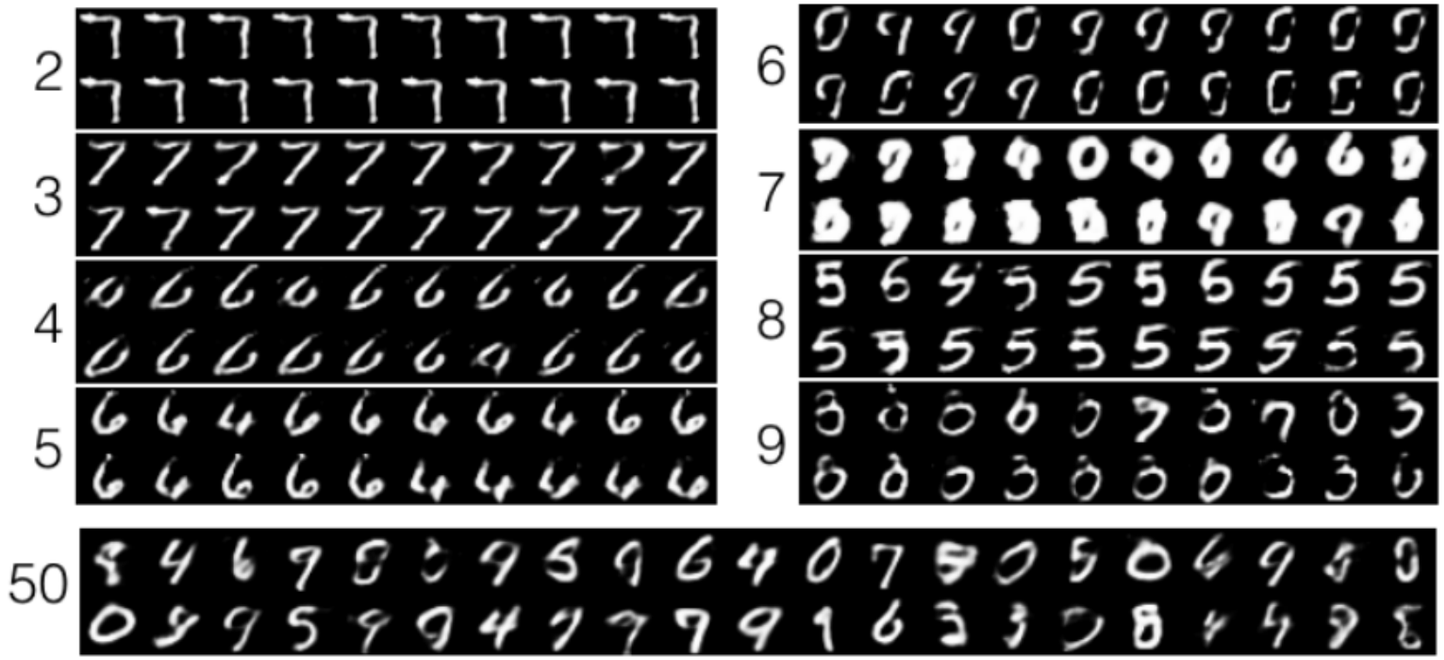


DPMM VAE



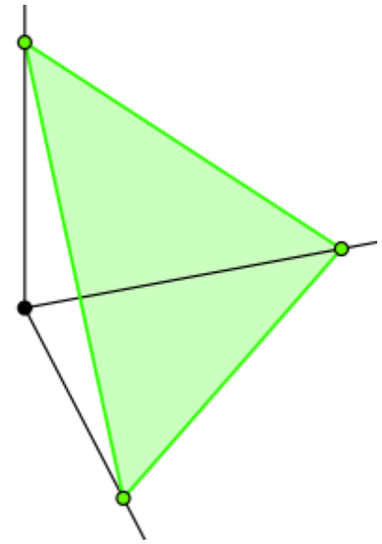
Results: MNIST Samples

DIMENSIONALITY

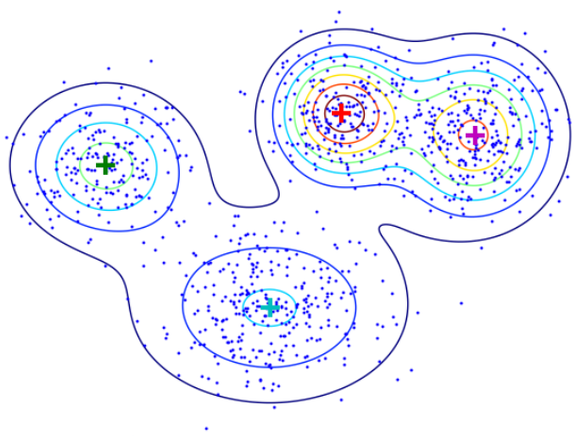


Truncation level of 50. Beta(1,5) prior.

STICK-BREAKING VAE

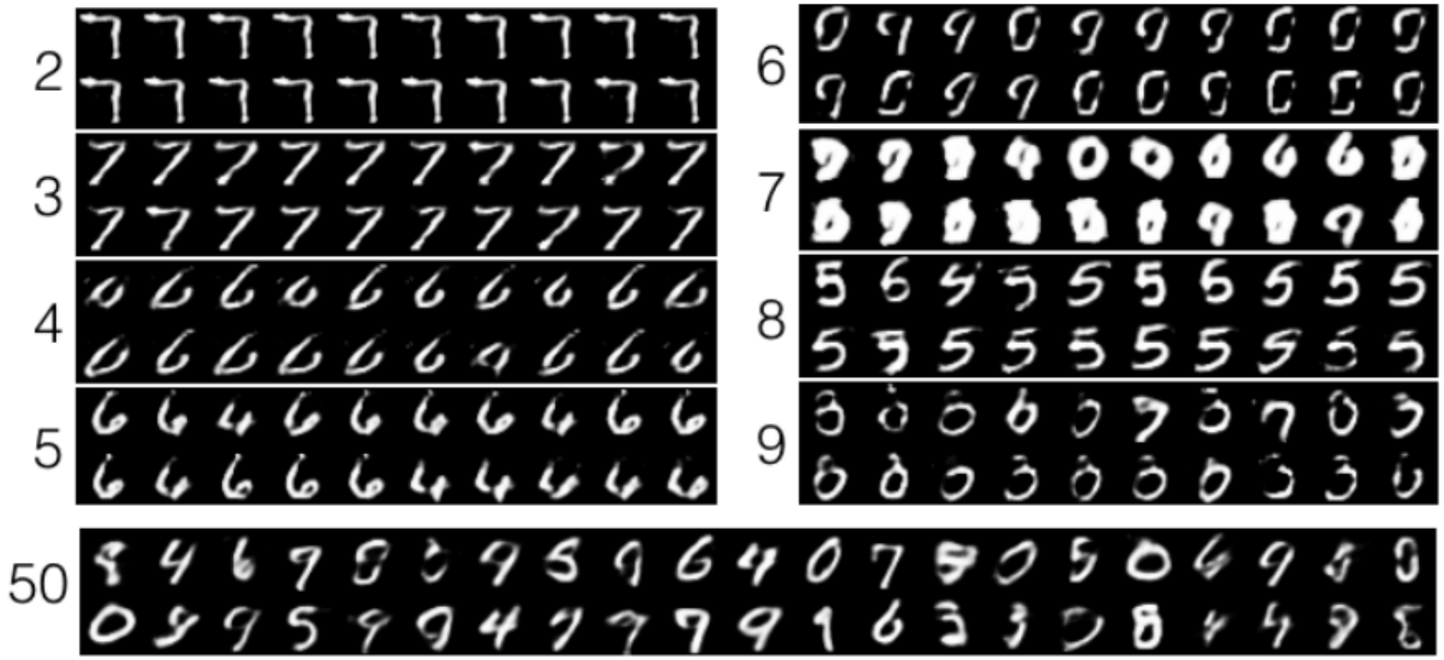


DPMM VAE

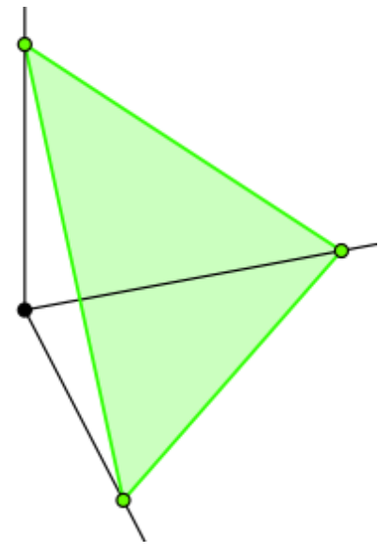


Results: MNIST Samples

DIMENSIONALITY



STICK-BREAKING VAE



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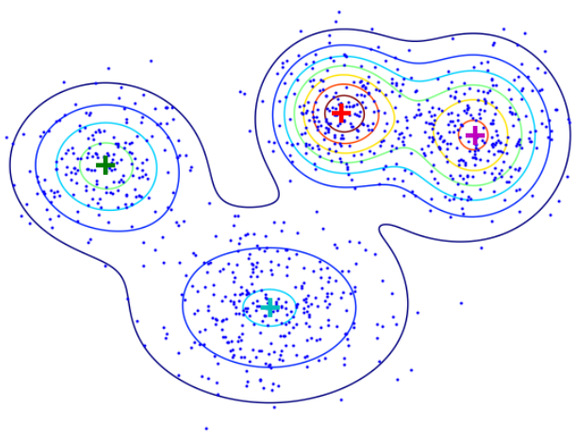
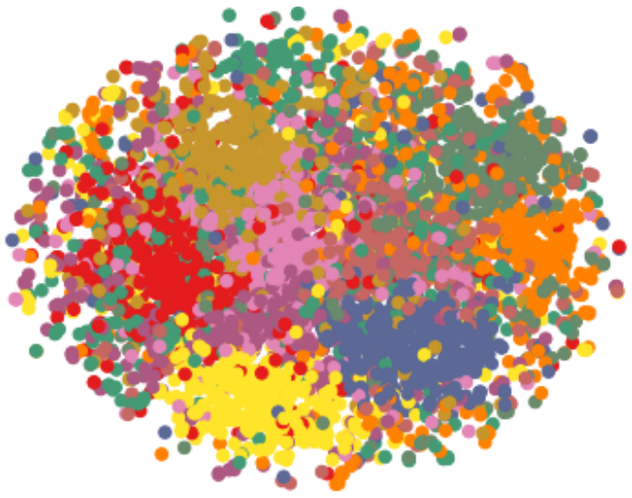


Samples from Component #1

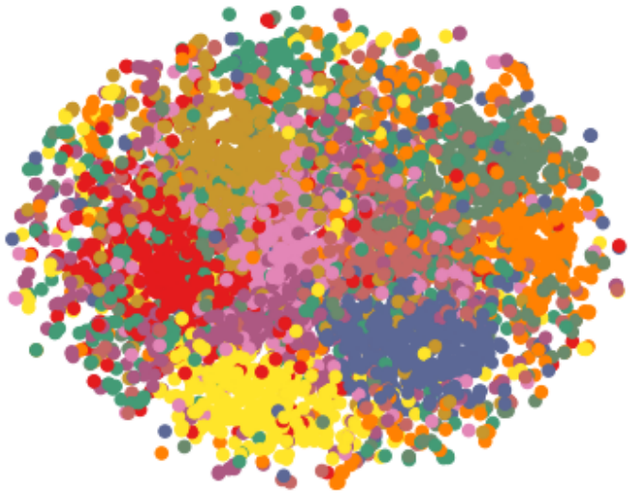
Samples from Component #5

Results: MNIST Latent Space



Gaussian Latent Space (t-SNE)

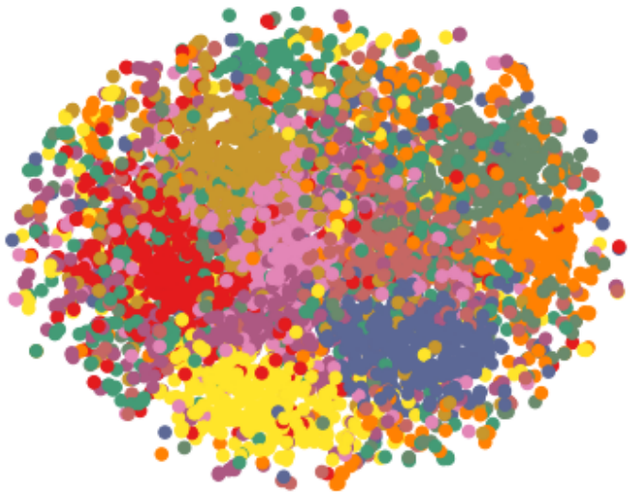
Results: MNIST Latent Space



Gaussian Latent Space (t-SNE)

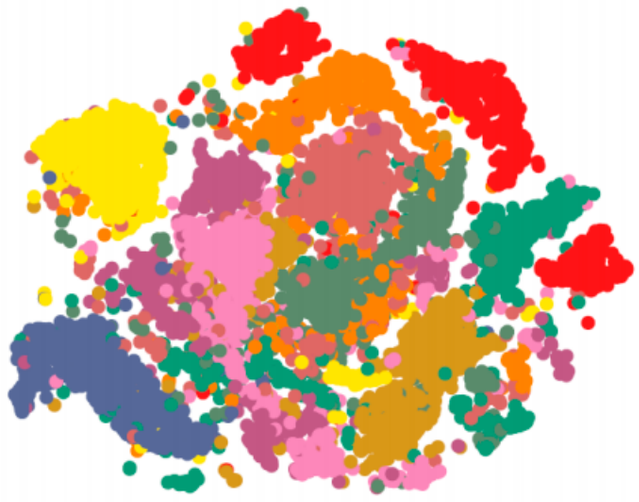
GEM Latent Space (t-SNE)

Results: MNIST Latent Space



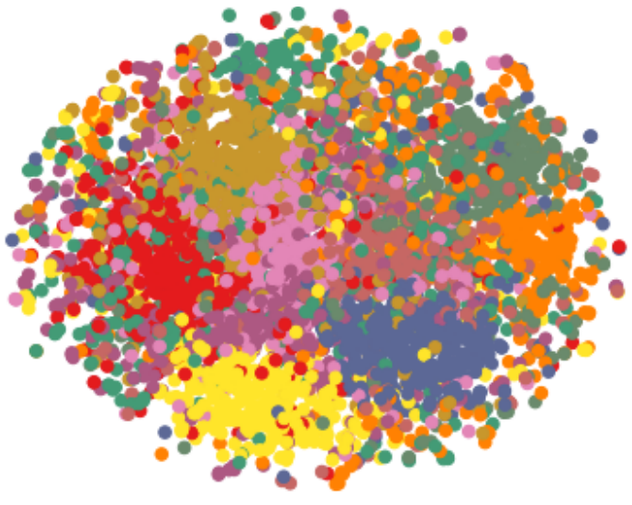
Gaussian Latent Space (t-SNE)

GEM Latent Space (t-SNE)

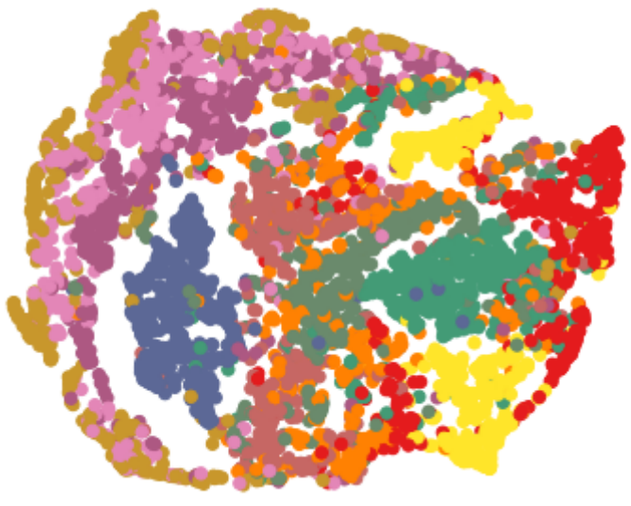


DPMM Latent Space (t-SNE)

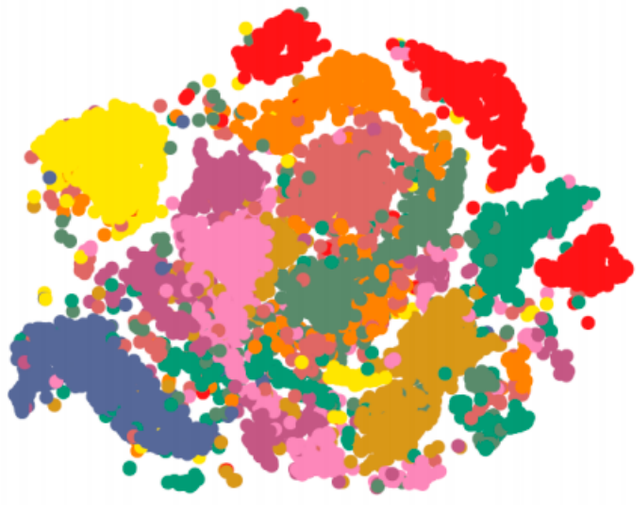
Results: MNIST Latent Space



Gaussian Latent Space (t-SNE)



GEM Latent Space (t-SNE)

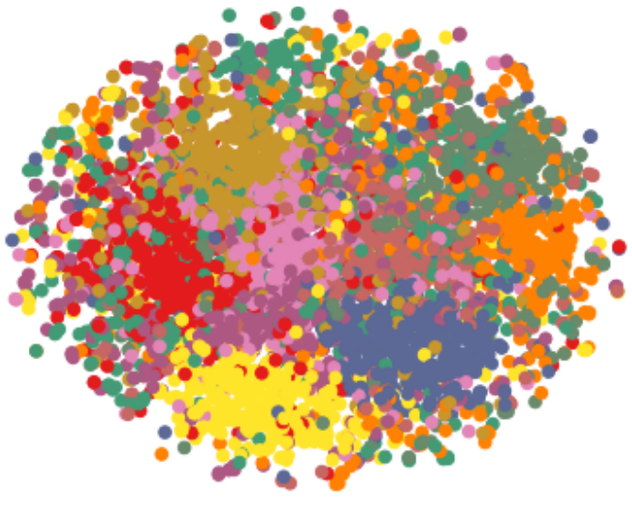


DPMM Latent Space (t-SNE)

	k=3	k=5	k=10
SB-VAE	9.34	8.65	8.90
DLGMM	9.14	8.38	8.42
Gauss VAE	28.4	20.96	15.33
GMVAE[6]	—	8.96	—

Error Rate of k-Nearest Neighbor Classifier on Latent Space

Results: MNIST Latent Space



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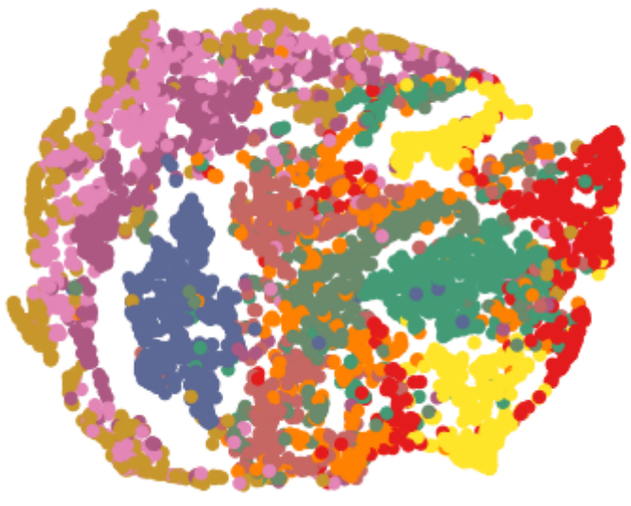

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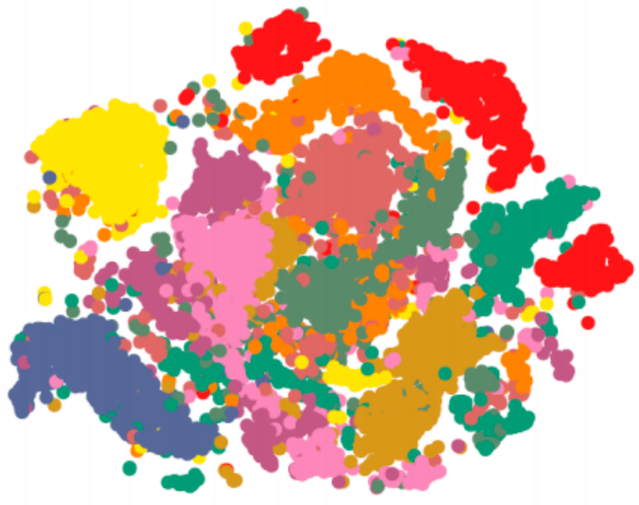

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Error Rate of k-Nearest Neighbor Classifier on Latent Space

Results: Likelihood and Semi-Supervised

HELD-OUT LIKELIHOOD

SEMI-SUPERVISED CLASSIFICATION

Results: Likelihood and Semi-Supervised

HELD-OUT LIKELIHOOD

	$-\log p_{\boldsymbol{\theta}}(\mathbf{x}_i)$	
	MNIST	OMNIGLOT
DLGMM (500d-3x25s)	**96.50**	123.50
DLDPMM (500d-17tx25s)	96.91	123.76
Gauss-VAE (500d-25s)	96.80	**119.18**
SB-VAE (500d-25t)	98.01	–

Negative log likelihood on test set (importance sampled)

SEMI-SUPERVISED CLASSIFICATION

Results: Likelihood and Semi-Supervised

HELD-OUT LIKELIHOOD

	$-\log p_{\boldsymbol{\theta}}(\mathbf{x}_i)$	
	MNIST	OMNIGLOT
DLGMM (500d-3x25s)	**96.50**	123.50
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SB-VAE (500d-25t)	98.01	–

Negative log likelihood on test set (importance sampled)

SEMI-SUPERVISED CLASSIFICATION

	MNIST (N=45,000)			**SVHN** (N=65,000)		
	10%	5%	1%	10%	5%	1%
SB-DGM	4.86$_{\pm.14}$	5.29$_{\pm.39}$	**7.34**$_{\pm.47}$	**32.08**$_{\pm4.00}$	**37.07**$_{\pm5.22}$	**61.37**$_{\pm3.60}$
Gauss-DGM	**3.95**$_{\pm.15}$	**4.74**$_{\pm.43}$	11.55$_{\pm2.28}$	36.08$_{\pm1.49}$	48.75$_{\pm1.47}$	69.58$_{\pm1.64}$
kNN	6.13$_{\pm.13}$	7.66$_{\pm.10}$	15.27$_{\pm.76}$	64.81$_{\pm.34}$	68.94$_{\pm.47}$	76.64$_{\pm.54}$

Error rate on test set when training with X% labeled.

Nonparametric version of (Kingma et al., NIPS 2014)'s M2 model

Priors for Neural Networks

CONDITIONAL MODEL: p(**W**)

NONPARAMETRIC

GP Equivalence [Neal, 1994]
ARD [Neal, 1994; MacKay, 1994]

INDUCTIVE BIAS

SUBJECTIVE BY PROXY

OBJECTIVE

OBJECTIVE

SUBJECTIVE

OBJECTIVE

INDUCTIVE BIAS

NONPARAMETRIC

Stick-Breaking [Nalisnick & Smyth, 2017]
DP-Mixture [Nalisnick et al., 2016]

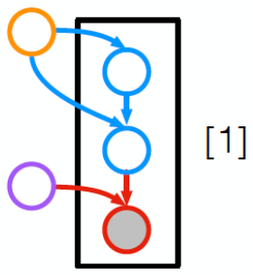
SUBJECTIVE

DENSITY NETWORK: p(**z**)

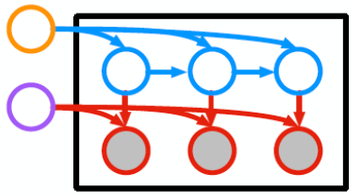
Future Directions and Summary

Future Directions

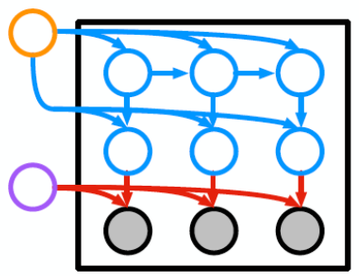
- **Structured Priors / Models:** [Johnson et al., 2016] demonstrated how to combine density networks and latent graphical models.


[1]

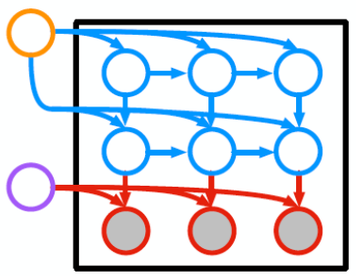
Gaussian mixture model


[2]

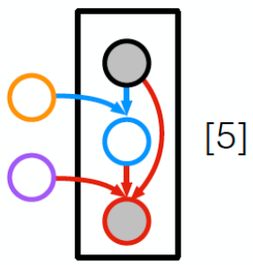
Linear dynamical system


[3]

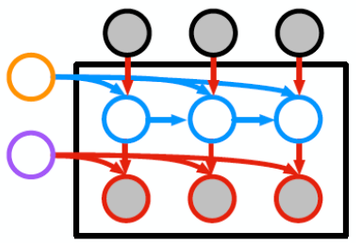
Hidden Markov model


[4]

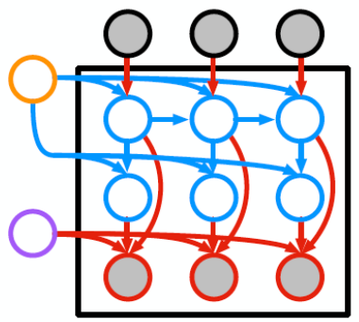
Switching LDS


[5]

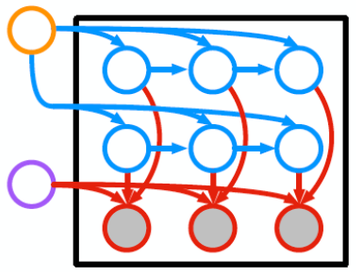
Mixture of Experts


[2]

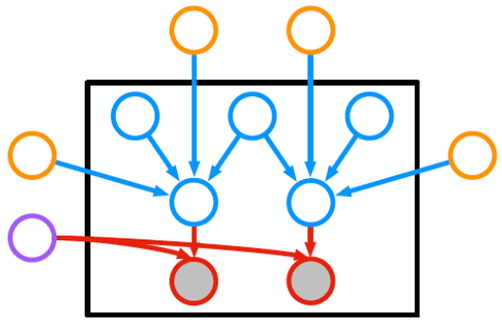
Driven LDS


[6]

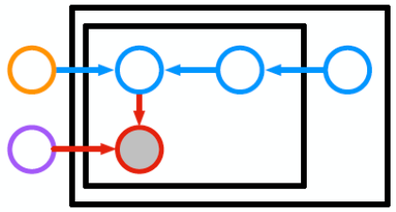
IO-HMM


[7]

Factorial HMM


[8,9]

Canonical correlations analysis


[10]

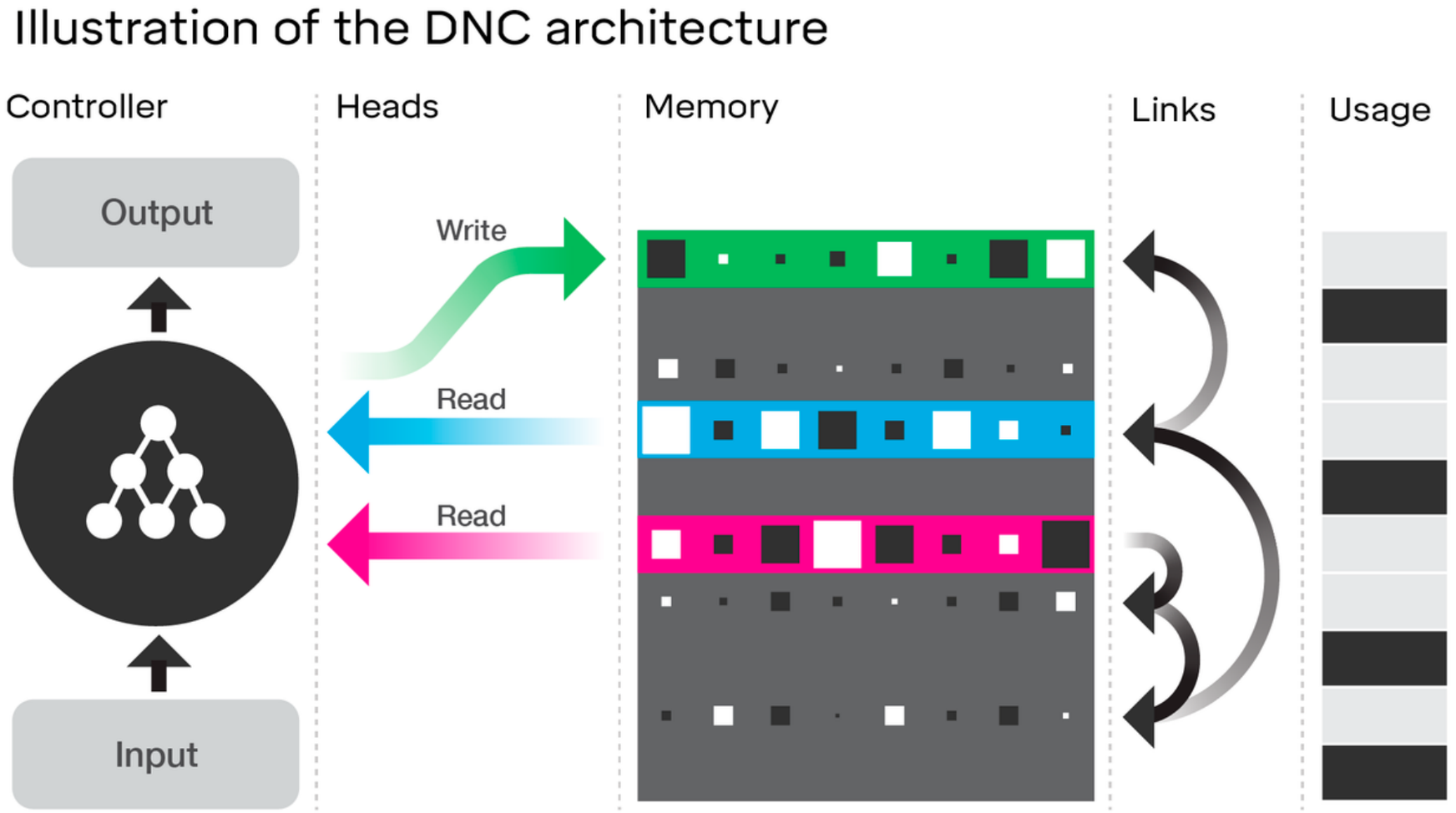
admixture / LDA / NMF


= Neural Network

From M. Johnson's DL summer school slides

Future Directions

- ‘**Neural Nonparametrics’:** Recent deep learning innovations such as *differentiable memory* [Graves et al., 2014] and *adaptive computation* [Graves, 2016] have the character of nonparametrics. I think they can be formalized with traditional BNP priors.



Summary

- [ ] **Bayesian neural networks** have the potential to quantify uncertainty, learn in sequential settings, and ease NN's hunger for data.

- [ ] **Choice of prior is important:** They endow the model with characteristics such as the ability to follow the data and grow in complexity.

- [ ] **Contributions presented:** Extended and explored *reference priors* and *nonparametric priors* for density networks.

Many Thanks to…

MY COMMITTEE



MY RESEARCH GROUP

UCI DATALAB

BREN:ICS
INFORMATION AND COMPUTER SCIENCES
UCIRVINE | UNIVERSITY of CALIFORNIA

Appendix

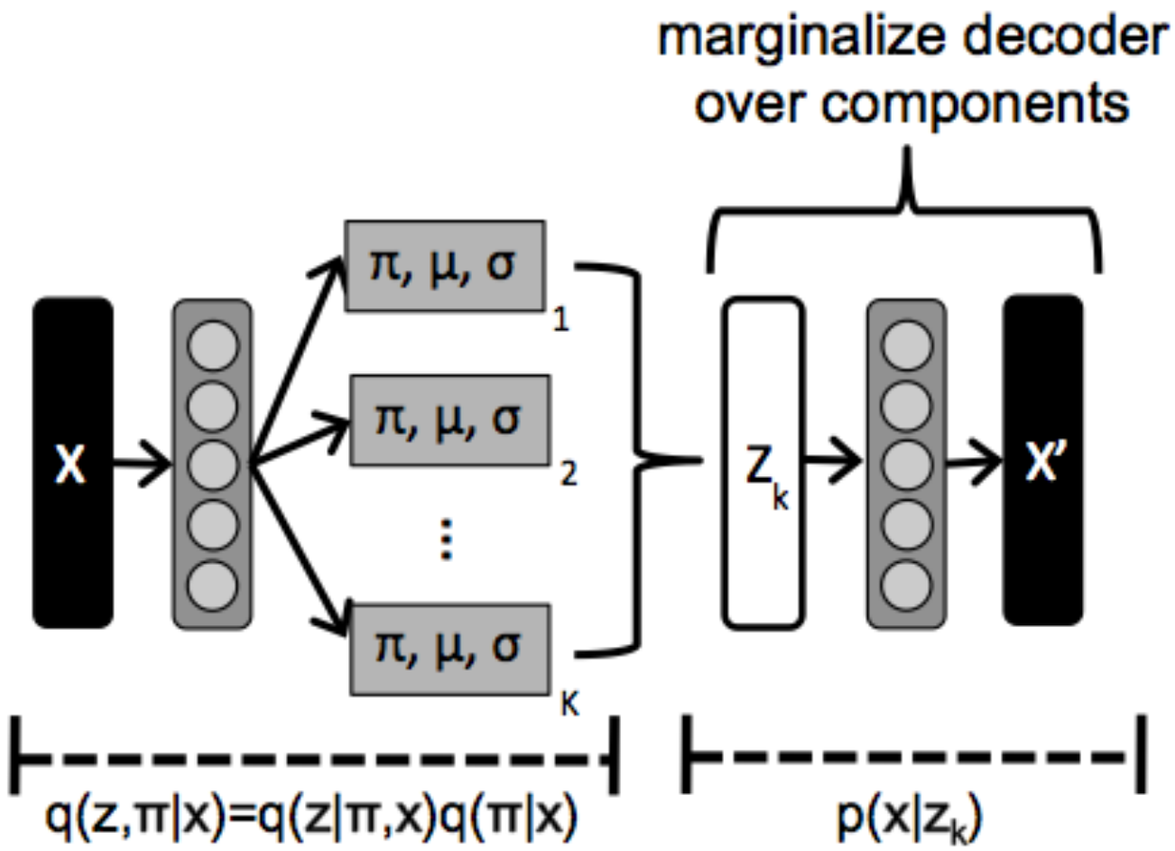
Approximating Reference Priors

Can re-write the Reference prior objective as:

$$
\begin{aligned}
p^*(\boldsymbol{\theta}) &= \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}} \int_{\mathcal{D}} p(\mathcal{D}) \int_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathcal{D}) \log \frac{p(\boldsymbol{\theta}|\mathcal{D})}{p(\boldsymbol{\theta})} d\boldsymbol{\theta} d\mathcal{D} \\
&= \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}} \int_{\boldsymbol{\theta}} p(\boldsymbol{\theta}) \int_{\mathcal{D}} p(\mathcal{D}|\boldsymbol{\theta}) \log \frac{p(\mathcal{D}|\boldsymbol{\theta})}{p(\mathcal{D})} d\mathcal{D} d\boldsymbol{\theta} \\
&= \underset{p(\boldsymbol{\theta})}{\operatorname{argmax}} \mathbb{E}_{p(\boldsymbol{\theta})} KLD[p(\mathcal{D}|\boldsymbol{\theta}) \,||\, p(\mathcal{D})].
\end{aligned}
$$

MODEL #2: Dirichlet Process Variational Autoencoder

(Nalisnick et al., 2016)



$$\mathcal{L}_{\text{SGVB}} = \sum_k \mu_{\pi_k} [\frac{1}{S} \sum_s \log p_{\boldsymbol{\theta}}(\mathbf{x}_i | \hat{\mathbf{z}}_{i,k,s}) + \mathbb{E}_{q_k}[\log p(\mathbf{z}_i)]]$$

$$- \text{KLD}[q(\boldsymbol{\pi}_k|\mathbf{x}_i)||p(\boldsymbol{\pi}_k)] - \frac{1}{S} \sum_s \log \sum_k \hat{\pi}_{i,k,s} q(\hat{\mathbf{z}}_{i,k,s}; \boldsymbol{\phi}_k)$$