Day 2
Probabilistic Models with Deep Neural Networks

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Masegosa, A. R., Cabañas, R., Langseth, H., Nielsen, T. D., & Salmern, A. (2019). Probabilistic Models with Deep Neural Networks. arXiv preprint arXiv:1908.03442.

Plan for this week

Day 1: Introduction to probabilistic programming languages

- Why do we need PPLs?
- Probabilistic programming in Pyro
- Hand-on exercises:
  - Probability Distributions in Pyro.
  - Probabilistic Models in Pyro.
  - Ice-cream Shop Model.

Day 2: Probabilistic Models with Deep Neural Networks

- Uncertainty in Machine Learning
- Variational Inference
- Supervised/Unsupervised Learning
- Hand-on exercises
  - Bayesian Neural Networks
  - Variational Auto-encoders

Uncertainty with Machine Learning

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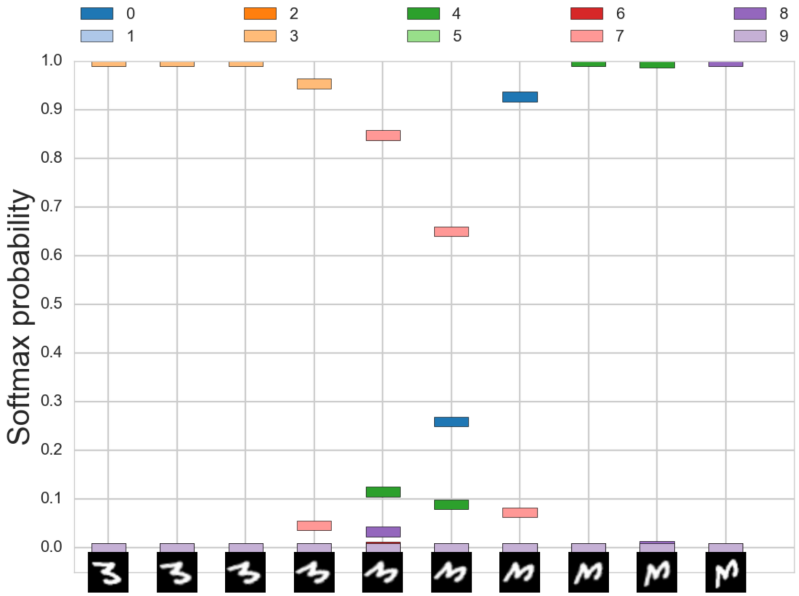

Why is important to model uncertainty?

- To assess **confidence in the predictions**.
- To know **what I don't knowWhy ilist**.
- **Big implications** in many problems.

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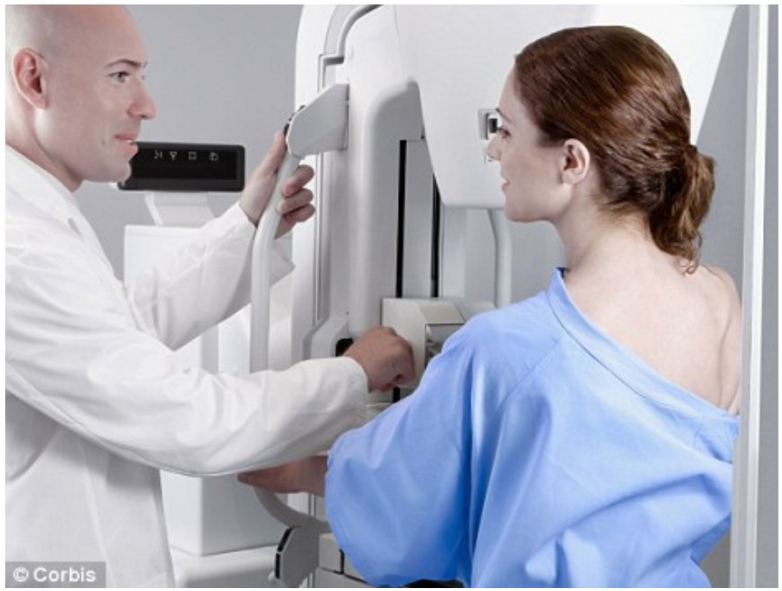

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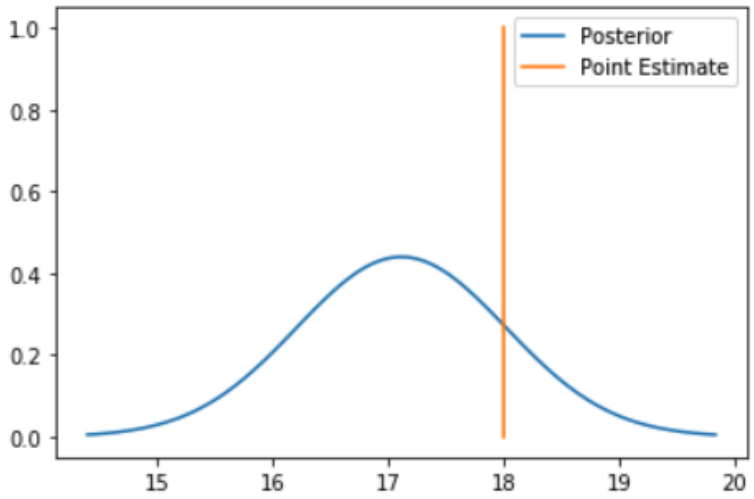
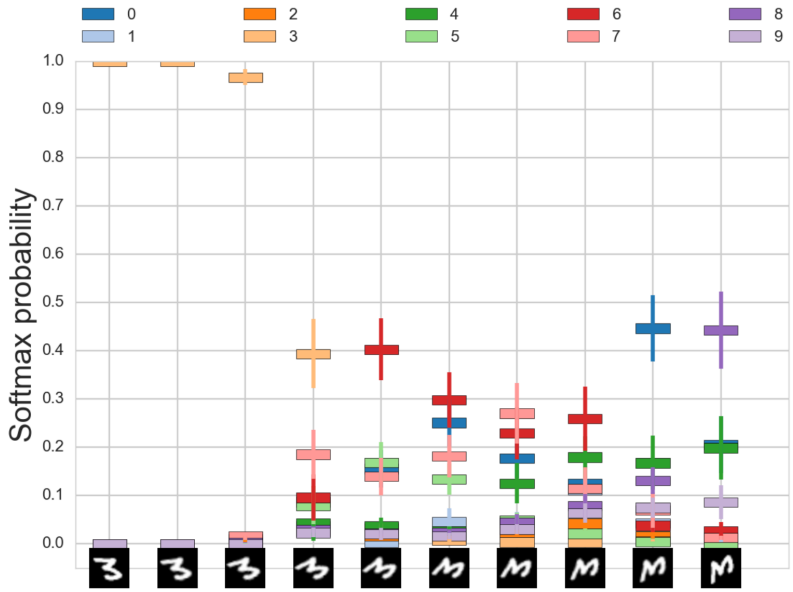



```
P(Temperature|Sensor=18.0) =
Normal(loc: 17.115509033203125, scale: 0.9070338010787964)
```

Probabilistic Models naturally quantify uncertainty

- Everything is defined in terms of **random variables**.
- **Standard language** to model uncertainty.



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Example

Real Data Example

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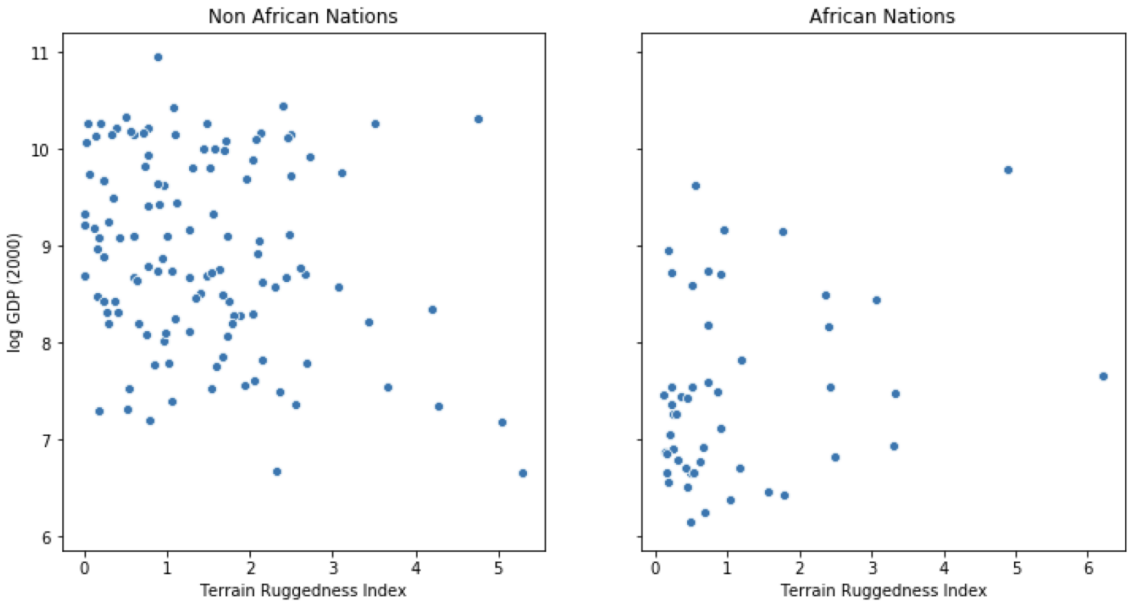

Relationship between topographic heterogeneity and GDP per capita

- Is Terrain ruggedness or **bad geography** is related to poorer economic performance outside of Africa?

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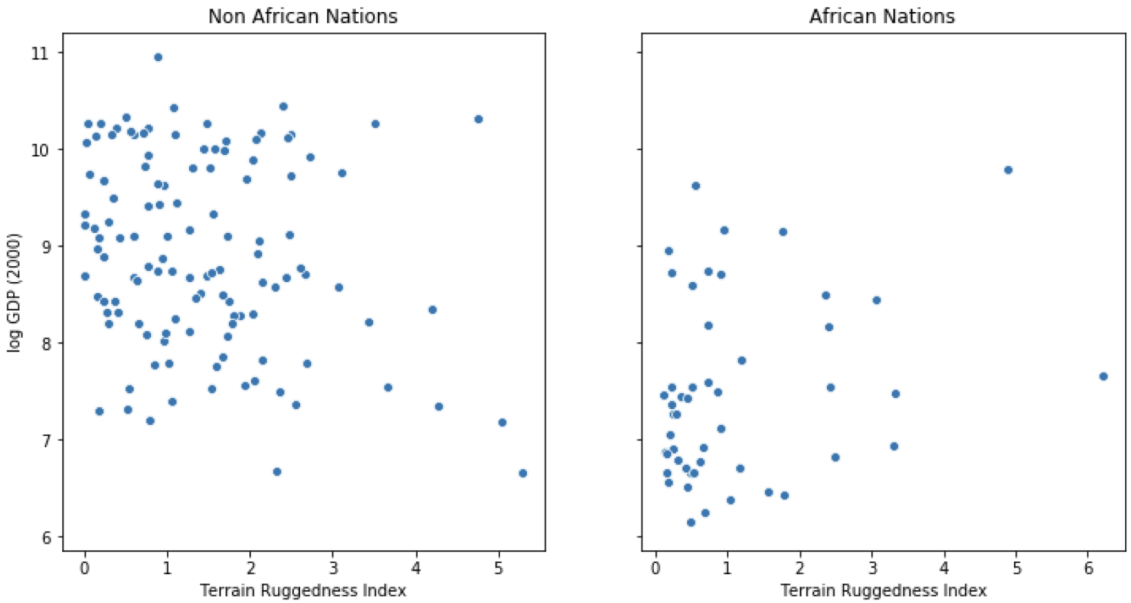

Relationship between topographic heterogeneity and GDP per capita

- Is Terrain ruggedness or **bad geography** is related to poorer economic performance outside of Africa?
- Does **rugged terrains** have had a reverse effect on income for African nations?

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$$y = w_0 + w_1 \cdot x$$

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`Day1/students_Bayesian_regression.ipynb`

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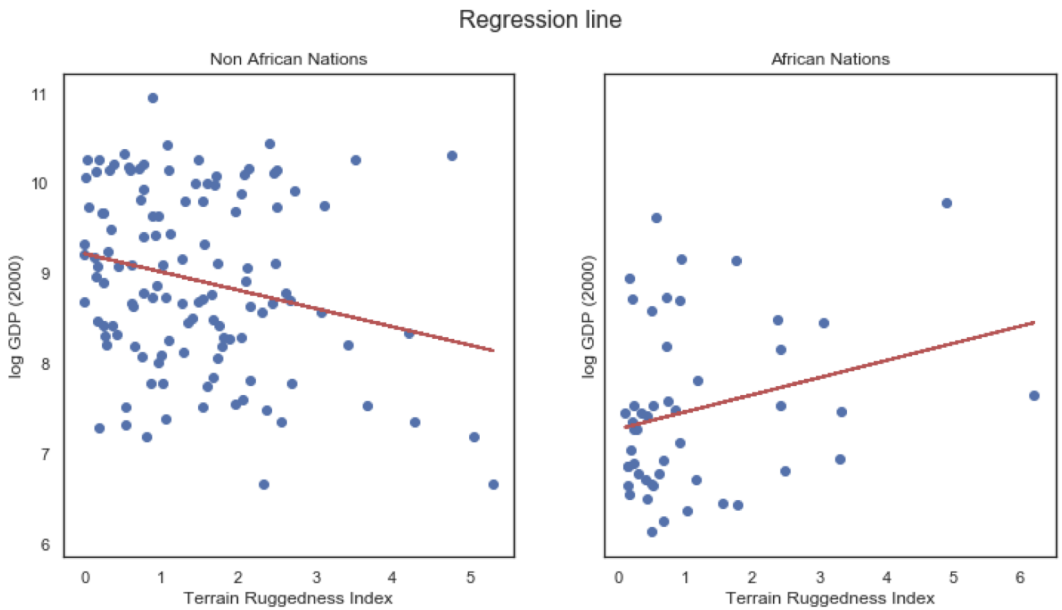

Linear Regression Model

- Negative slope for Non African Nations.
- Positive slope for African Nations.

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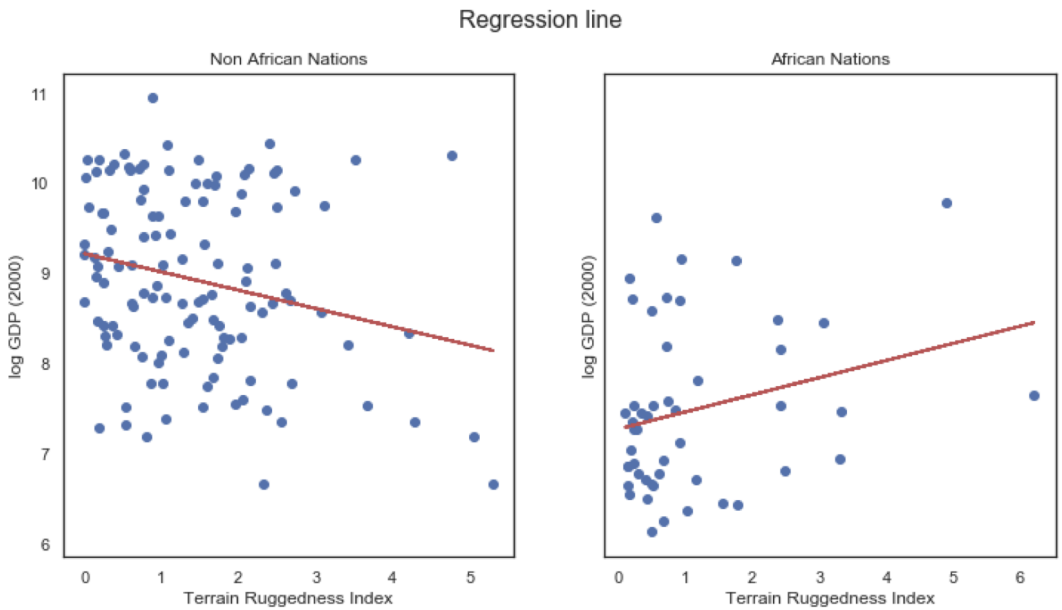

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Are we 100% sure about the conclusion?

Bayesian Machine Learning

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3. **We compute the posterior (Bayes' rule)**:

$$p(w_0, w_1, \sigma^2|D) = \frac{\prod_{i=1}^{n} p(y_i|x_i, w_0, w_1, \sigma^2) p(w_0, w_1, \sigma^2)}{p(y_1, \ldots, y_n|x_1, \ldots, x_n)}$$

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Day1/students_Bayesian_regression.ipynb

Exercise: Bayesian Logistic Regression

- Predicts whether a country is African or not based on ruggedness and GDP.

`Day1/students_Bayesian_Regression.ipynb`

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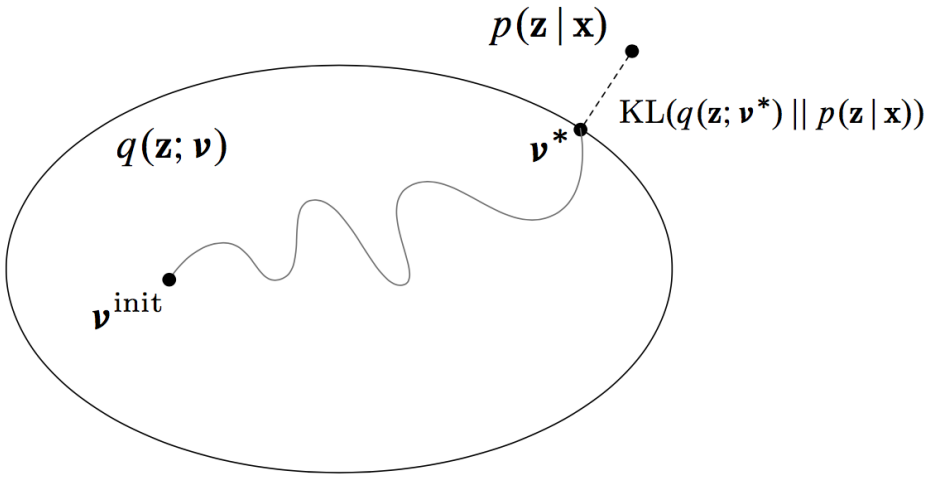
We have to use **approximate posterior inference**.

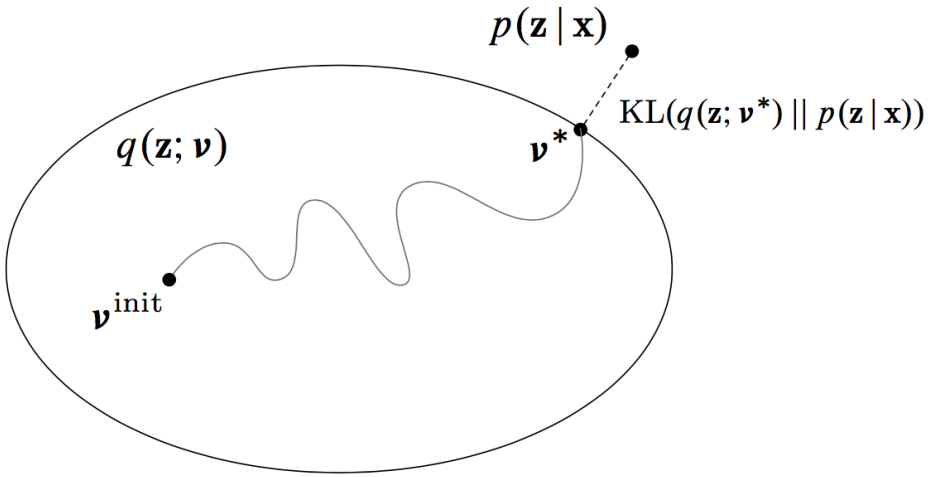
Variational Inference



- **Variational Inference** is an approximate method,

$$q(\mathbf{z}|\boldsymbol{\nu}) \approx p(\mathbf{z}|\mathbf{x})$$

  - $q(\mathbf{z}|\boldsymbol{\nu})$ is a simpler distribution (e.g. diagonal covariance matrix, unimodal).



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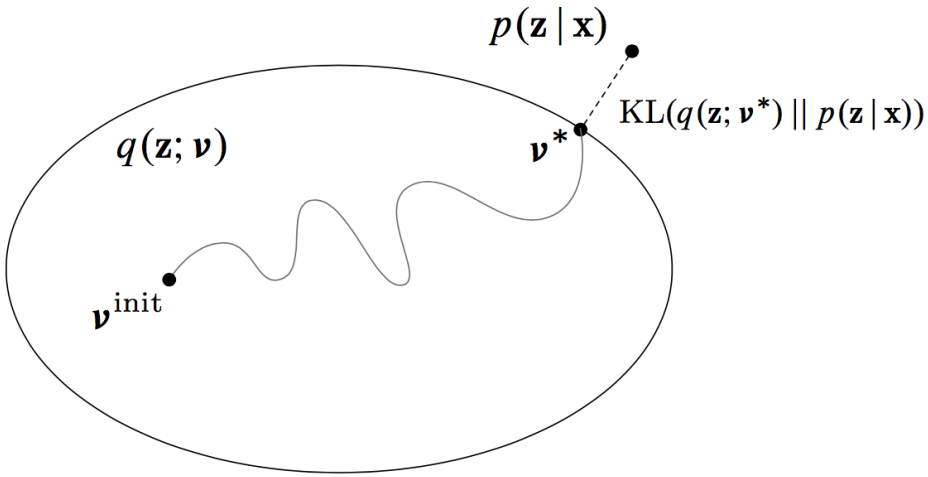

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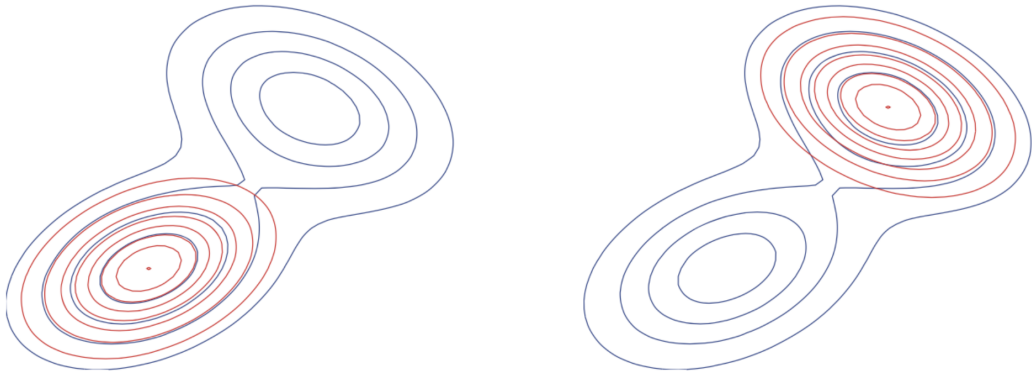

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- The above minimization problem is **equivalent to maximize the ELBO function**,

$$\boldsymbol{\nu}^{\star} = \arg\max_{\nu} \mathcal{L}(\boldsymbol{\nu})$$

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4. Use the variational approximation as a **proxy**,

$$q(\mathbf{z}|\boldsymbol{\nu}) \approx p(\mathbf{z}|\mathbf{x})$$

Variational Inference in Pyro

```
#The observatons
obs = {'sensor': torch.tensor(18.0)}

def model(obs):
    temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
    sensor = pyro.sample('sensor', dist.Normal(temp, 1.0), obs=obs['sensor'])
```

Pyro's Model

- We have a **probabilistic model**,

$$p(temp) = \mathcal{N}(15.0, 2.0)$$
$$p(sensor|temp) = \mathcal{N}(sensor, 2.0)$$

```python
#The guide
def guide(obs):
    a = pyro.param("mean", torch.tensor(0.0))
    b = pyro.param("scale", torch.tensor(1.), constraint=constraints.positive)
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Pyro's Guides

- We want to compute the **posterior**, $p(temp|sensor = 18.0)$
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- We define, $q(temp|\boldsymbol{\nu}) = \mathcal{N}(\boldsymbol{\nu}_a, \boldsymbol{\nu}_b)$
- **Guide's requirements**:
  - Model and Guide have both **same input signature**.
  - All **unobserved sample statements** in the model must appear in the guide.

```
pyro.clear_param_store()
svi = pyro.infer.SVI(model=temperature_model,
                     guide=guide,
                     optim=SGD({"lr": 0.001, "momentum":0.1}),
                     loss=Trace_ELBO())

for t in range(num_steps):
    svi.step(obs)
```

Pyro's Variational Inference

- We run **optimization** to solve,

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Exercise: Pyro implementation for a simple Gaussian model

1. Implement a Pyro's **model** for a Normal distribution with prior over mean and (inverse) of variance. The variable x is always observed.

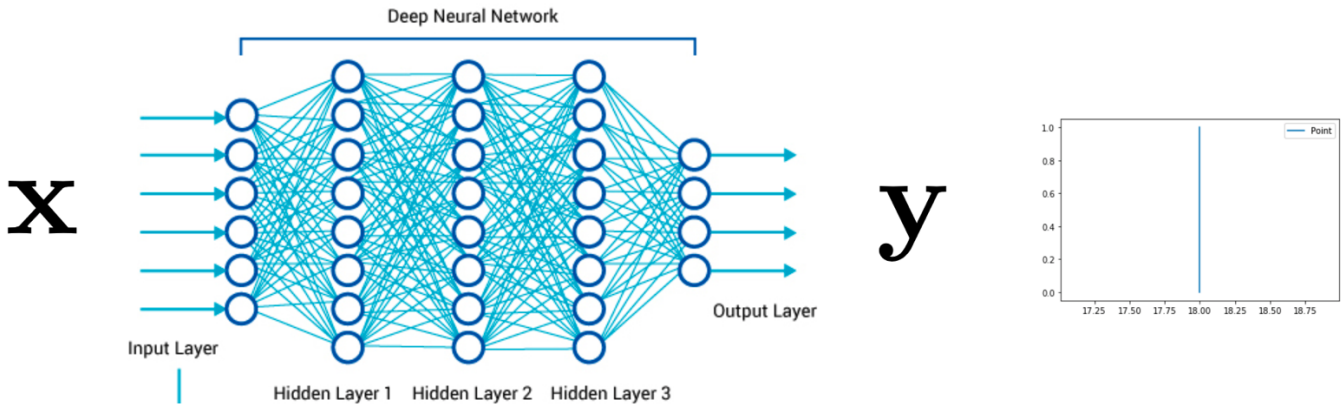
$$
\begin{aligned}
p(\mu) &= \text{Normal}(0, 10000.0) \\
p(\gamma) &= \text{Gamma}(1, 1) \\
p(x \mid \mu, \gamma) &= \text{Norma}(\mu, 1/\gamma)
\end{aligned}
$$

2. Define a Pyro's **guide** for approximating the posterior,

$$p(\mu, \gamma | \mathbf{x})$$

`Session2/student_simple_model.ipynb`

Supervised Probabilistic Models with Deep Neural Networks



Neural Network

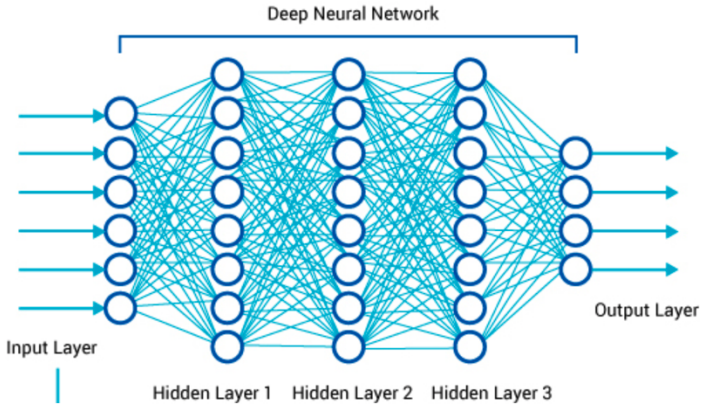
- $h(\cdot;\theta)$ encodes a neural network (i.e. a non-linear function).

$$\mathbf{y} = h(\mathbf{x};\theta)$$

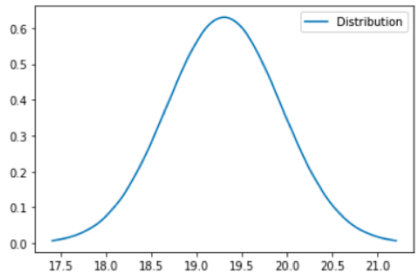
- Loss minimization,

$$\arg\min_{\theta} \sum_{i=1}^{n} \ell(h(\mathbf{x}_i;\theta), \mathbf{y}_i)$$

$\mathbf{x}$



$p(y|h(\mathbf{x};\theta))$

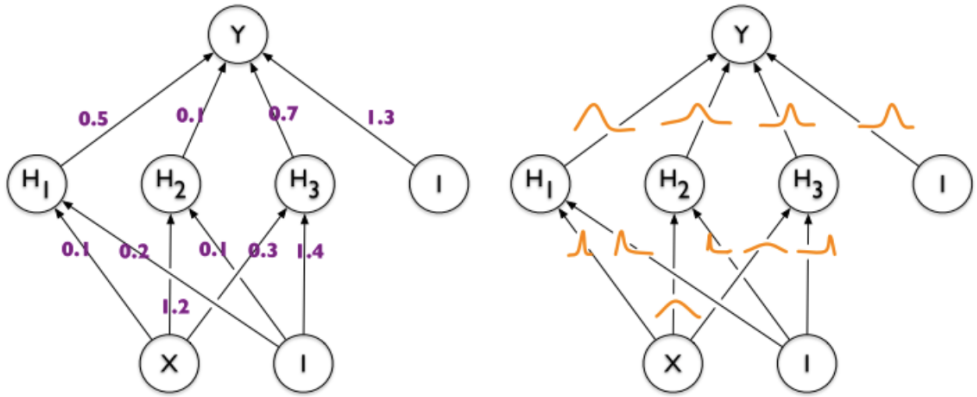


Bayesian Neural Network

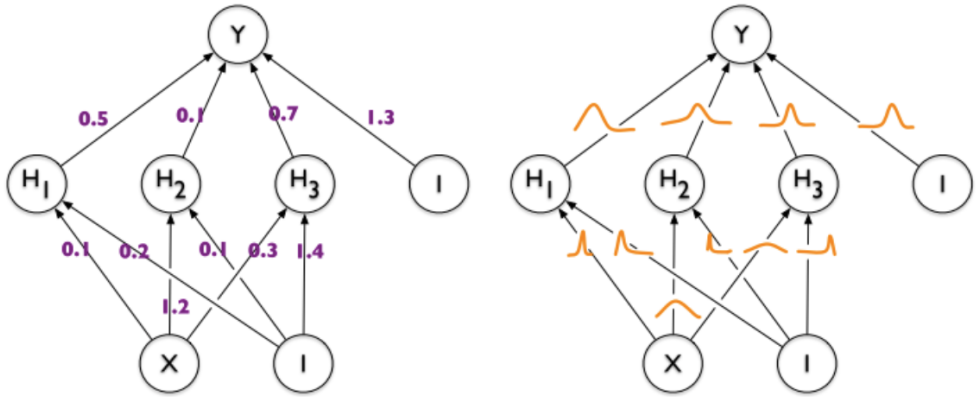
- E.g. Neural regressor,

$$p(y|\mathbf{x},\theta) = \mathcal{N}(\mu = h(\mathbf{x};\theta_h), \sigma^2 = g(\mathbf{x};\theta_g))$$

$h(\cdot;\theta)$ encodes a neural network.



Bayesian Neural Network



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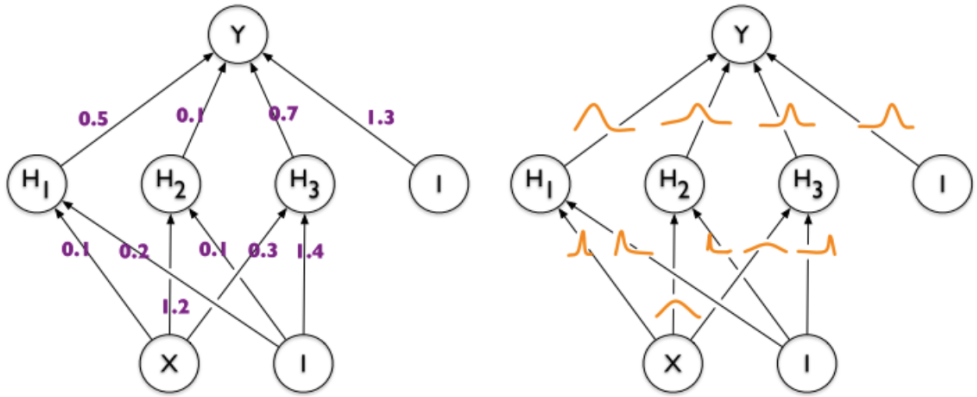

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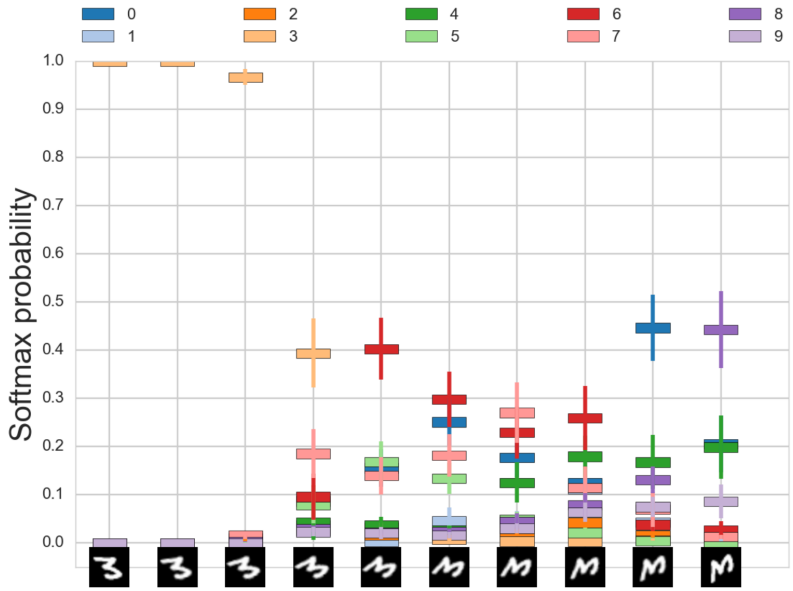
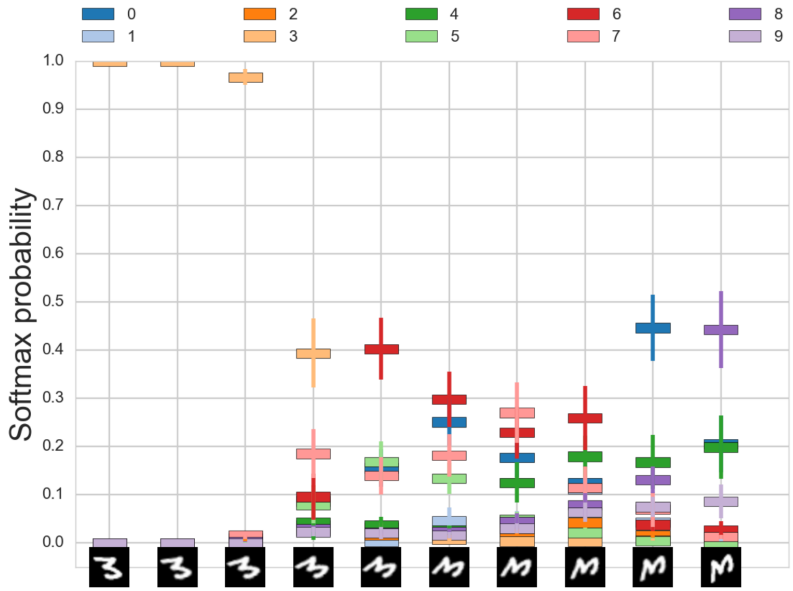
- Bayesian predictive is an **ensemble of neural networks**,

$$p(y|\mathbf{x}) = \int p(y|\mathbf{x}, \theta) q(\theta|\boldsymbol{\nu}^\star)$$
$$\approx \frac{1}{M} \sum_{\theta_j \sim q(\theta|\boldsymbol{\nu}^\star)} p(y|\mathbf{x}, \theta_j)$$



Bayesian Neural Networks

- Capture the uncertainty.
- Better identify low confidence predictions (**They know what they don't know**).



Bayesian Neural Networks

- Capture the uncertainty.
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Unsupervised Probabilistic Models with Deep Neural Networks

$$\mathbf{z} \sim p(\mathbf{z})$$
$$\mathbf{x} \sim p(\mathbf{x}|h(\mathbf{z};\theta))$$

Bayesian Neural Network

- $h(\cdot;\theta)$ encodes a neural network.
- E.g. Neural regressor,

$$p(y|\mathbf{x}) = \mathcal{N}(\mu = h(\mathbf{x};\theta_h), \quad \sigma^2 = g(\mathbf{x};\theta_g))$$

- Variational Inference,

$$\boldsymbol{\nu}^\star = \arg\min_{\nu} KL\big(q(\theta|\boldsymbol{\nu})||p(\theta|\mathbf{x})\big)$$

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