Probabilistic Programming with Deep Neural Networks

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https://andresmasegosa.github.io/
https://pgmlab.github.io/

This material jointly made with Thomas D. Nielsen (AAU).

Plan for this week

Day 1: Introduction to probabilistic programming languages

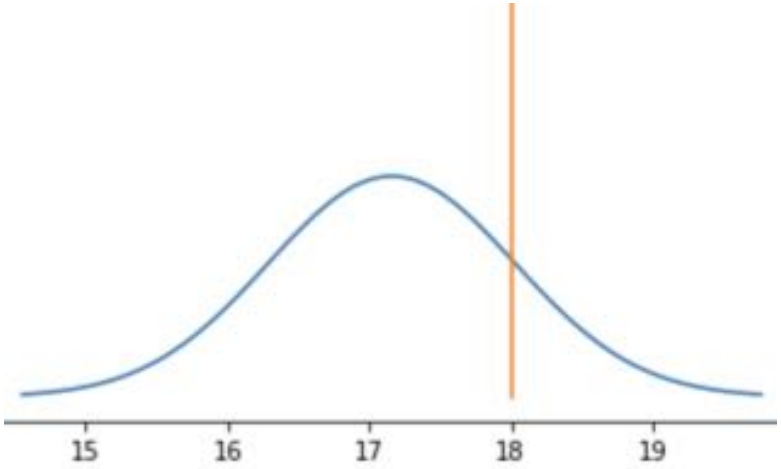
- Why do we need PPLs?
- Probabilistic programming in Pyro
- Hand-on exercises:
  - Probability Distributions in Pyro.
  - Probabilistic Models in Pyro.

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

What is a PPL?

What is a probabilistic model?



Normal Distribution

What is a probabilistic model?

VQ-VAE-2

What is a PPL?

```
import tensorflow as tf
import tensorflow_probability as tfp

# Pretend to load synthetic data set.
features = tfp.distributions.Normal(loc=0., scale=1.).sample(int(100e3))
labels = tfp.distributions.Bernoulli(logits=1.618 * features).sample()

# Specify model.
model = tfp.glm.Bernoulli()

# Fit model given data.
coeffs, linear_response, is_converged, num_iter = tfp.glm.fit(
    model_matrix=features[:, tf.newaxis],
    response=tf.cast(labels, dtype=tf.float32),
    model=model)
# ==> coeffs is approximately [1.618] (We're golden!)
```

Probabilistic Programming Language (PPL)

- An attempt to **unify probabilistic modeling and general programming languages**.

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- A programming paradigm to define **general probabilistic models (mixing deterministic + stochastic functions)**.

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Probabilistic Programming Language (PPL)

- An attempt to **unify probabilistic modeling and general programming languages**.
- A programming paradigm to define **general probabilistic models (mixing deterministic + stochastic functions)**.
- Make probabilistic modeling more **applicable and powerful**.

Why PPLs?

Why do we need PPLs?

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- Reason 1: Try to democratize the development of AI systems.

Why do we need PPLs?

- Reason 1: Try to democratize the development of AI systems.
- Reason 2: Try to make AI systems safer.

Reason 1: Try to democratize the development of AI systems.

DARPA's Fund Call for PPLs in Artificial Intelligence.

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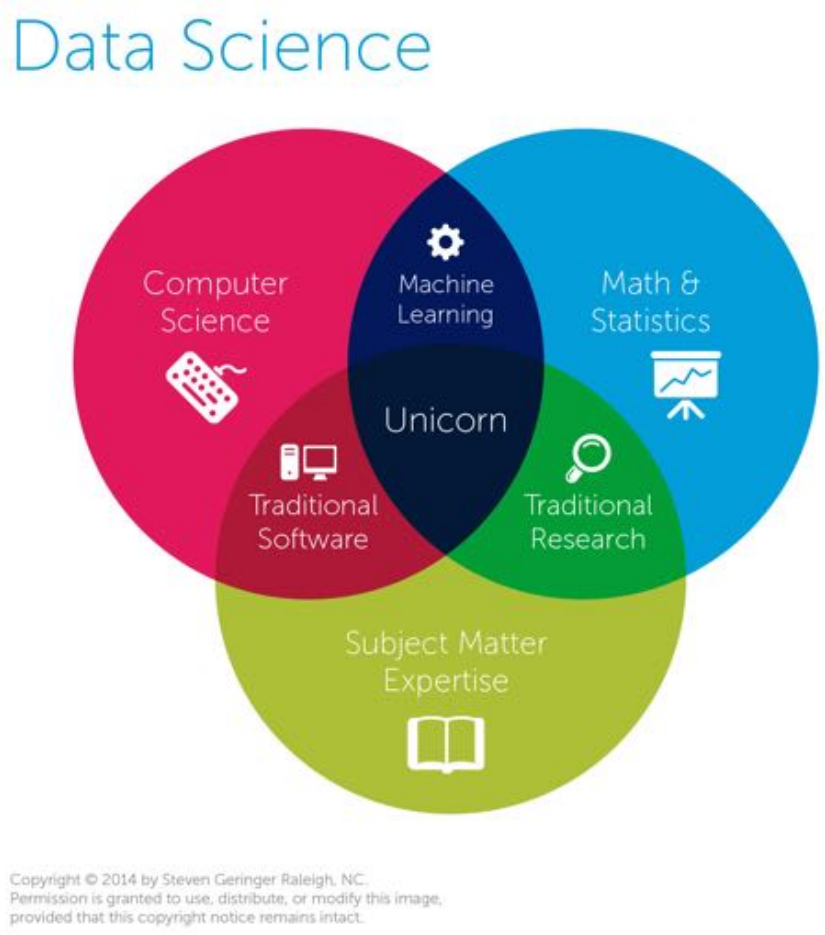
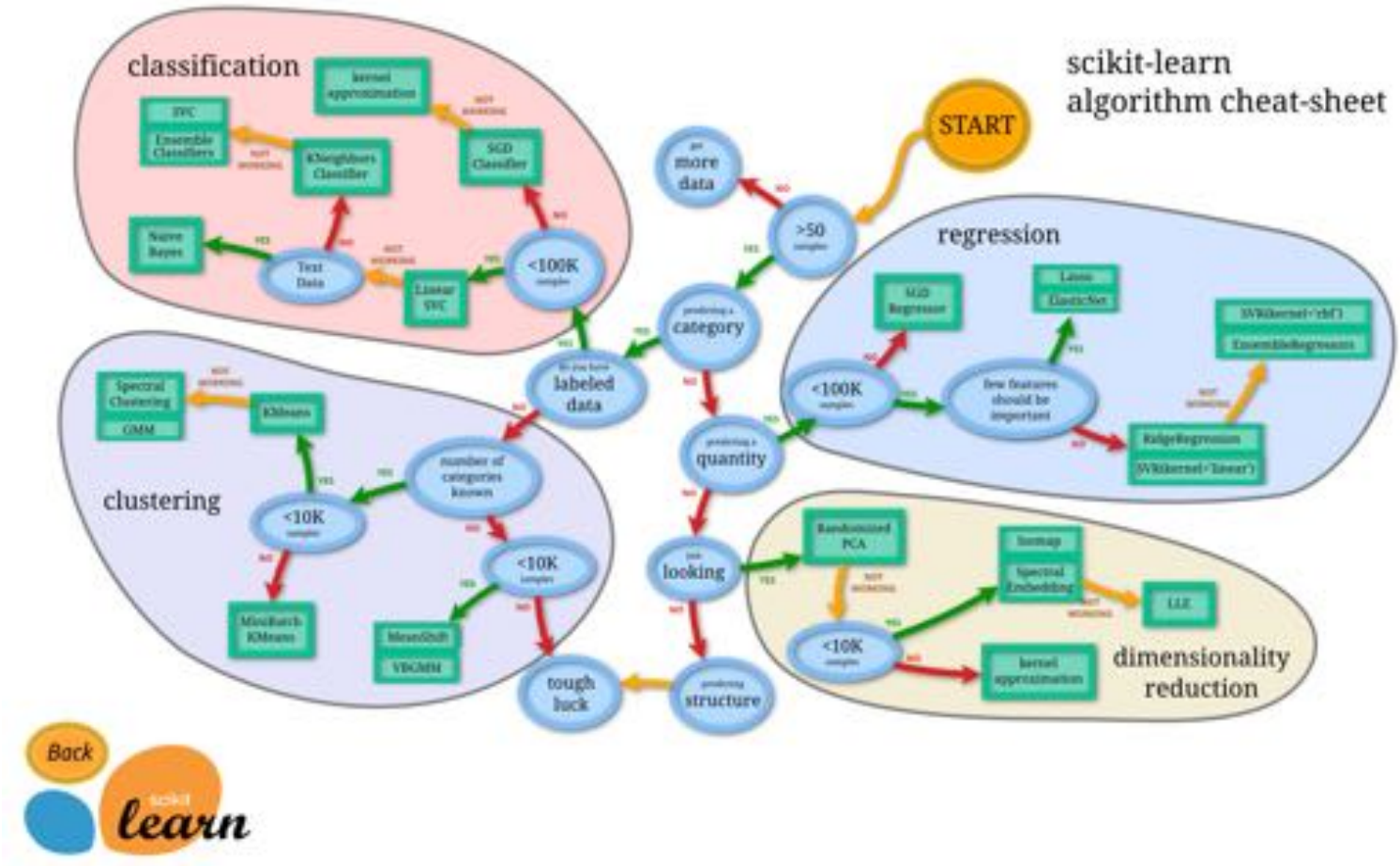
The development of machine learning systems requires enormous efforts.



The development of machine learning systems requires enormous efforts.

- **It requires of highly qualified experts.**

Why PPLs?

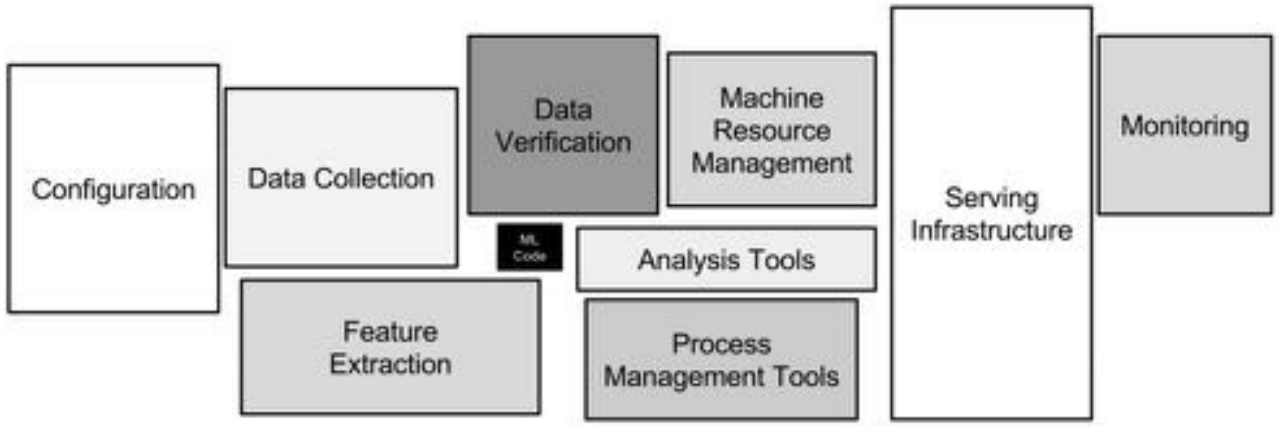


The development of machine learning applications requires enormous effort.

- It is necessary to have highly qualified experts.
- **It is difficult to find the ML model most suitable for an application.**

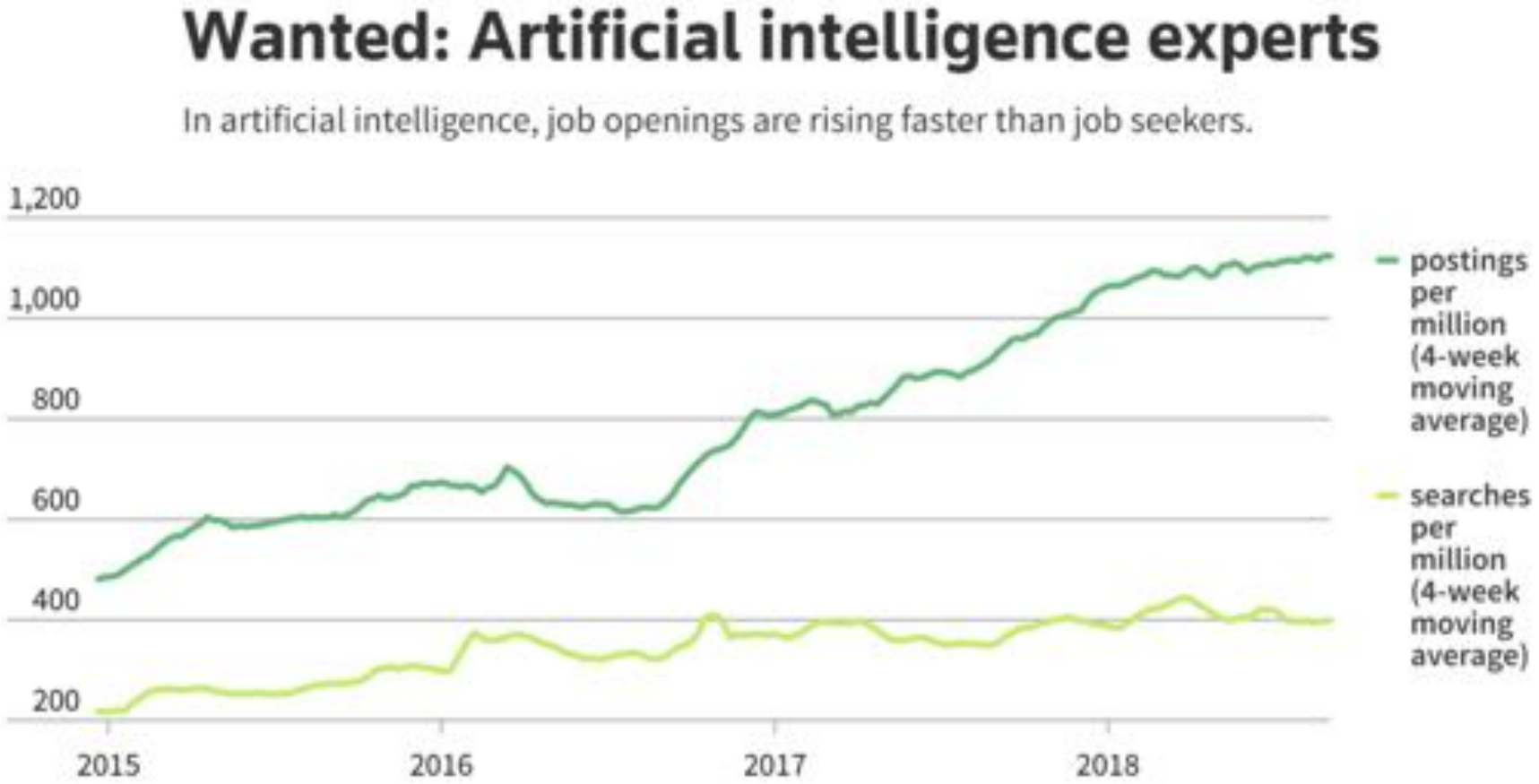
Hidden Technical Debt in Machine Learning Systems

D. Sculley, Gary Holt, Daniel Golovin, Eugene Davydov, Todd Phillips
{dsculley,gholt,dgg,edavydov,toddphillips}@google.com
Google, Inc.



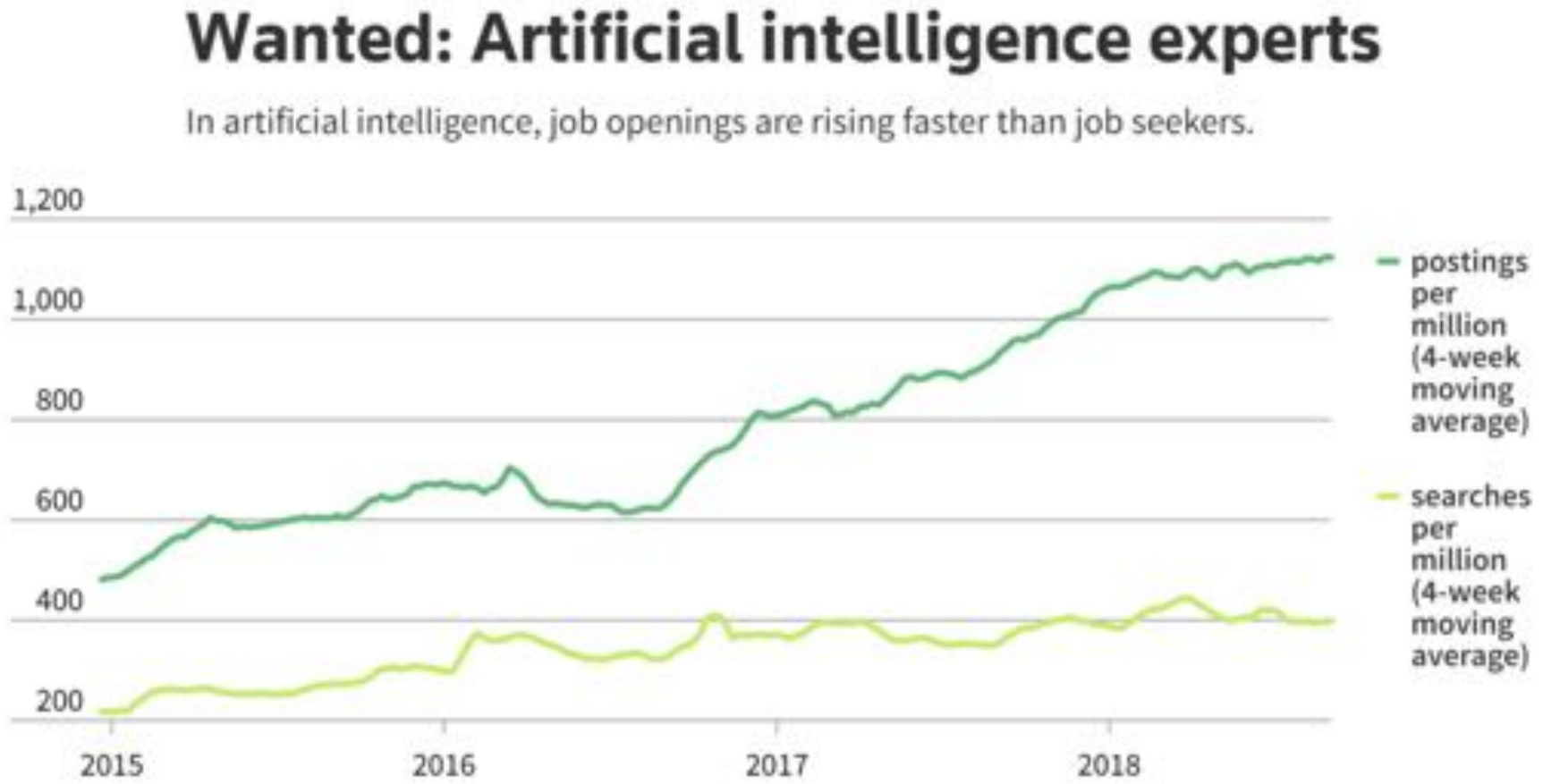
The development of machine learning applications requires enormous effort.

- It is necessary to have highly qualified experts.
- It is difficult to find the ML model most suitable for an application.
- **Programming a ML model is a complex task where many problems are intermingled**.



Consequences:

- Shortage of AI experts (and high salaries).



Consequences:

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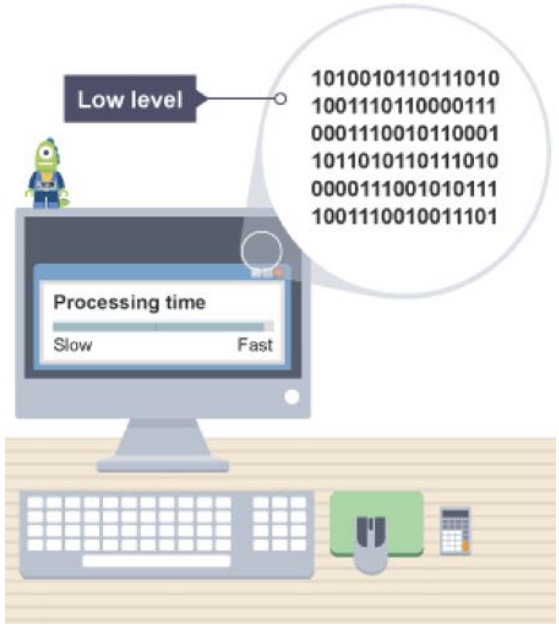
- Only big corporations have the resources for developing ML systems.

Why PPLs?



Similar situation than 50 years ago:

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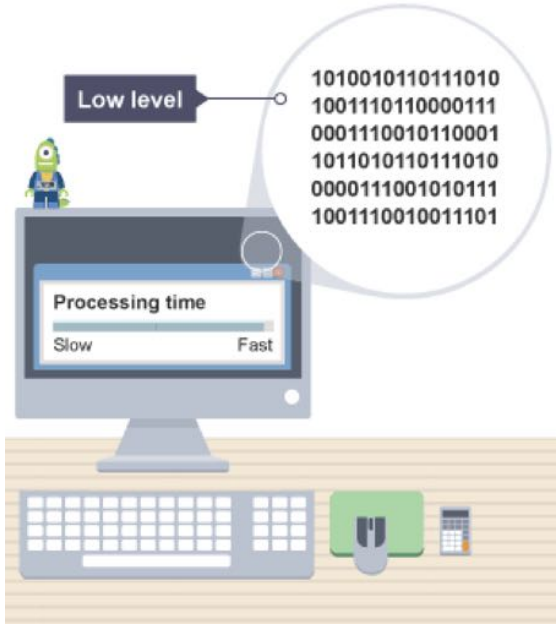

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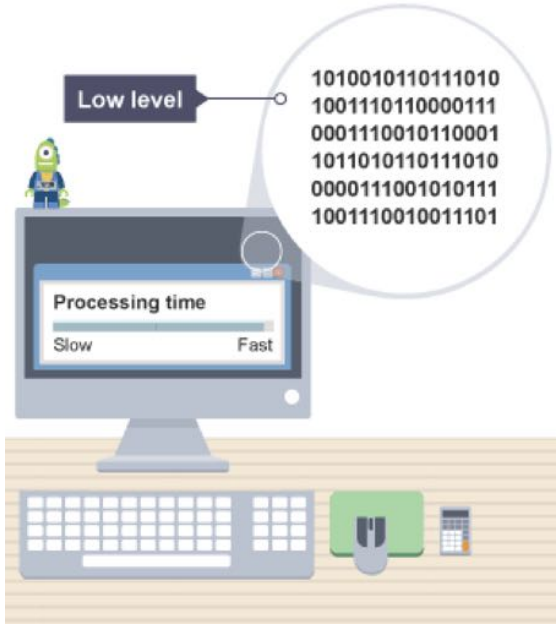

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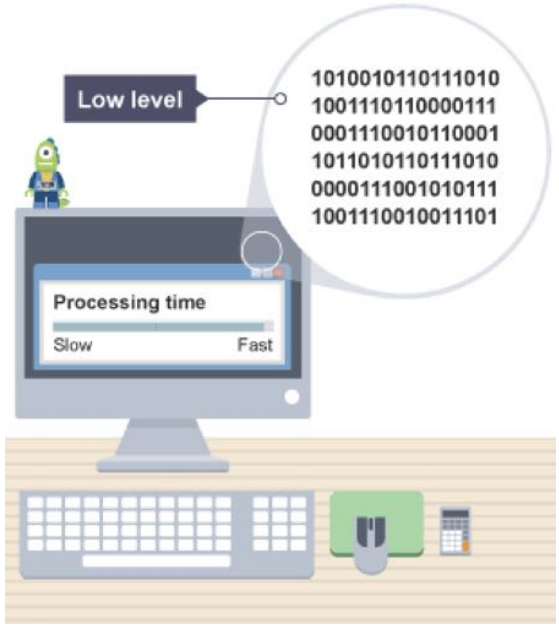

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- People used to program in low-level programming languages.
- Programming was complex and demand high-expertise.
- Focus on application and low-level hardware details.

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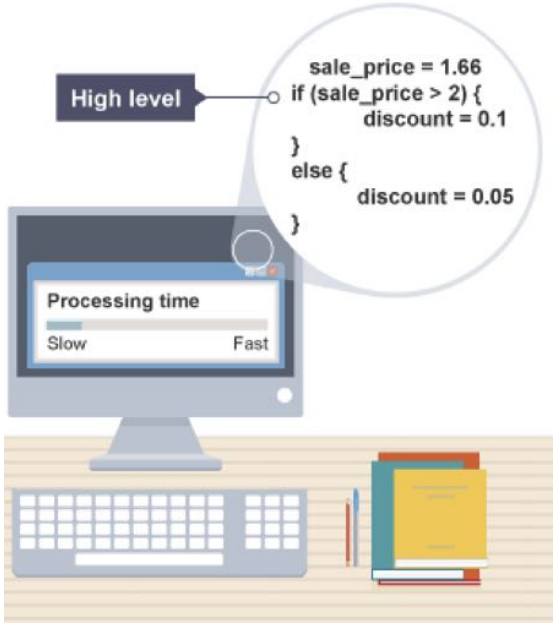

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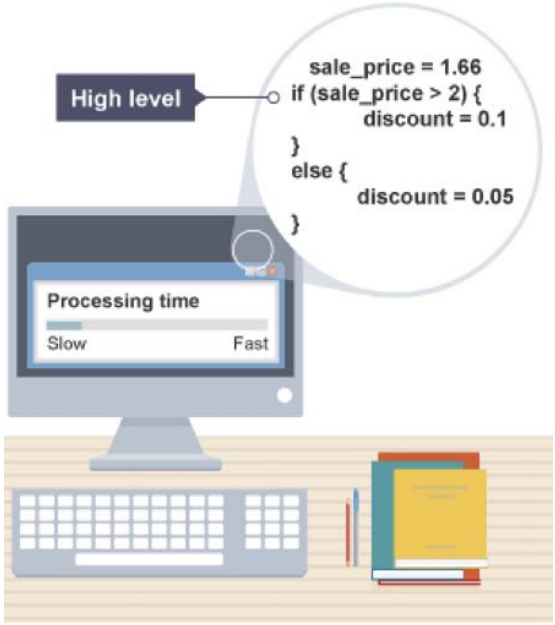

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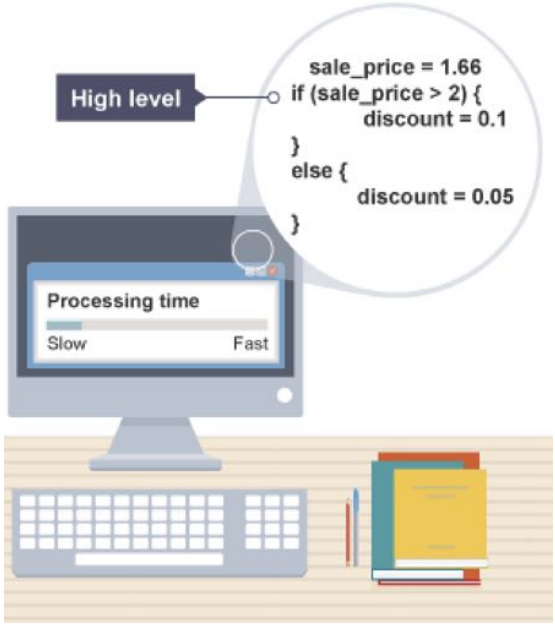

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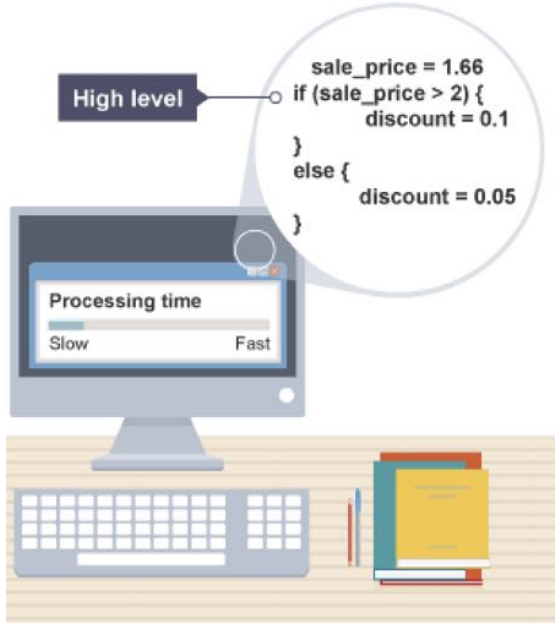

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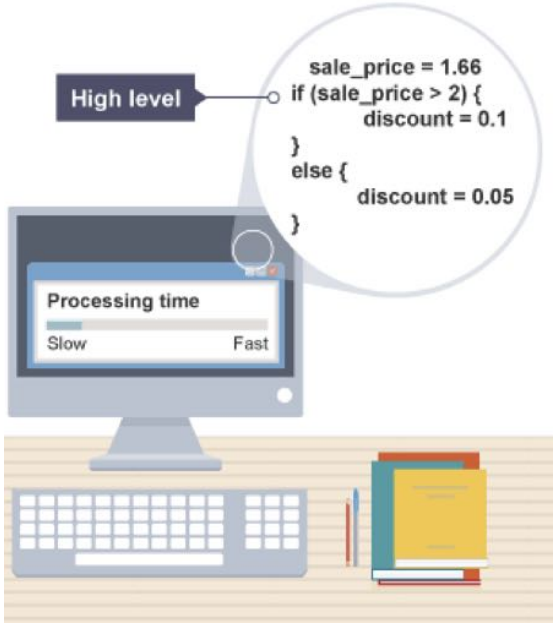

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- "Democratization" of the software development.

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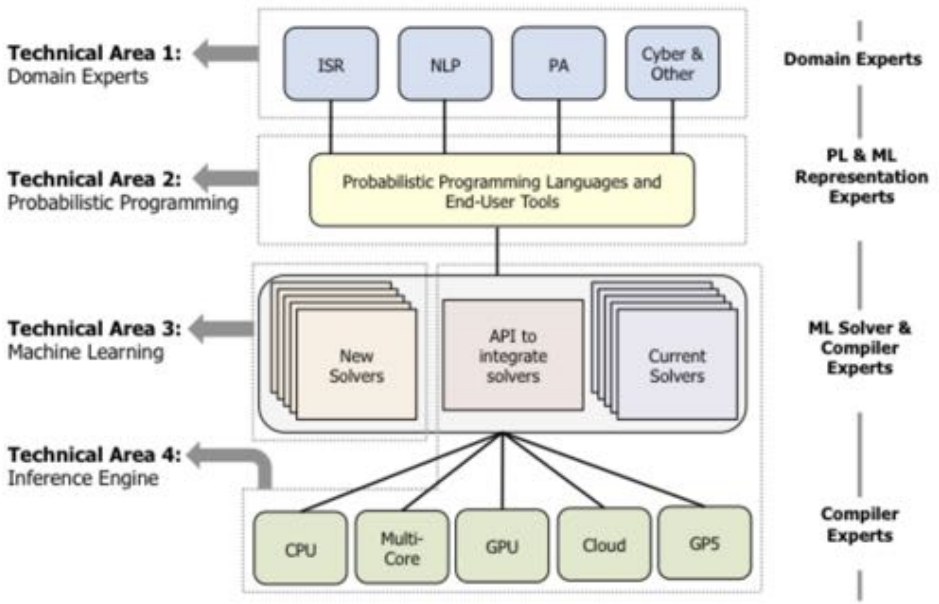

PPLs as high-level programming languages for **machine learning systems**:

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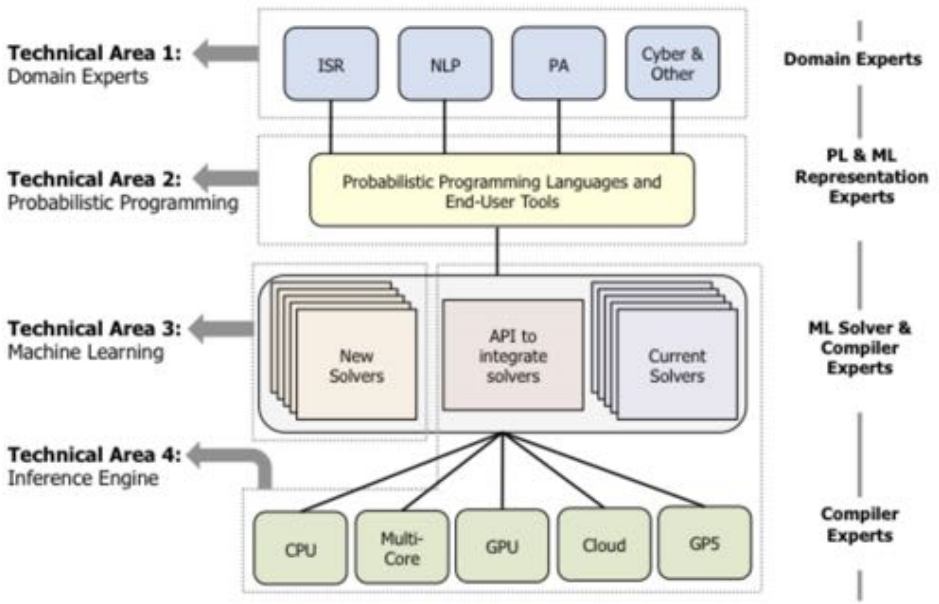

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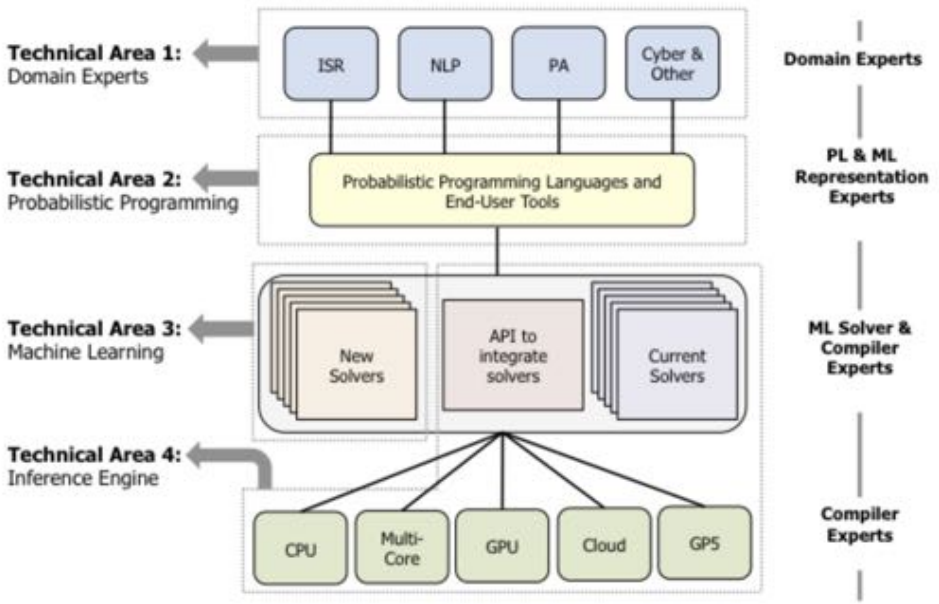

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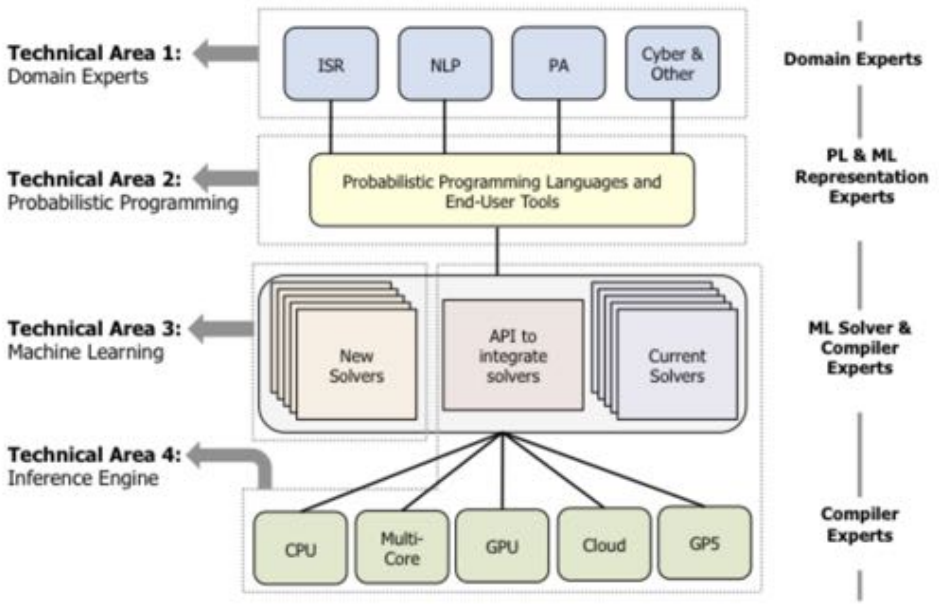

PPLs as high-level programming languages for **machine learning systems**:

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- Compile experts will focus on running these ML solvers on specialized hardware.

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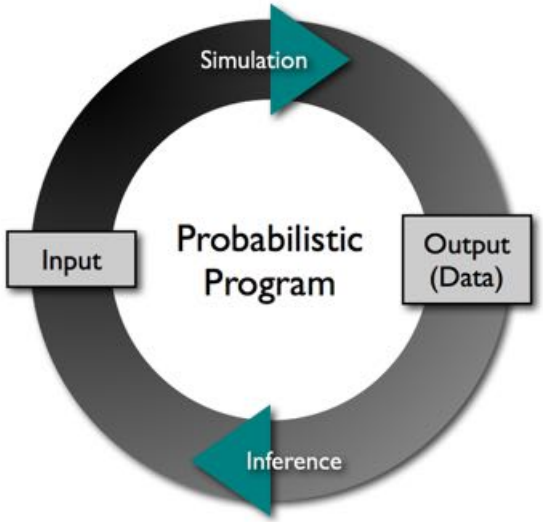

Benefits of PPLs:

- Simplify machine learning model code.

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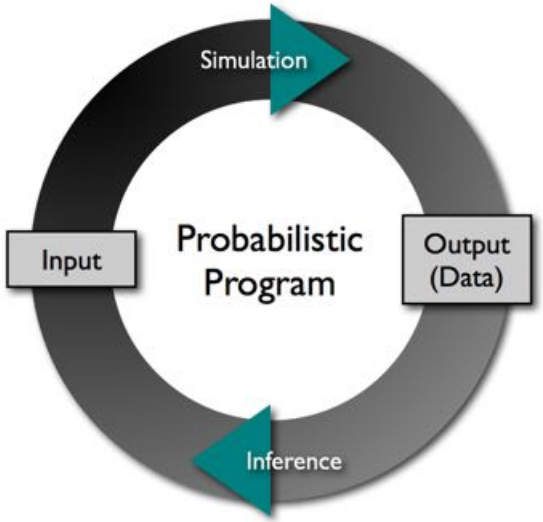

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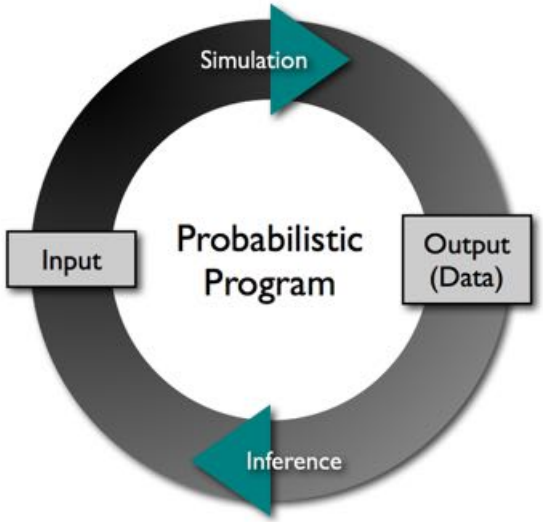

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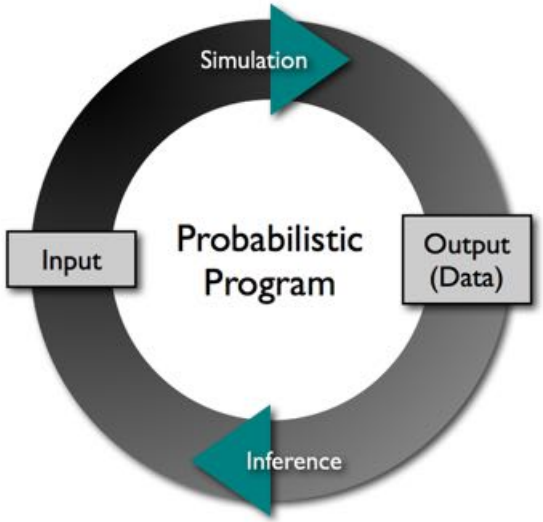

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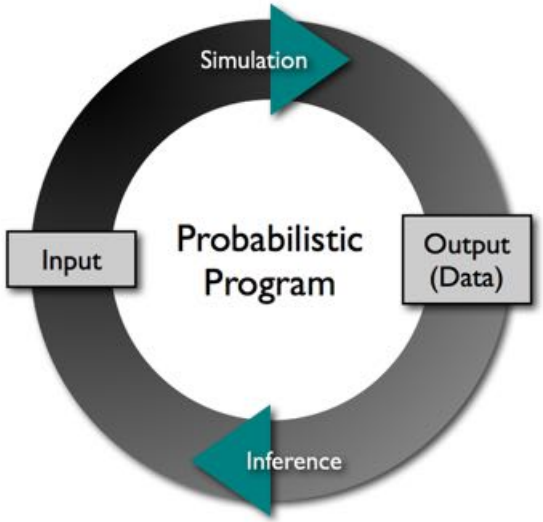

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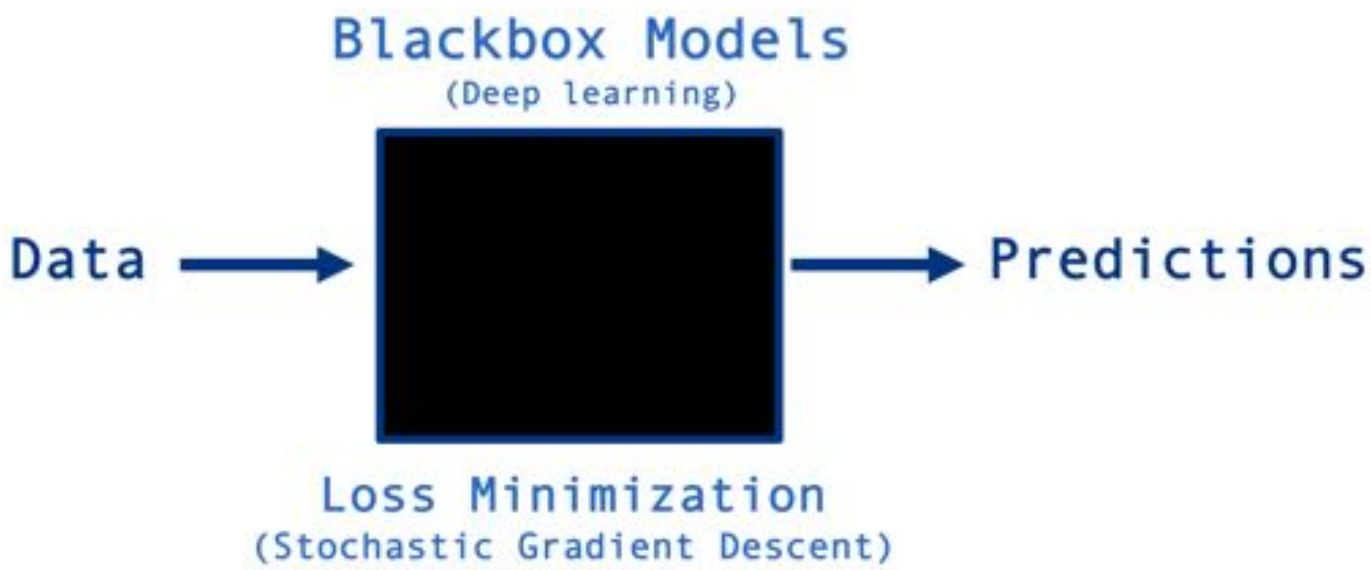
- "Democratization" of the development of ML systems.

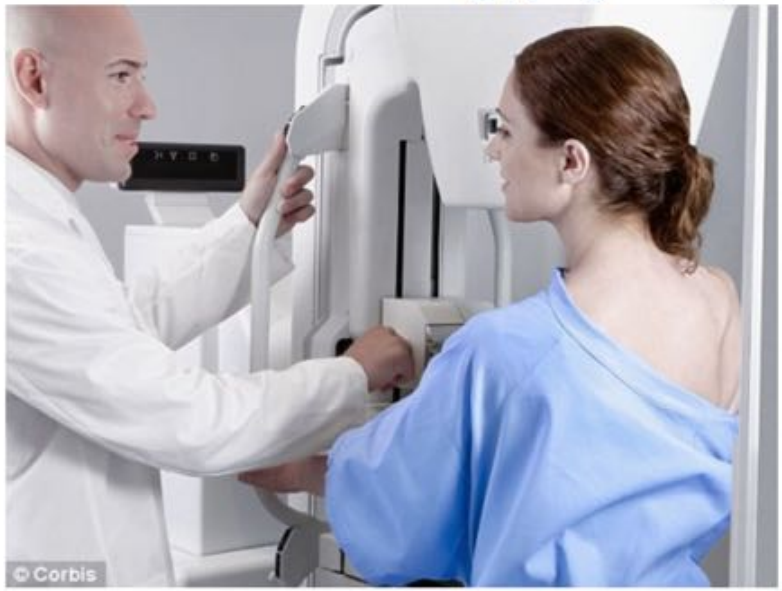
Reason 2: Try to make AI systems safer



Deep Learning Based AI Systems :

- **Issue 1**: Hard to **interpret**.
- **Issue 2**: No possible to know **how sure they are** in a particular prediction.
- Enormously **limit** the application of AI to many **real life problems**.

Today AI



AI in Health Care:

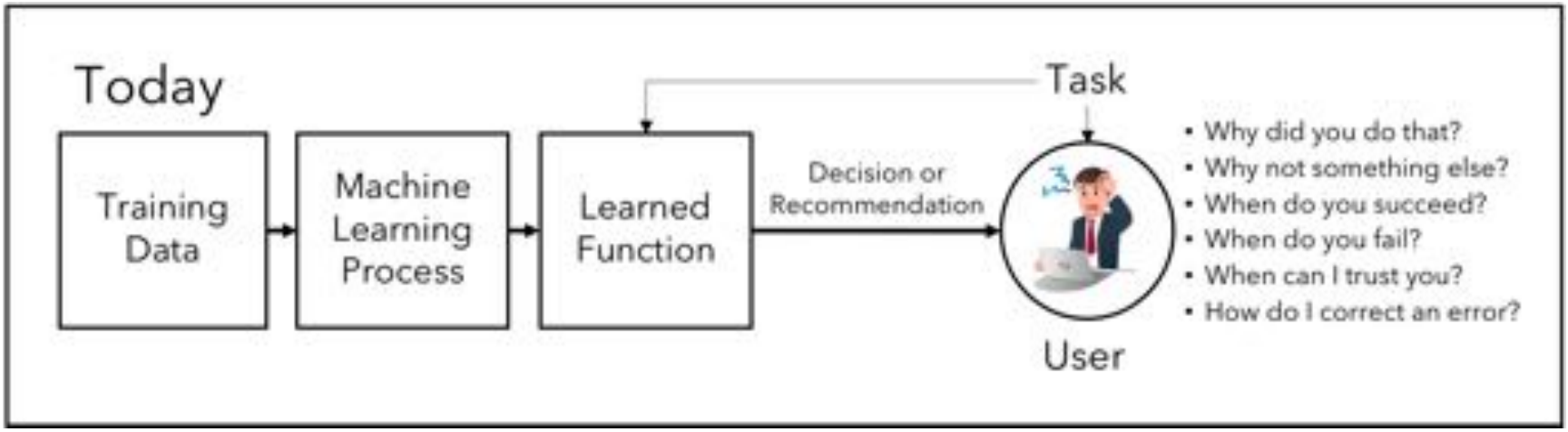
- Patients **need to know** why they are prescribed some treatment.
- An doctor can supervise the machine (**humans in the loop**).
- Extensible to any safe-critical system.

Today AI

AI in Automated Systems:

- The system should detect when it is in a **completely new situation**.
- Let a **human take the control**.

XAI: Explainable AI



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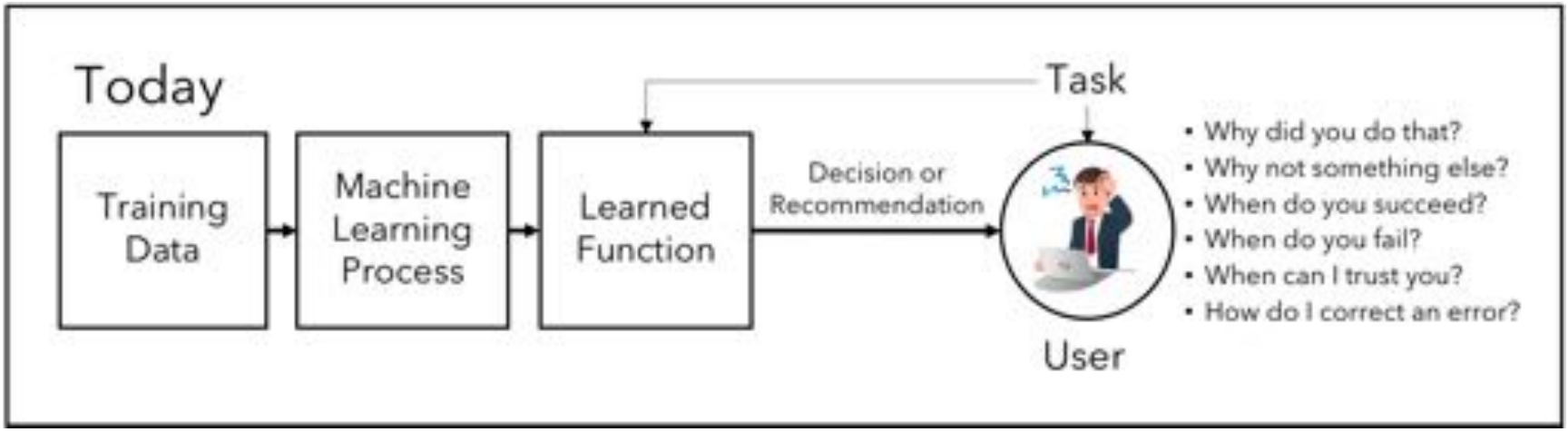

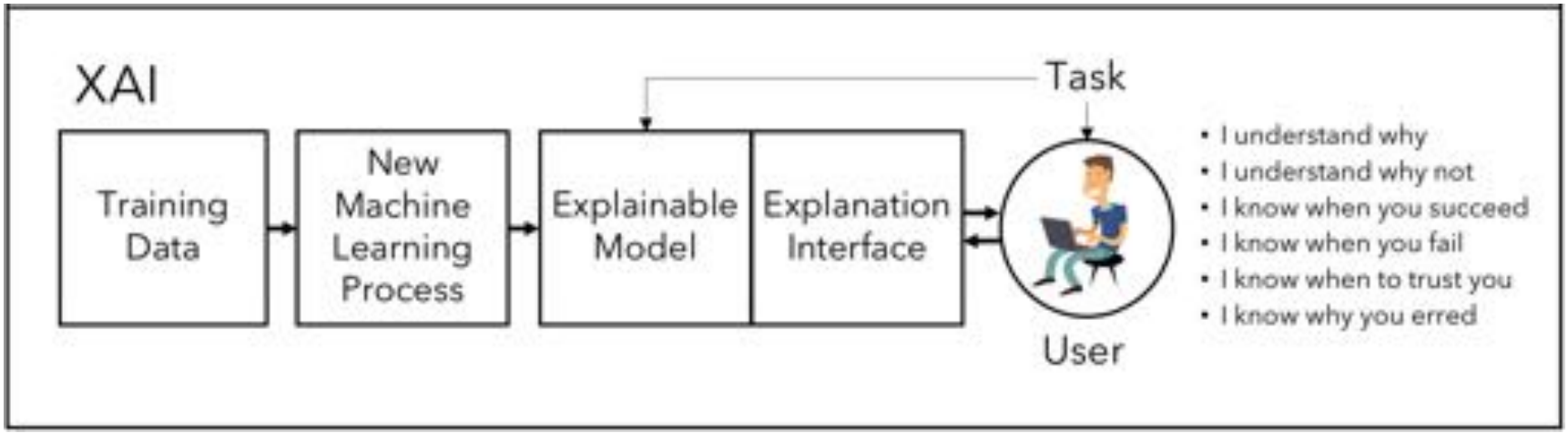

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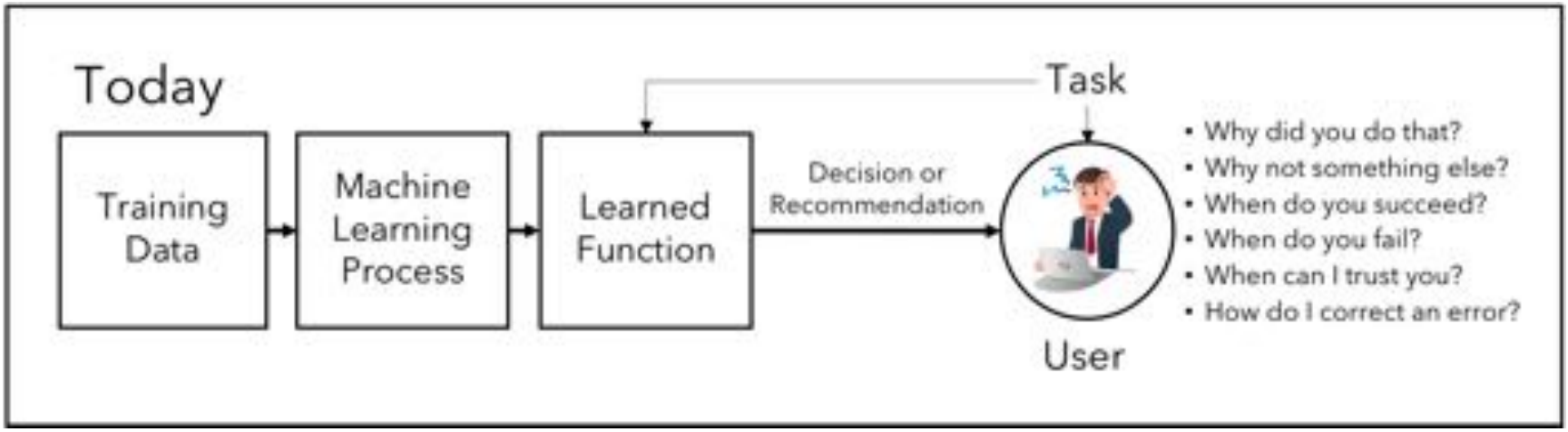
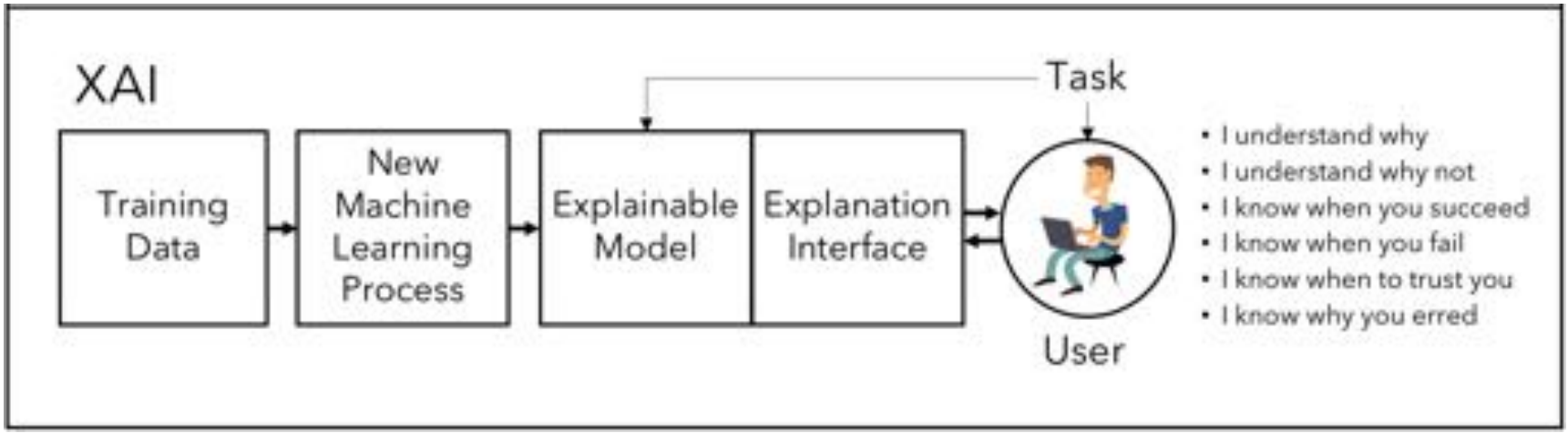
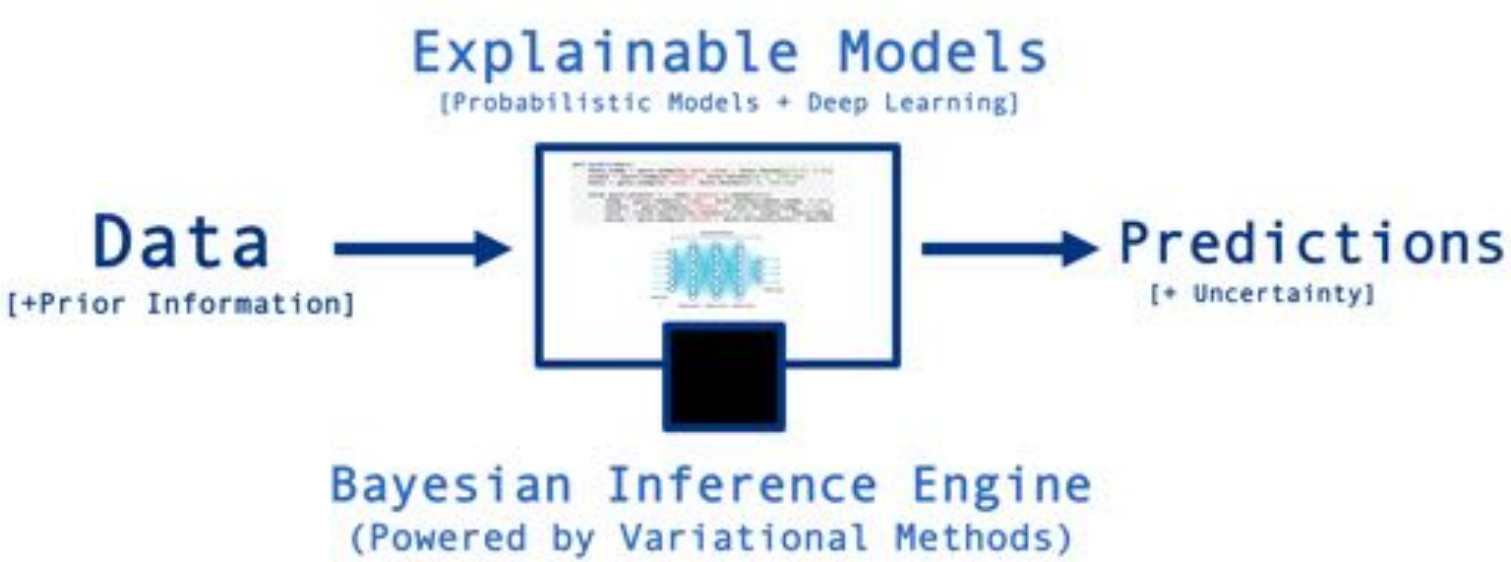




DARPA's Fund Call for XAI projects.

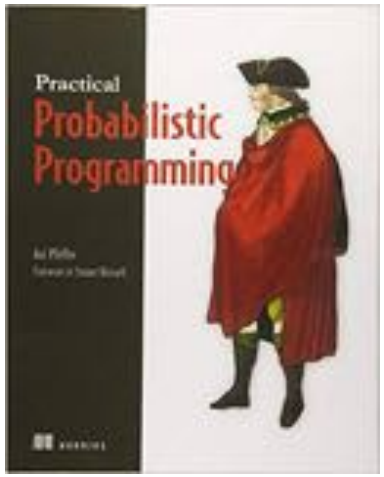
Explainable AI



PPL based Systems :

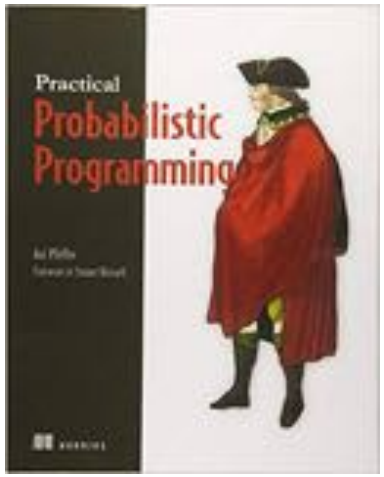
- Addressing Issue 1: PPLs provide **transparent** model description.
- Addressing Issue 2: PPLs provide **uncertainty estimation** both in models and predictions.

Brief Historical Review of PPLs



1st Generation of PPLs :

- Bugs, WinBugs, Jags, Figaro, etc.



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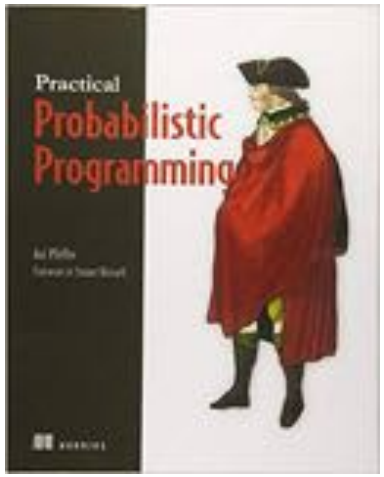

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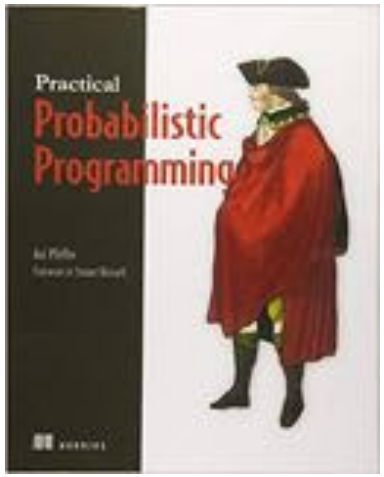

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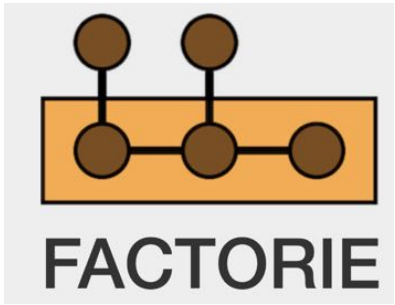
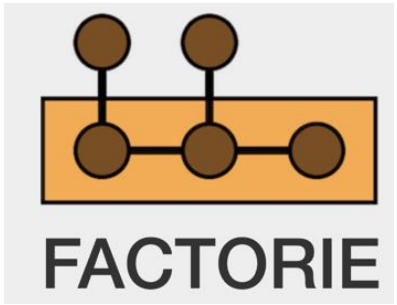


2nd Generation of PPLs :

- Infer.net, Factorie, Amidst, etc.



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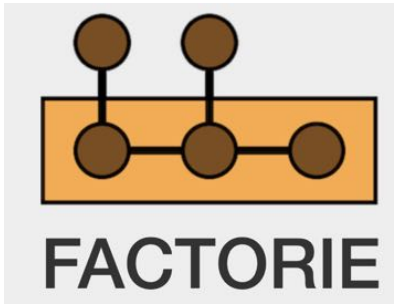

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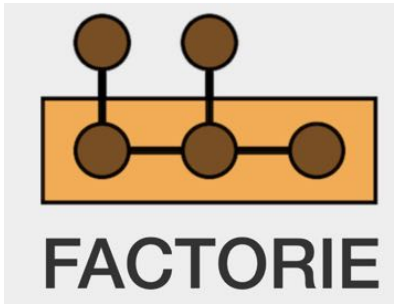

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- **Restricted** probabilistic model family (i.e. factor graphs, conjuage exponential family, etc.)



3rd Generation of PPLs :

- TensorFlow Probability, Pyro, PyMC3, InferPy, etc.



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- TensorFlow Probability, Pyro, PyMC3, InferPy, etc.
- **Black Box Variational Inference** and Hamiltonian Monte-Carlo.



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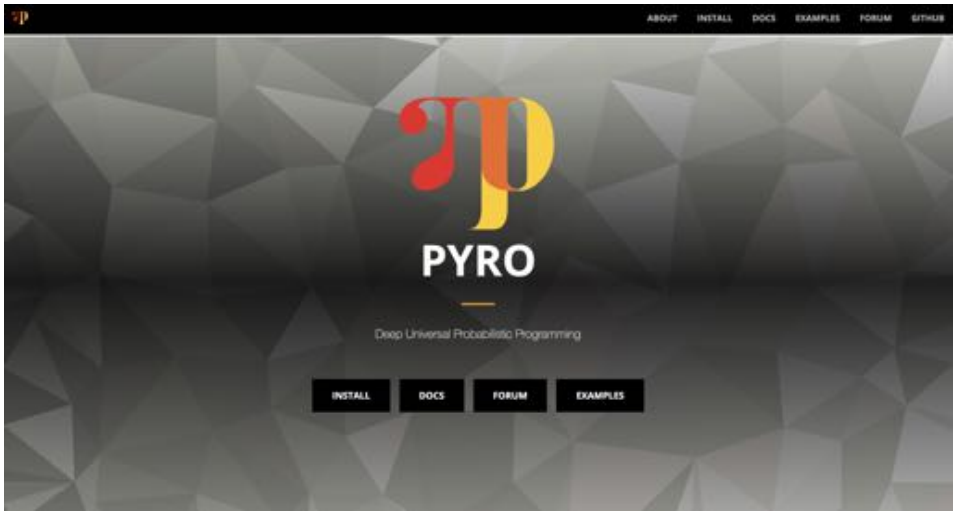
- Allow the inclusion of **deep neural networks**.



3rd Generation of PPLs :

- TensorFlow Probability, Pyro, PyMC3, InferPy, etc.
- **Black Box Variational Inference** and Hamiltonian Monte-Carlo.
- They did **scale** to large data samples/high-dimensional models.
- **Turing-complete** probabilistic programming languages.
- Allow the inclusion of **deep neural networks**.
- Rely on **deep learning frameworks** (TensorFlow, Pytorch, Theano, etc).

Pyro


ABOUT
INSTALL
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EXAMPLES
FORUM
GITHUB
PYRO
Deep Universal Probabilistic Programming
INSTALL
DOCS
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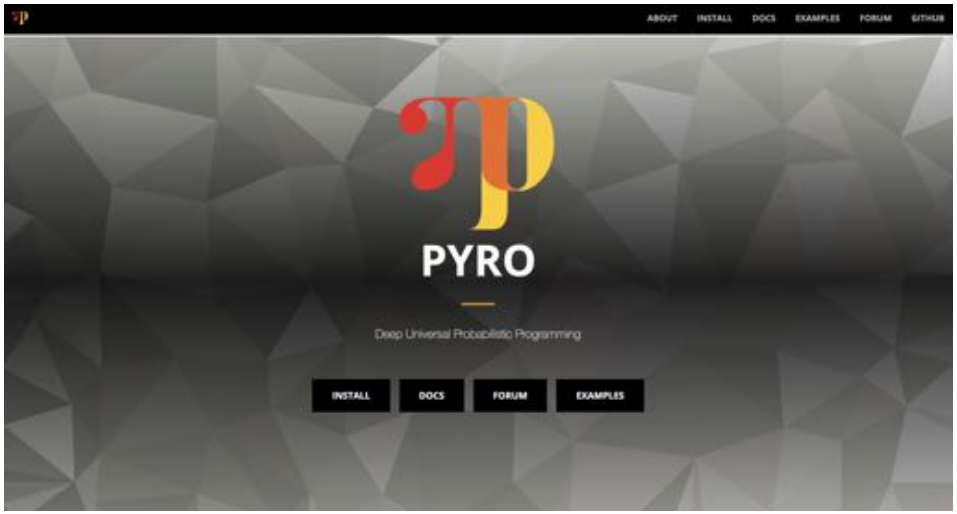
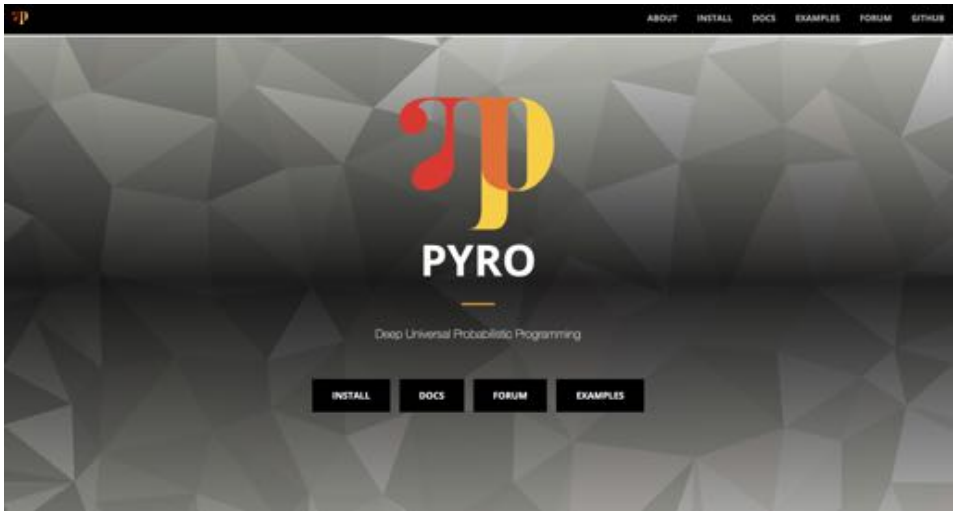
EXAMPLES



Pyro's main features (`www.pyro.ai`) :

- Developed by **UBER** (the car riding company).



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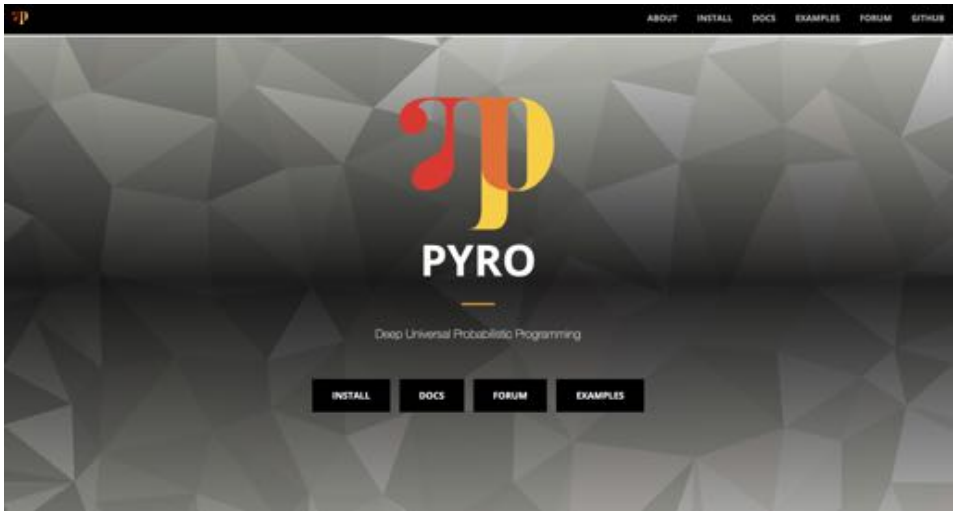

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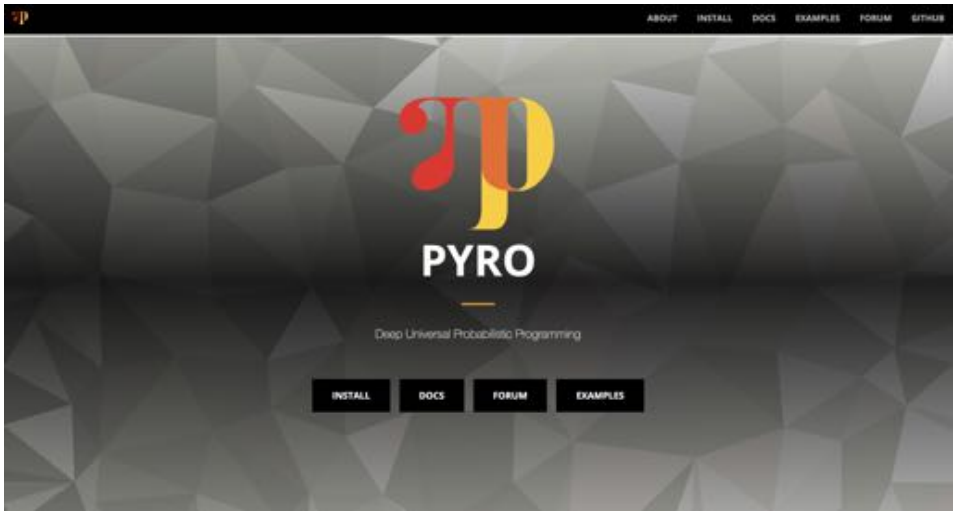
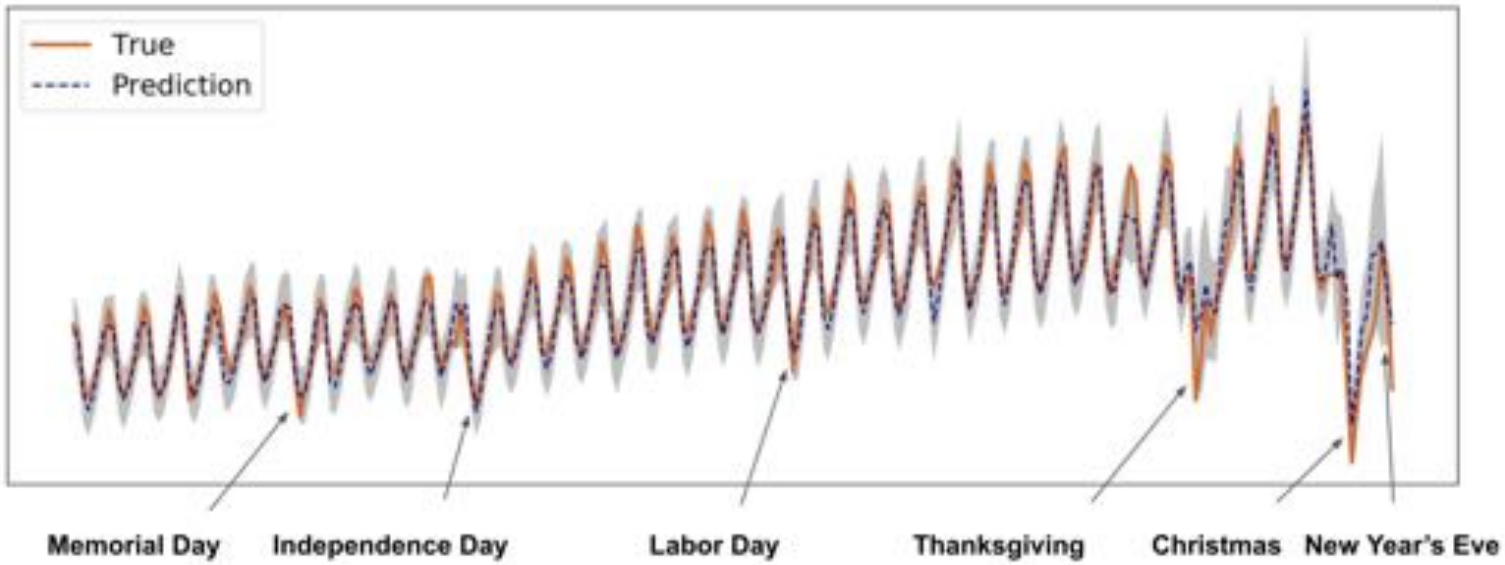


Pyro's main features (`www.pyro.ai`) :

- Developed by **UBER** (the car riding company).
- Focus on **probabilistic models with deep neural networks**.
- Rely on **Pytorch** (Deep Learning Framework).
- Enable **GPU** accelaration and distributed learning.

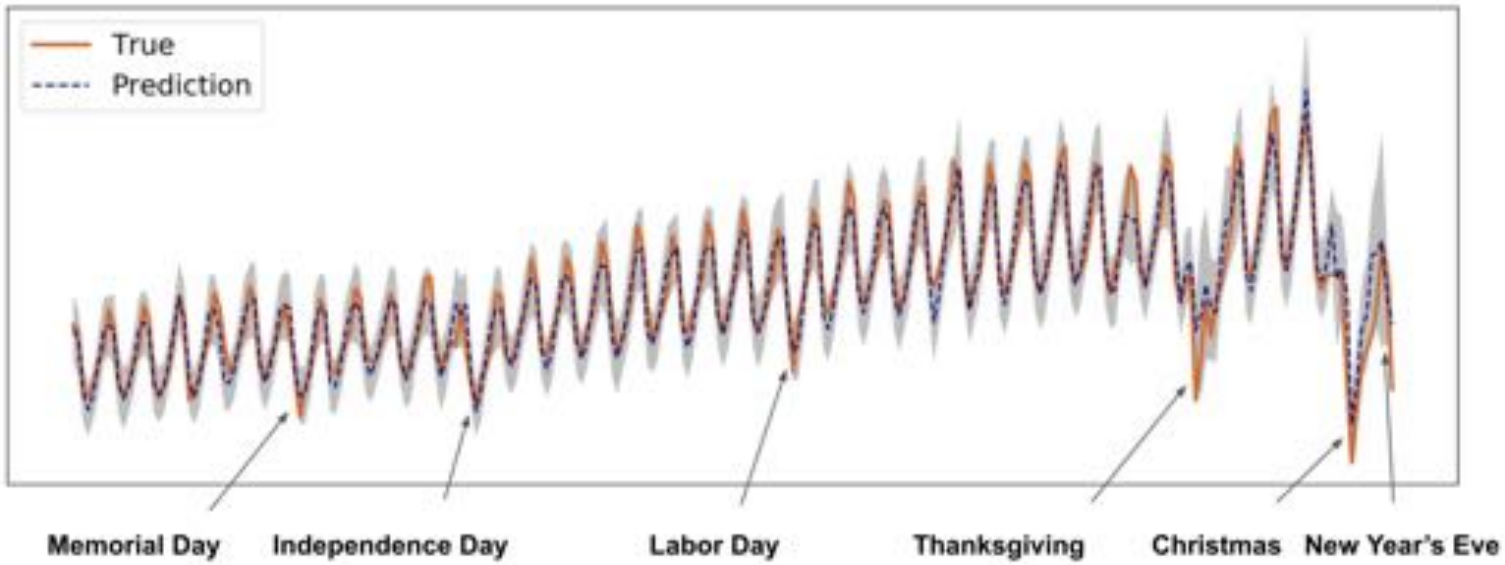
Pyro at UBER



Demand Prediction with Pyro:

- Demand prediction is **critical** for user experience, resource allocation, etc.

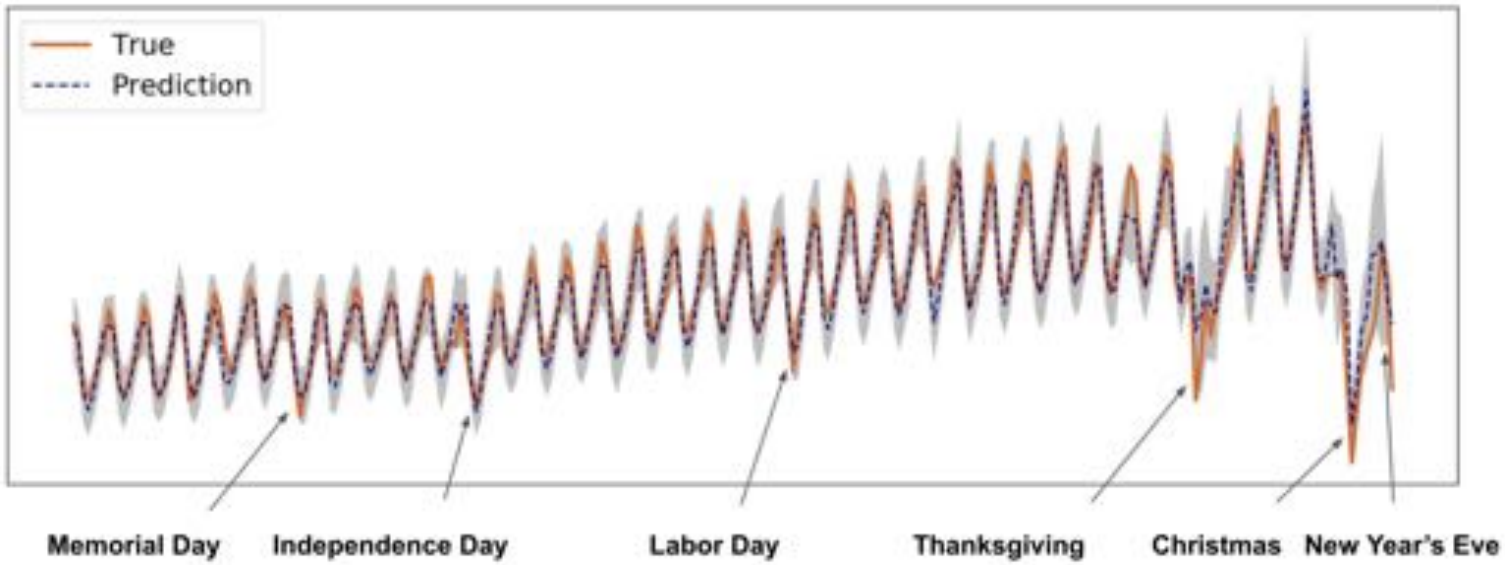
Pyro at UBER



Demand Prediction with Pyro:

- Demand prediction is **critical** for user experience, resource allocation, etc.
- LSTM powerful for time series modelling.

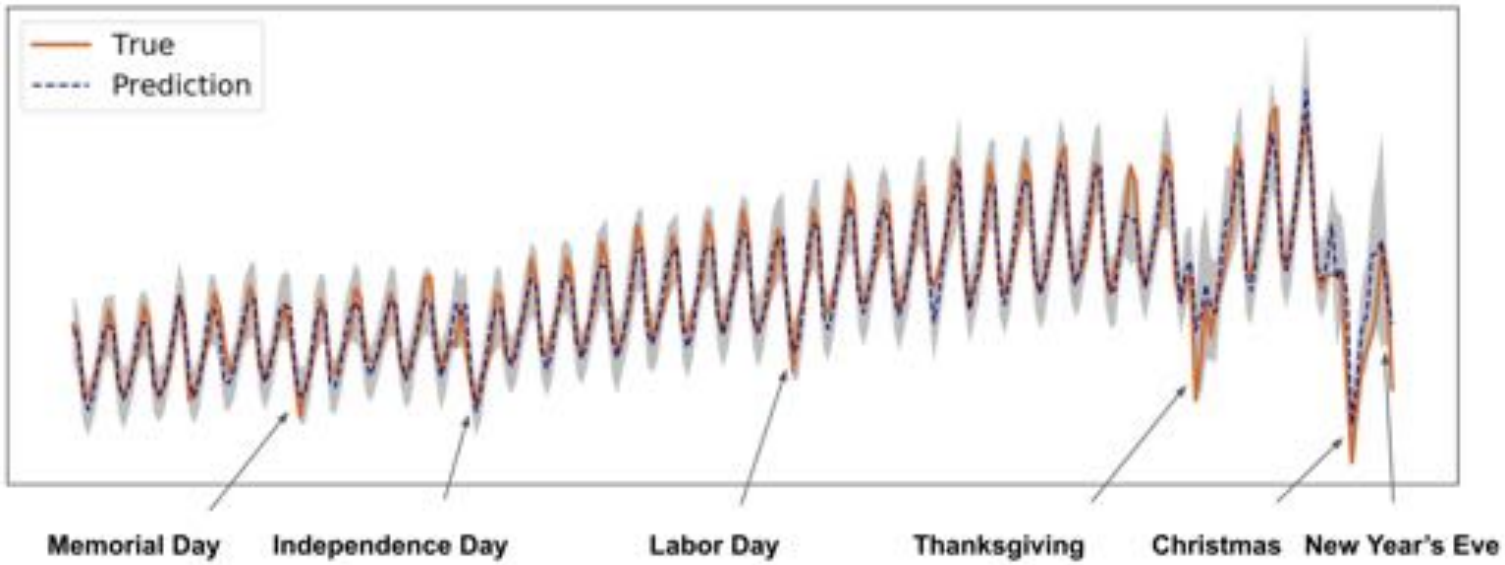
Pyro at UBER



Demand Prediction with Pyro:

- Demand prediction is **critical** for user experience, resource allocation, etc.
- LSTM powerful for time series modelling.
- Prediction at **special events** is challenging: weather, population growth, etc.

Pyro at UBER



Demand Prediction with Pyro:

- Demand prediction is **critical** for user experience, resource allocation, etc.
- LSTM powerful for time series modelling.
- Prediction at **special events** is challenging: weather, population growth, etc.
- Bayesian LSTM provides **uncertainty estimation**.

Pyro's Distributions

```
In [3]: normal = dist.Normal(0,1)
        normal

Out[3]: Normal(loc: 0.0, scale: 1.0)
```

Pyro's distributions (`http://docs.pyro.ai/en/stable/distributions.html`) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.

```
In [15]: sample = normal.sample()
         sample

Out[15]: tensor(0.4908)
```

Pyro's distributions (`http://docs.pyro.ai/en/stable/distributions.html`) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.
- Samples from the distributions are Pytorch's Tensor objects (i.e. multidimensional arrays).

```
In [17]: sample = normal.sample(sample_shape=[3,4,5])
         sample.shape

Out[17]: torch.Size([3, 4, 5])
```

Pyro's distributions (http://docs.pyro.ai/en/stable/distributions.html) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.
- Samples from the distributions are Pytorch's Tensor objects (i.e. multidimensional arrays).

```
In [19]: torch.sum(normal.log_prob(sample))
Out[19]: tensor(-85.1003)
```

Pyro's distributions (http://docs.pyro.ai/en/stable/distributions.html) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.
- Samples from the distributions are Pytorch's Tensor objects (i.e. multidimensional arrays).
- Operations, like log-likelihood, are defined over tensors (with GPU acceleration powered by Pytorch).

```
In [9]: normal = dist.Normal(torch.tensor([1.,2.,3.]),1.)
        normal

Out[9]: Normal(loc: torch.Size([3]), scale: torch.Size([3]))
```

Pyro's distributions (`http://docs.pyro.ai/en/stable/distributions.html`) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.
- Samples from the distributions are Pytorch's Tensor objects (i.e. multidimensional arrays).
- Operations, like log-likelihood, are defined over tensors (with GPU acceleration powered by Pytorch).
- Multiple distributions can be embedded in single object (to define efficient vectorized operations).

```
In [10]: normal.sample()

Out[10]: tensor([2.0592, 2.4035, 3.1918])
```

Pyro's distributions (http://docs.pyro.ai/en/stable/distributions.html) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.
- Samples from the distributions are Pytorch's Tensor objects (i.e. multidimensional arrays).
- Operations, like log-likelihood, are defined over tensors (with GPU acceleration powered by Pytorch).
- Multiple distributions can be embedded in single object (to define efficient vectorized operations).

```
In [11]: normal.log_prob(normal.sample())

Out[11]: tensor([-0.9402, -1.2113, -2.3214])
```

Pyro's distributions (`http://docs.pyro.ai/en/stable/distributions.html`) :

- Wide range of distributions: Normal, Beta, Cauchy, Dirichlet, Gumbel, Poisson, Pareto, etc.
- Samples from the distributions are Pytorch's Tensor objects (i.e. multidimensional arrays).
- Operations, like log-likelihood, are defined over tensors (with GPU acceleration powered by Pytorch).
- Multiple distributions can be embedded in single object (to define efficient vectorized operations).

Now it is your turn!

Open the Notebook and Play around

- Test that you have installed the basic packages.
- Test that you can run the first lines of code.
- Play a bit with the code in Section 1 of the notebook.

`Day1/students_PPLs_Intro.ipynb`

`https://github.com/PGM-Lab/ASML-Tbilisi`

Pyro's Models

```
In [12]: def model():
             temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
             return temp

         print(model())
         print(model())
```

```
tensor(12.3926)
tensor(22.5272)
```

Pyro's models (http://pyro.ai/examples/intro_part_i.html) :

- A probabilistic model is defined as a **stochastic function**.

In [12]:
```
def model():
    temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
    return temp

print(model())
print(model())
```

```
tensor(12.3926)
tensor(22.5272)
```

Pyro's models (http://pyro.ai/examples/intro_part_i.html) :

- A probabilistic model is defined as a **stochastic function**.
- Each random variable is associated to a **primitive stochastic function** using the construct **pyro.sample(...)**.

```
In [21]: def model():
             temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
             sensor = pyro.sample('sensor', dist.Normal(temp, 1.0))
             return (temp, sensor)

         out1 = model()
         out1

Out[21]: (tensor(15.8576), tensor(16.9907))
```

Pyro's models (http://pyro.ai/examples/intro_part_i.html) :

- A **stochastic function** can be defined as a composition of **primitive stochastic functions**.

```
In [21]: def model():
             temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
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         out1 = model()
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Out[21]: (tensor(15.8576), tensor(16.9907))
```

Pyro's models (`http://pyro.ai/examples/intro_part_i.html`) :

- A **stochastic function** can be defined as a composition of **primitive stochastic functions**.
- We define the **joint probability distribution**:

$$p(\texttt{sensor}, \texttt{temp}) = p(\texttt{sensor}|\texttt{temp})p(\texttt{temp})$$

Pyro's Inference

In [22]:
```
#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 inference (http://pyro.ai/examples/intro_part_ii.html) :

- We can introduce observations (e.g. sensor $= 18.0$).

In [27]:
```
#Run inference
svi(model,guide,obs, plot=True)

#Print results
print("P(Temperature|Sensor=18.0) = ")
print(dist.Normal(pyro.param("mean").item(), pyro.param("scale").item()))
print("")
```

Pyro's inference (http://pyro.ai/examples/intro_part_ii.html) :

- We can introduce observations (e.g. sensor $= 18.0$).
- We can query the **posterior probability distribution**:

$$p(\texttt{temp}|\texttt{sensor} = 18) = \frac{p(\texttt{sensor} = 18|\texttt{temp})p(\texttt{temp})}{\int p(\texttt{sensor} = 18|\texttt{temp})p(\texttt{temp})d\texttt{temp}}$$

```
In [27]: #Run inference
svi(model,guide,obs, plot=True)

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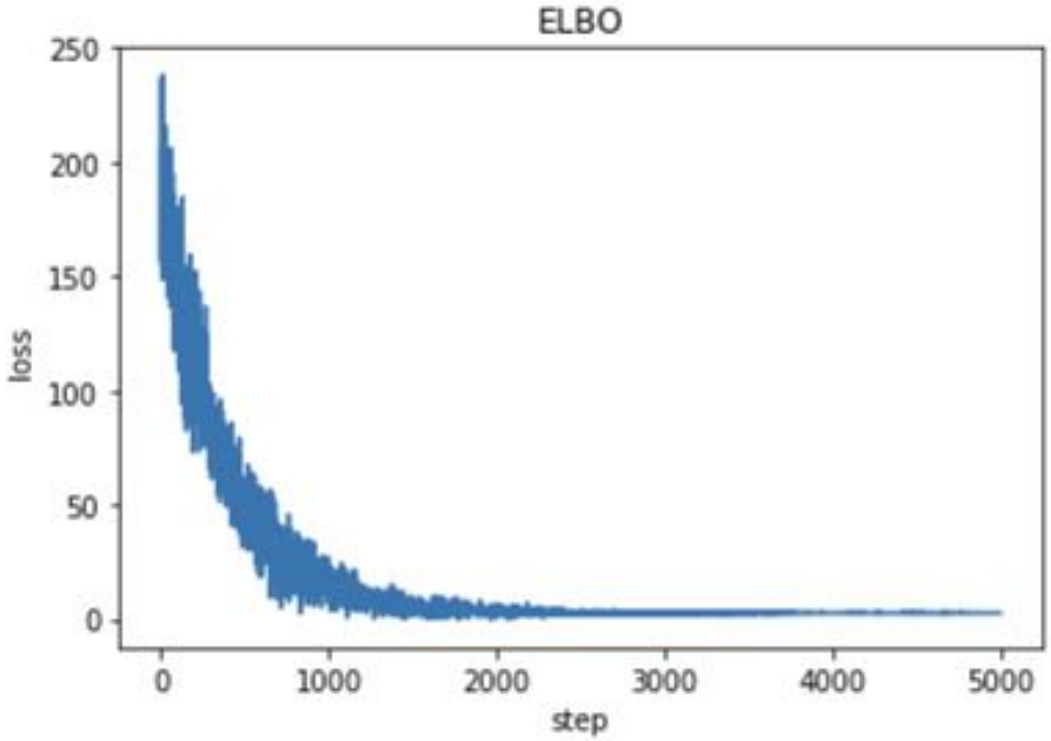
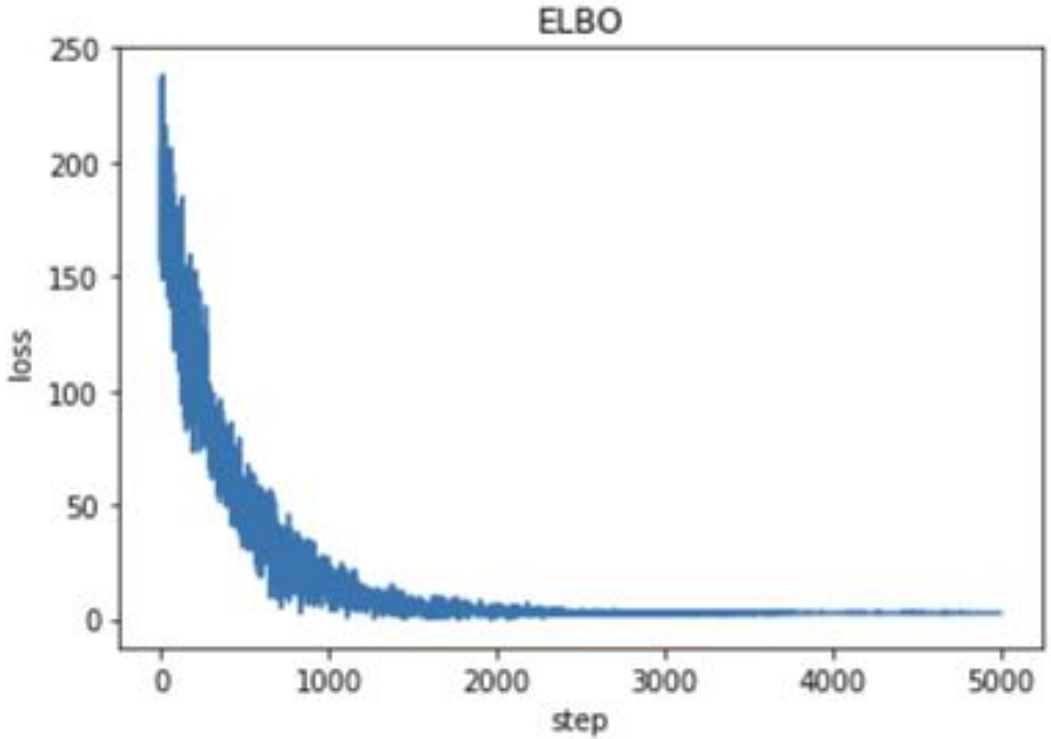
- Guide is an auxiliary method needed for inference (more details in the coming sessions).




```
P(Temperature|Sensor=18.0) =
Normal(loc: 17.39859390258789, scale: 0.9089401960372925)
```




```
P(Temperature|Sensor=18.0) =
Normal(loc: 17.39859390258789, scale: 0.9089401960372925)
```

Details on the inference method will be given on the following sessions.

Exercise 1: Change in the precision of the temperature sensor

- The precision of our temperature sensor is reflected in the **variance/scale** of the Normal distribution of the **sensor** variable.
- What happens if we get a **more precise temperature sensor**? Assume it has a variance/scale equal to 0.5.

`Day1/students_PPLs_Intro.ipynb`

`https://github.com/PGM-Lab/ASML-Tbilisi`

In [ ]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    for i in range(0,obs['sensor'].shape[0]):
        temp = pyro.sample(f'temp_{i}', dist.Normal(15.0, 2.0))
        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's inference (http://pyro.ai/examples/intro_part_ii.html) :

- What if we have a **bunch of observations**, $\mathrm{s} = \{s_1, \ldots, s_n\}$

In [ ]:
```
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        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's inference (`http://pyro.ai/examples/intro_part_ii.html`) :

- What if we have a **bunch of observations**, $\mathrm{s} = \{s_1, \ldots, s_n\}$
- A random variable is created for each observation (using a **for-loop**).

In [ ]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    for i in range(0,obs['sensor'].shape[0]):
        temp = pyro.sample(f'temp_{i}', dist.Normal(15.0, 2.0))
        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's inference (http://pyro.ai/examples/intro_part_ii.html) :

- What if **we do not know the average temperature**?

```
In [28]: #The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    mean_temp = pyro.param('mean_temp', torch.tensor(15.0))
    for i in range(0,obs['sensor'].shape[0]):
        temp = pyro.sample(f'temp_{i}', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's inference (`http://pyro.ai/examples/intro_part_ii.html`) :

- What if **we do not know the average temperature**?
- We can introduce a **parameter** using **pyro.param** construct.

```
In [32]: #Run inference
svi(model, guide, obs, num_steps=1000)

#Print results
print("Estimated Mean Temperature")
print(pyro.param("mean_temp").item())
```

```
Estimated Mean Temperature
19.129146575927734
```

Pyro's inference (`http://pyro.ai/examples/intro_part_ii.html`) :

- And **learn the parameter** with the same general inference algorithm.

$$\mu_t = \arg\max_{\mu} \ln p(s_1, \ldots, s_n | \mu)$$

- Details about the inference algorithm will be given in the next sessions.

In [28]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    mean_temp = pyro.param('mean_temp', torch.tensor(15.0))
    for i in range(0,obs['sensor'].shape[0]):
        temp = pyro.sample(f'temp_{i}', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's inference (http://pyro.ai/examples/intro_part_ii.html) :

- What if **we want to capture uncertainty about the estimation of the average temperature**?

In [176]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    mean_temp = pyro.sample('mean_temp', dist.Normal(15.0, 2.0))
    for i in range(obs['sensor'].shape[0]):
        temp = pyro.sample(f'temp_{i}', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's inference (http://pyro.ai/examples/intro_part_ii.html) :

- What if **we want to capture uncertainty about the estimation of the average temperature**?
- We can model this parameter with a **random variable**.

In [162]:
```
import time

#Run inference
start = time.time()
svi(model, guide, obs, num_steps=1000)

#Print results
print("P(mean_temp|Sensor=[18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1]) =")
print(dist.Normal(pyro.param("mean").item(), pyro.param("scale").item()))
print("")
end = time.time()
print(f"{(end - start)} seconds")
```

```
P(mean_temp|Sensor=[18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1]) =
Normal(loc: 19.199871063232422, scale: 0.6046891212463379)

10.298431873321533 seconds
```

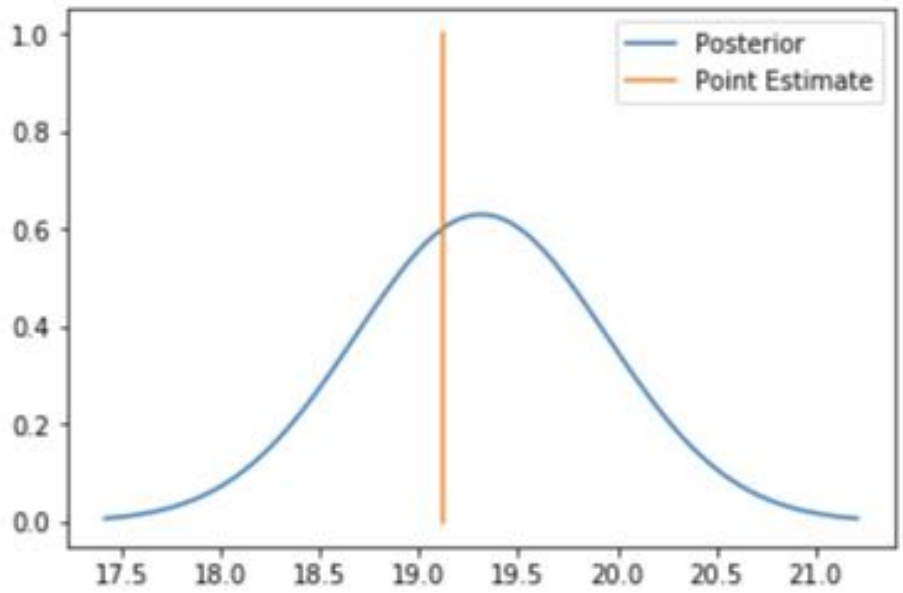
Pyro's inference (`http://pyro.ai/examples/intro_part_ii.html`) :

- And **learn the distribution** with the same general inference algorithm.

$$p(\mu_t | s_1, \ldots, s_{10})$$

- Details about the inference algorithm will be given in the next sessions.

f



Pyro's inference (`http://pyro.ai/examples/intro_part_ii.html`) :

- And **learn the distribution** with the same general inference algorithm.

$$p(\mu_t | s_1, \ldots, s_{10})$$

- Details about the inference algorithm will be given in the next sessions.

Defining Conditional Independences in Pyro

In [176]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    mean_temp = pyro.sample('mean_temp', dist.Normal(15.0, 2.0))
    for i in range(obs['sensor'].shape[0]):
        temp = pyro.sample(f'temp_{i}', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample(f'sensor_{i}', dist.Normal(temp, 1.0), obs=obs['sensor'][i])
```

Pyro's cond. independeces (http://pyro.ai/examples/svi_part_ii.html) :

- Sensor variables are **independent** given temperature mean, μ_t.

$$p(s_1, t_1, ..., s_{10}, t_{10}|\mu_t) = \prod_{i=1}^{10} p(s_i, t_i|\mu_t)$$

```
In [37]: #The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1])}

def model(obs):
    mean_temp = pyro.sample('mean_temp', dist.Normal(15.0, 2.0))
    with pyro.plate('a', obs['sensor'].shape[0]):
        temp = pyro.sample('temp', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample('sensor', dist.Normal(temp, 1.0), obs=obs['sensor'])
```

Pyro's cond. independeces (http://pyro.ai/examples/svi_part_ii.html) :

- Sensor variables are **independent** given temperature mean, μ_t.

$$p(s_1, t_1, ..., s_{10}, t_{10}|\mu_t) = \prod_{i=1}^{10} p(s_i, t_i|\mu_t)$$

- We can use **Pyro's plate construct** to introduce this independence.

In [165]:
```
#Run inference
start = time.time()
svi(model, guide, obs, num_steps=1000)

#Print results
print("P(mean_temp|Sensor=[18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1]) =")
print(dist.Normal(pyro.param("mean").item(), pyro.param("scale").item()))
print("")
end = time.time()
print(f"{(end - start)} seconds")
```

```
P(mean_temp|Sensor=[18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1]) =
Normal(loc: 19.300748825073242, scale: 0.6379732489585876)

2.81210994720459 seconds
```

Pyro's cond. independeces (`http://pyro.ai/examples/svi_part_ii.html`) :

- We get large gains in efficiency due to **vectorized operations**.
- Execution time without *plate* is over 10s.

Now it is your turn!

- Exercise 2: The role of the **number of observations** in learning.

- Exercise 3: The role of the **prior distribution** in learning.

`Day1/students_PPLs_Intro.ipynb`

Toy Example: Ice-cream shop

Toy Example

Defining Machine Learning models with PPLs:

- We have an ice-cream shop and we record the ice-cream sales and the average temperature of the day.
- We know temperature affects the sales of ice-creams.
- We want to precisely find out how temperature affects ice-cream sales.

In [49]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1]),
       'sales': torch.tensor([46., 47., 49., 44., 50., 54., 51., 52., 49., 53.])}

def model(obs):
    mean_temp = pyro.sample('mean_temp', dist.Normal(15.0, 2.0))

    with pyro.plate('a', obs['sensor'].shape[0]):
        temp = pyro.sample('temp', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample('sensor', dist.Normal(temp, 1.0), obs=obs['sensor'])
```

Ice-cream Shop Model:

- We have observations from temperature and sales.

```
In [43]: #The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19.5, 20.1]),
       'sales': torch.tensor([46., 47., 49., 44., 50., 54., 51., 52., 49., 53.])}

def model(obs):
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        sales = pyro.sample('sales', dist.Poisson(??????), obs=obs['sales'])
```

Ice-cream Shop Model:

- We have observations from temperature and sales.
- Sales are modeled with a **Poisson distribution**.

In [201]:
```
#The observatons
obs = {'sensor': torch.tensor([18., 18.7, 19.2, 17.8, 20.3, 22.4, 20.3, 21.2, 19
       'sales': torch.tensor([46., 47., 49., 44., 50., 54., 51., 52., 49., 53.]

def model(obs):
    mean_temp = pyro.sample('mean_temp', dist.Normal(15.0, 2.0))
    alpha = pyro.sample('alpha', dist.Normal(0.0, 100.0))
    beta = pyro.sample('beta', dist.Normal(0.0, 100.0))

    with pyro.plate('a', obs['sensor'].shape[0]):
        temp = pyro.sample('temp', dist.Normal(mean_temp, 2.0))
        sensor = pyro.sample('sensor', dist.Normal(temp, 1.0), obs=obs['sensor']
        rate = torch.max(torch.tensor(0.001), alpha + beta*temp)
        sales = pyro.sample('sales', dist.Poisson(rate), obs=obs['sales'])
```

Ice-cream Shop Model:

- We have observations from temperature and sales.
- Sales are modeled with a **Poisson distribution**.
- The rate of the Poisson **linearly depends of the real temperature**.

In [48]:
```
#Run inference
svi(model, guide, obs, num_steps=1000)

#Print results
print("Posterior Temperature Mean")
print(dist.Normal(pyro.param("mean").item(), pyro.param("scale").item()))
print("")
print("Posterior Alpha")
print(dist.Normal(pyro.param("alpha_mean").item(), pyro.param("alpha_scale").item()))
print("")
print("Posterior Beta")
print(dist.Normal(pyro.param("beta_mean").item(), pyro.param("beta_scale").item()))
```

```
Posterior Temperature Mean
Normal(loc: 19.311052322387695, scale: 0.6258021593093872)

Posterior Alpha
Normal(loc: 19.773971557617188, scale: 1.8541947603225708)

Posterior Beta
Normal(loc: 1.5178951025009155, scale: 0.1155082955956459)
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Ice-cream Shop Model:

- We run the **(variational) inference engine** and get the results.

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```

Ice-cream Shop Model:

- We run the **(variational) inference engine** and get the results.
- With PPLs, we only care about modeling, **not about the low-level details** of the machine-learning solver.

Exercise 4: Introduce Humidity in the Icecream shop model

- Assume we also have a bunch of humidity senor measurements.
- Assume the sales are also linearly influenced by the humidity.
- **Extend the above model in order to integrate all of that**.

`Day1/students_PPLs_Intro.ipynb`

Day 2
Probabilistic Models with Deep Neural Networks

Andrés Masegosa

Department of Mathematics
University of Almería
Spain

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

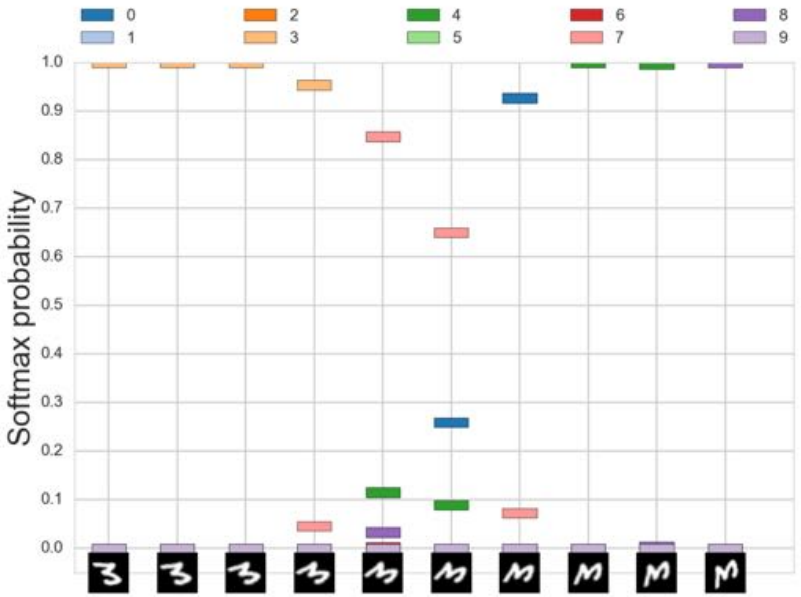
- Why do we need PPLs?
- Probabilistic programming in Pyro
- Hand-on exercises:
  - Probability Distributions in Pyro.
  - Probabilistic Models in Pyro.
  - Ice-cream Shop Model.

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

Uncertainty with Machine Learning



(Louizos et al, 2017)

Why is important to model uncertainty?

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

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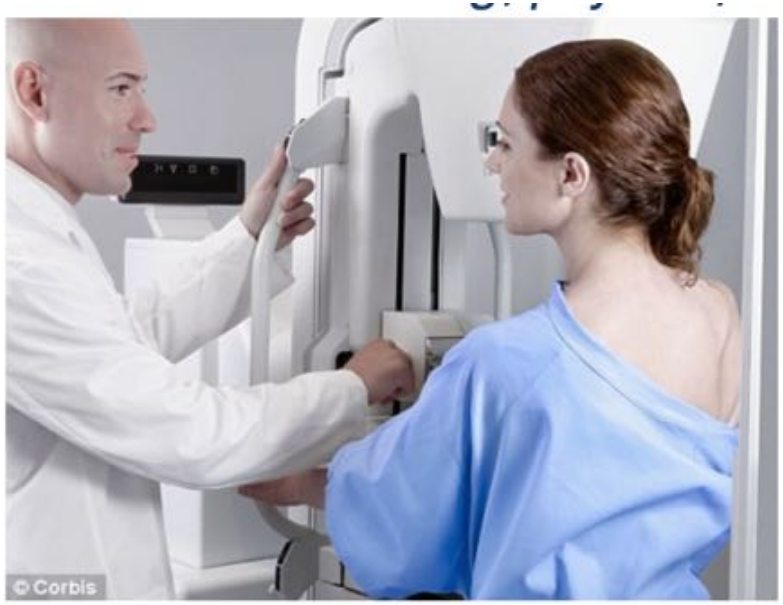

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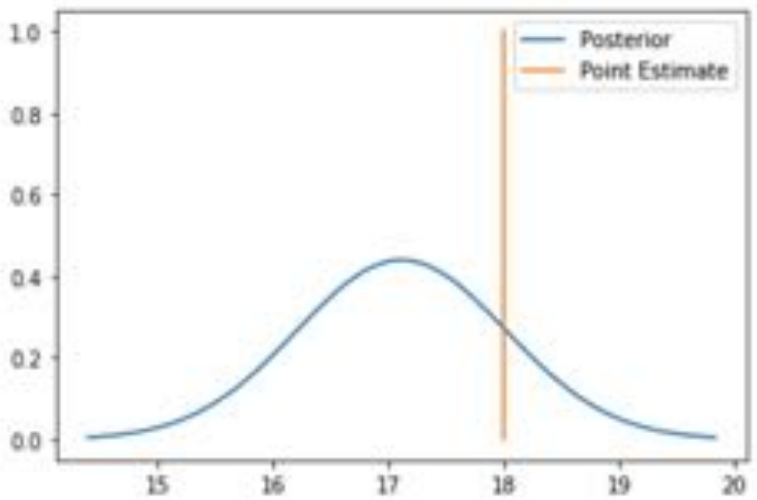
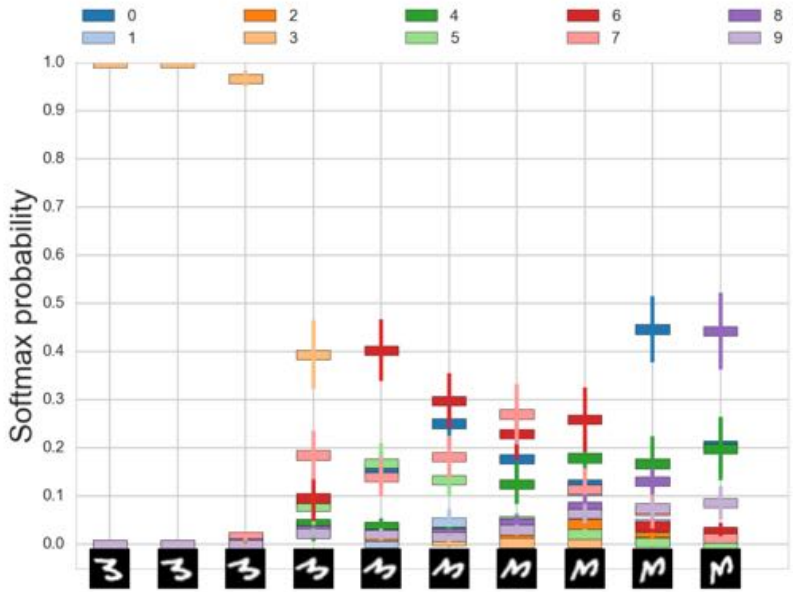



```
P(Temperature|Sensor=18.0) =
Normal(loc: 17.115509033203125, scale: 0.9070338010787964)
```

Probabilistic Models naturally quantify uncertainty

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

Uncertainty with Machine Learning



(Louizos et al, 2017)

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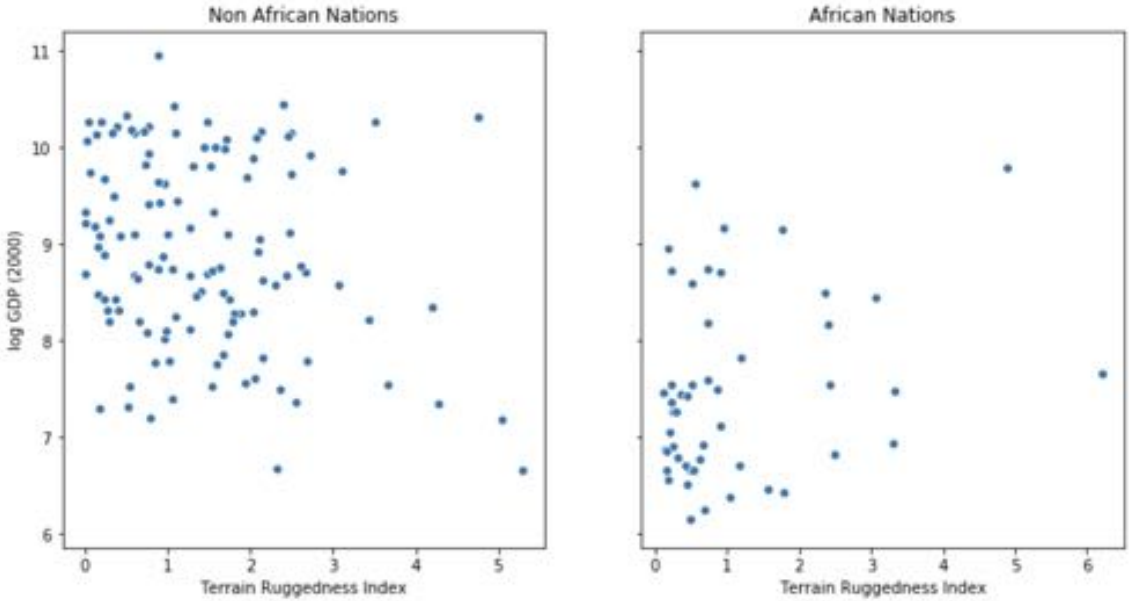
Example

Real Data Example

Nunn, N. & Puga, D., Ruggedness: The blessing of bad geography in Africa, Review of Economics and Statistics 94(1), Feb. 2012



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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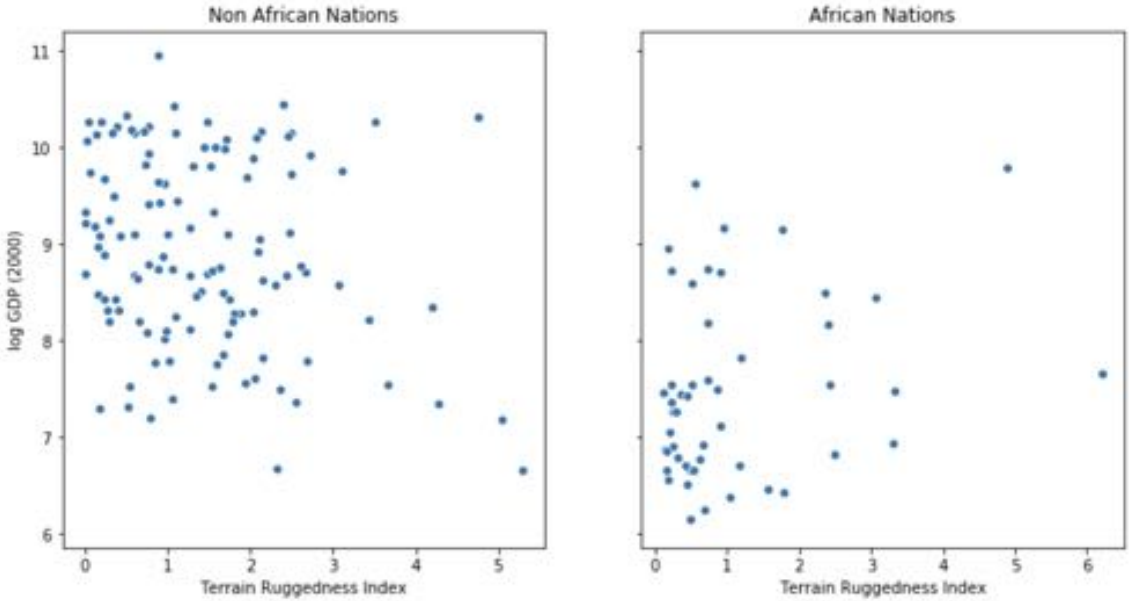

Relationship between topographic heterogeneity and GDP per capita

- 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?

1. **Linear Regression Model**:

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

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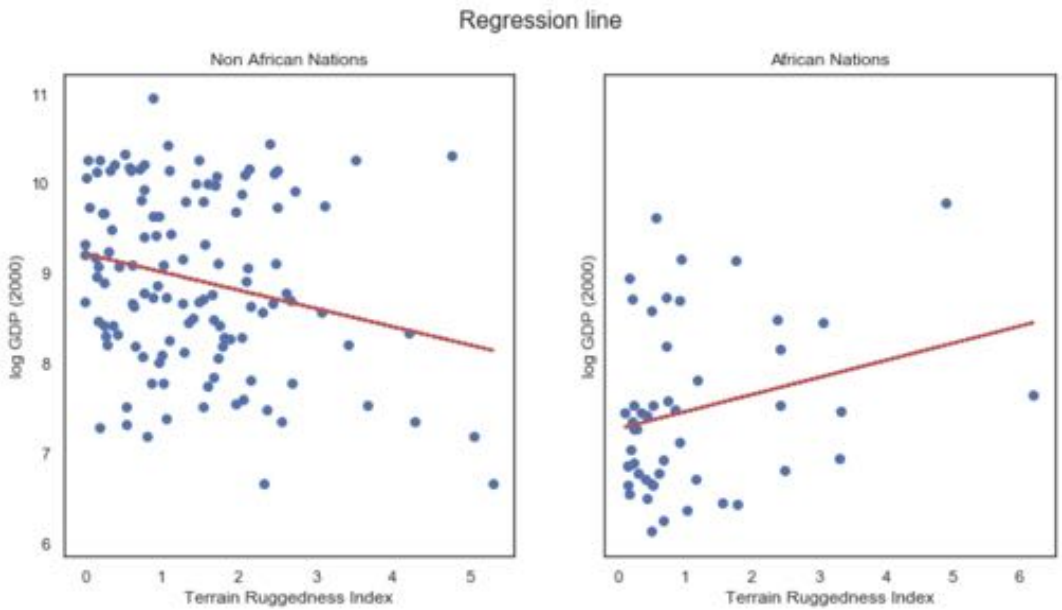
Day2/students_Bayesian_regression.ipynb

Real Data Example



Linear Regression Model

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

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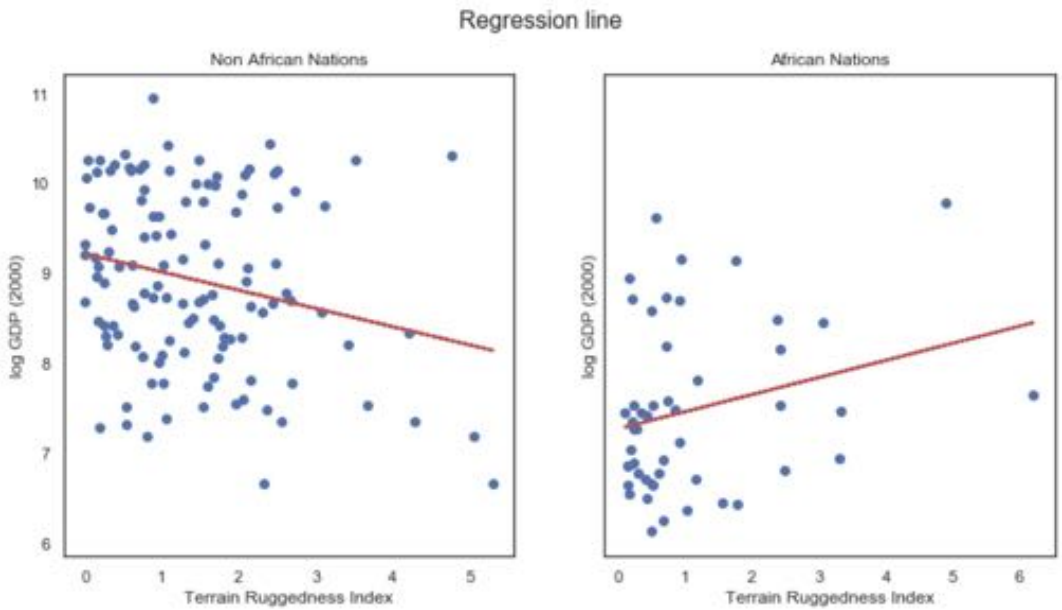

Linear Regression Model

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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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Day2/students_Bayesian_regression.ipynb

Exercise: Bayesian Logistic Regression

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

`Day2/students_Bayesian_Regression.ipynb`

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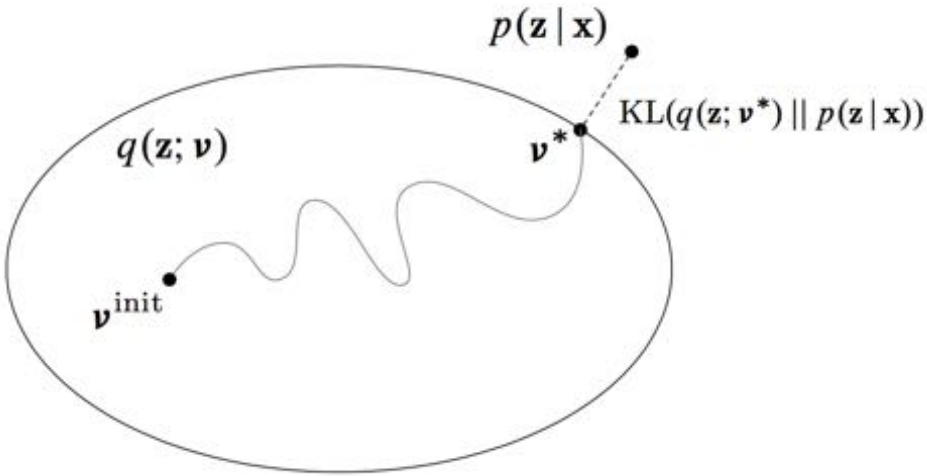
We have to use **approximate posterior inference**.

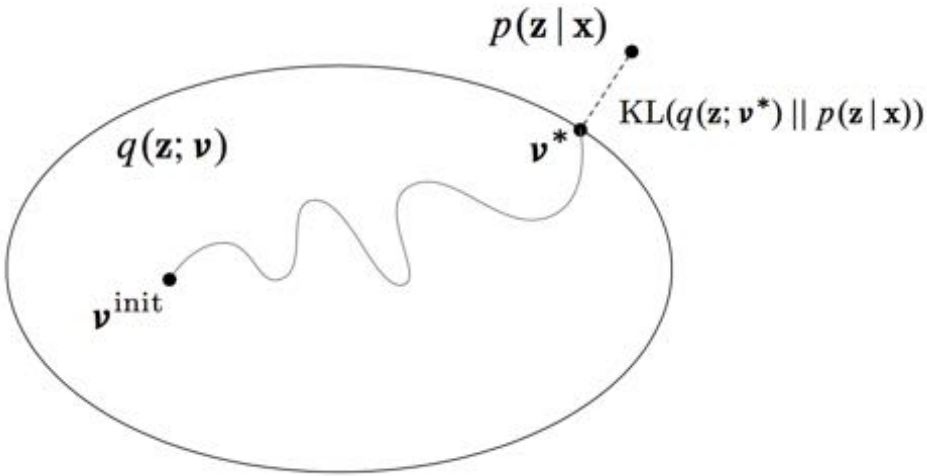
Variational Inference



- **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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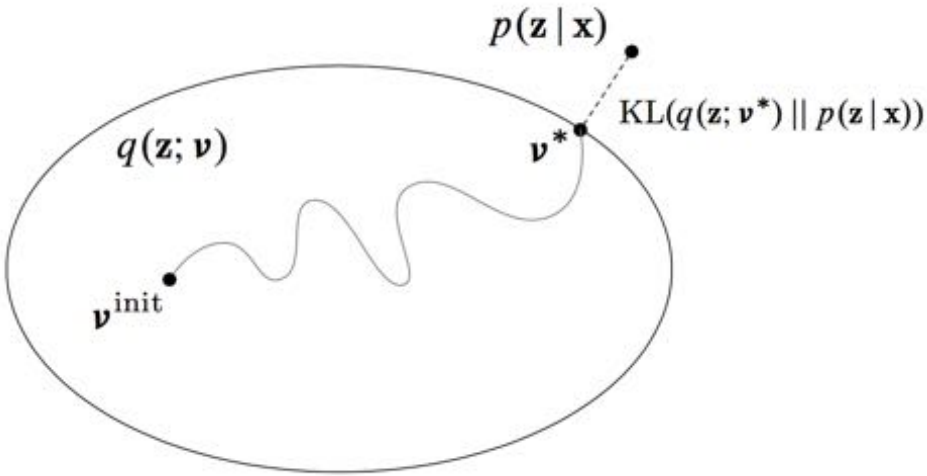

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- Solve using a **optimization algorithm** (i.e. gradient descent).

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

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

1. Define a tractable approximating **variational family**,

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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**,

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

```
#The guide
def guide(obs):
    a = pyro.param("mean", torch.tensor(0.0))
    b = pyro.param("scale", torch.tensor(1.), constraint=constraints.positive)
    temp = pyro.sample('temp', dist.Normal(a, b))
```

Pyro's Guides

- We want to compute the **posterior**, $p(temp|sensor = 18.0)$
- We define, $q(temp|\boldsymbol{\nu}) = \mathcal{N}(\boldsymbol{\nu}_a, \boldsymbol{\nu}_b)$

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Pyro's Guides

- We want to compute the **posterior**, $p(temp|sensor = 18.0)$
- 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,

$$\boldsymbol{\nu}^{\star} = \arg\min_{\nu} KL\big(q(temp|\boldsymbol{\nu})||p(temp|sensor = 18.0)\big)$$

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Exercise: Pyro implementation for a simple Gaussian model

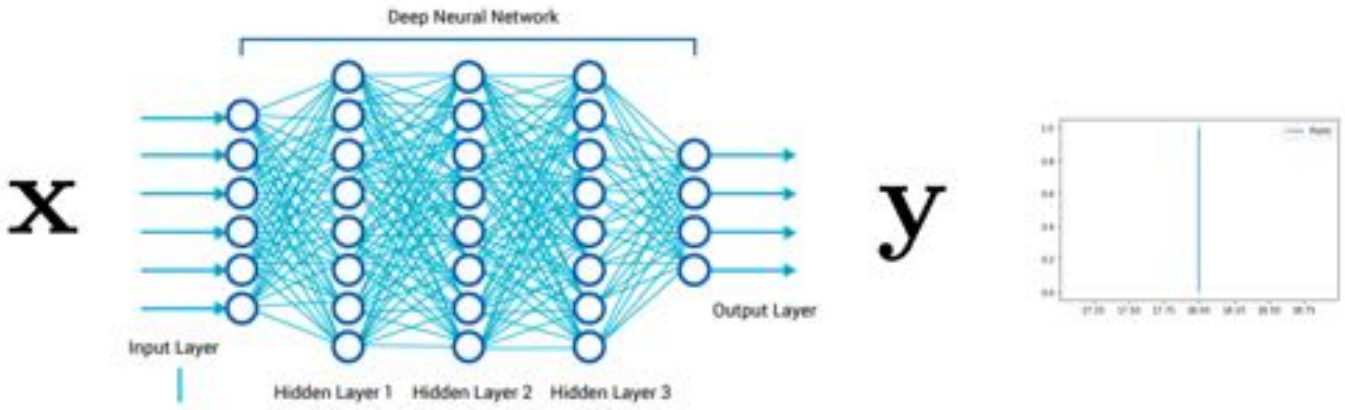
1. Implement a Pyro's **model** for a Normal distribution with prior over mean and (inverse) of variance. The variable x is always observed.

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

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

$$
\begin{aligned}
q(\mu) &= \text{Norma}(\boldsymbol{\nu}_{\mu}, \boldsymbol{\nu}_{\sigma^2}) \\
q(\gamma) &= \text{Gammal}(\boldsymbol{\nu}_{\alpha}, \boldsymbol{\nu}_{\beta})
\end{aligned}
$$

`Day2/student_simple_model.ipynb`



Neural Network

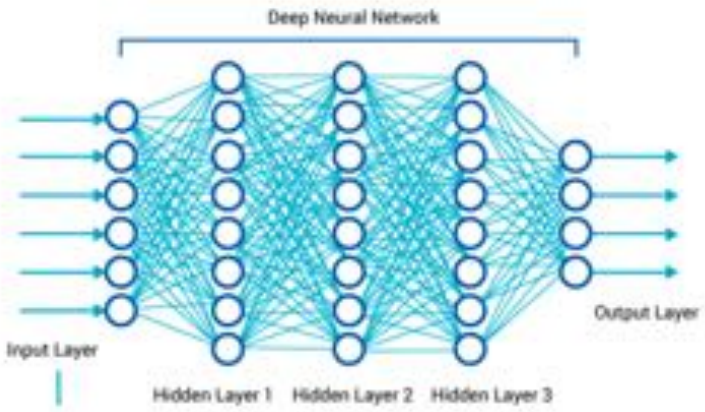
- $h(\cdot;\theta)$ encodes a neural network (i.e. a non-linear function).

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

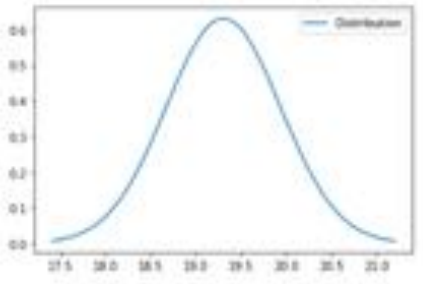
- Loss minimization,

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

$\mathbf{x}$



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

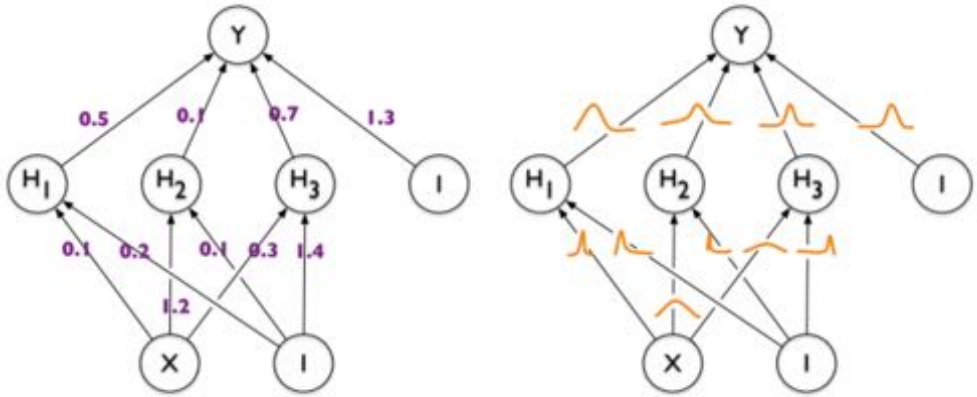


Bayesian Neural Network

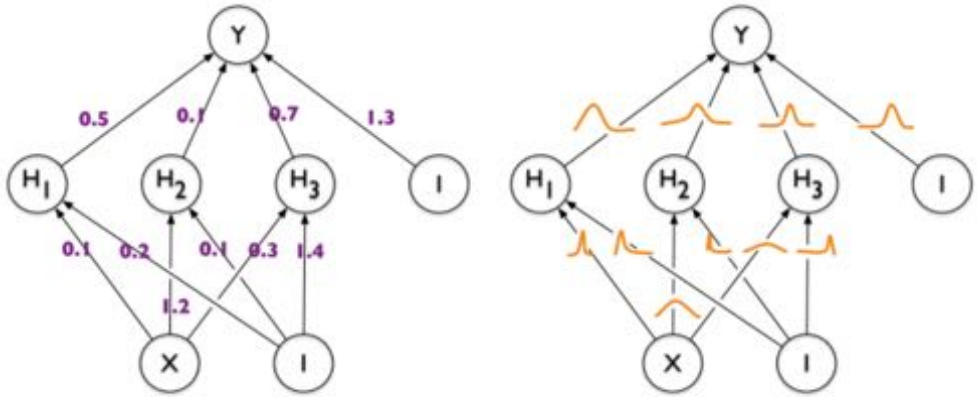
- E.g. Neural regressor,

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

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



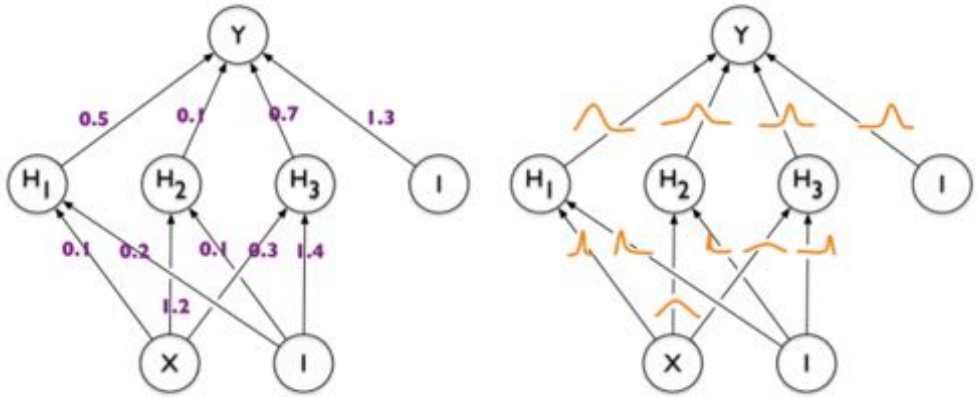
Bayesian Neural Network



Bayesian Neural Network

- **Variational Inference**,

$$\boldsymbol{\nu}^{\star} = \arg\min_{\nu} KL\big(q(\theta|\boldsymbol{\nu})||p(\theta|\mathbf{y}_1, \mathbf{x}_1, \ldots, \mathbf{y}_n, \mathbf{x}_n)\big)$$



Bayesian Neural Network

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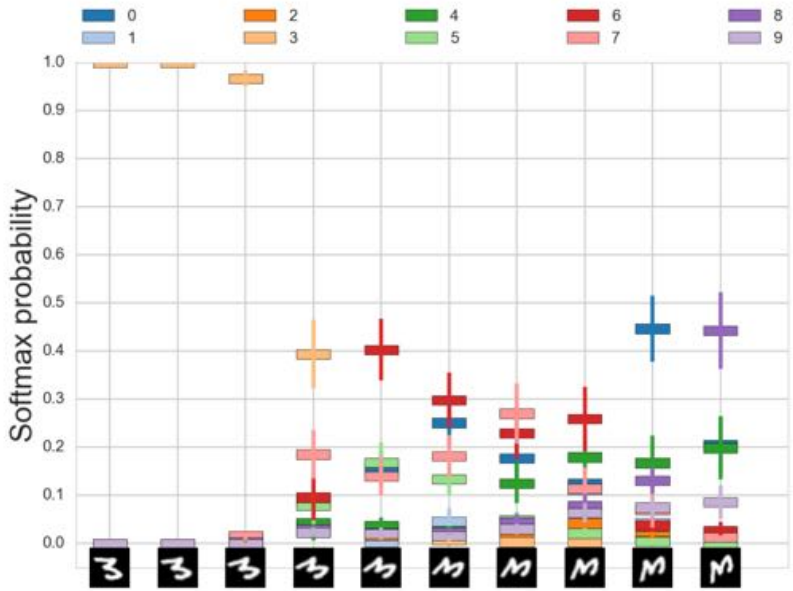
- Bayesian predictive is an **ensemble of neural networks**,

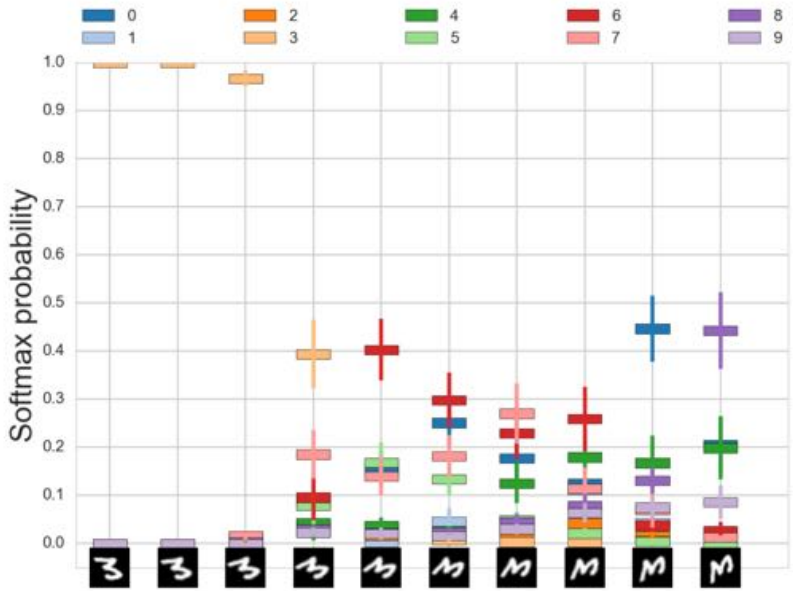
$$\begin{aligned} p(y|\mathbf{x}) &= \int p(y|\mathbf{x}, \theta) q(\theta|\boldsymbol{\nu}^\star) d\theta \\ &\approx \frac{1}{M} \sum_{\theta_j \sim q(\theta|\boldsymbol{\nu}^\star)} p(y|\mathbf{x}, \theta_j) \end{aligned}$$



(Louizos et al, 2017)

Bayesian Neural Networks

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



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Bayesian Neural Networks

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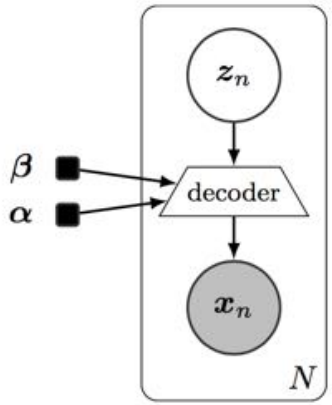
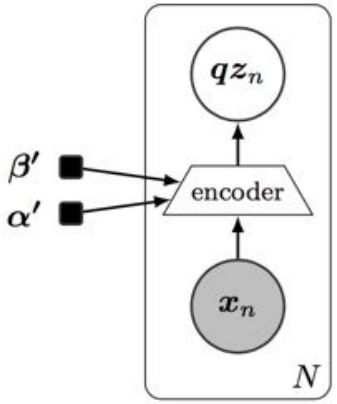
Day2/BayesianNeuralNetworks.ipynb

Unsupervised Probabilistic Models with Deep Neural Networks



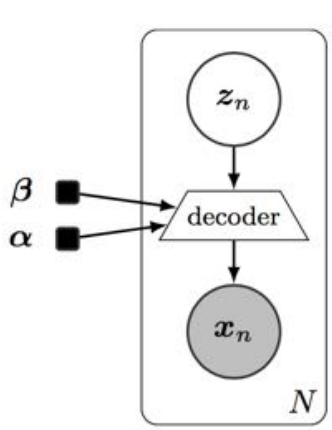
$p(\mathbf{x}|\mathbf{z}, \theta)$



$q(\mathbf{z}|\mathbf{x}, \phi)$

Unsepervised Learning with Deep Neural Networks

- **No labeled data** (extract structure from data).



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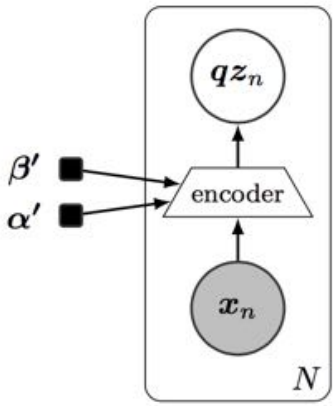

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Unsepervised Learning with Deep Neural Networks

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$$\mathbf{z} \sim p(\mathbf{z})$$
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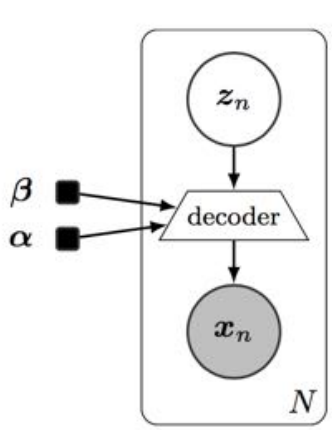

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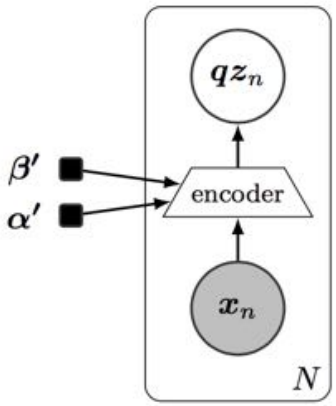

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Unsupervised Learning

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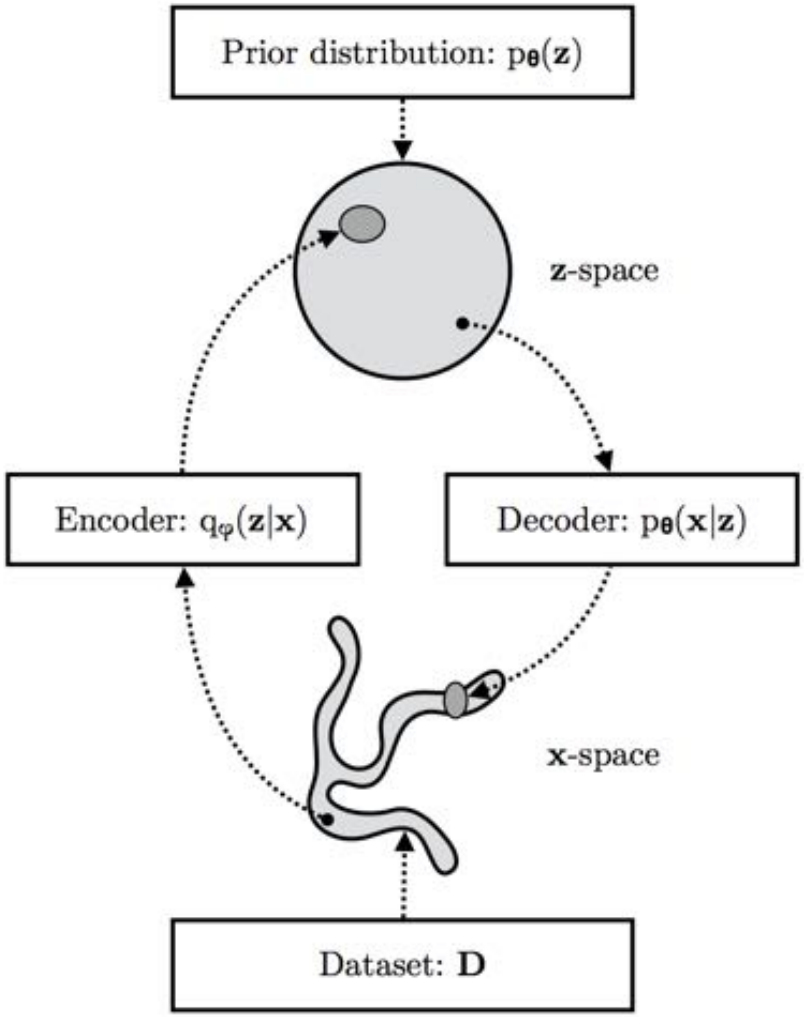
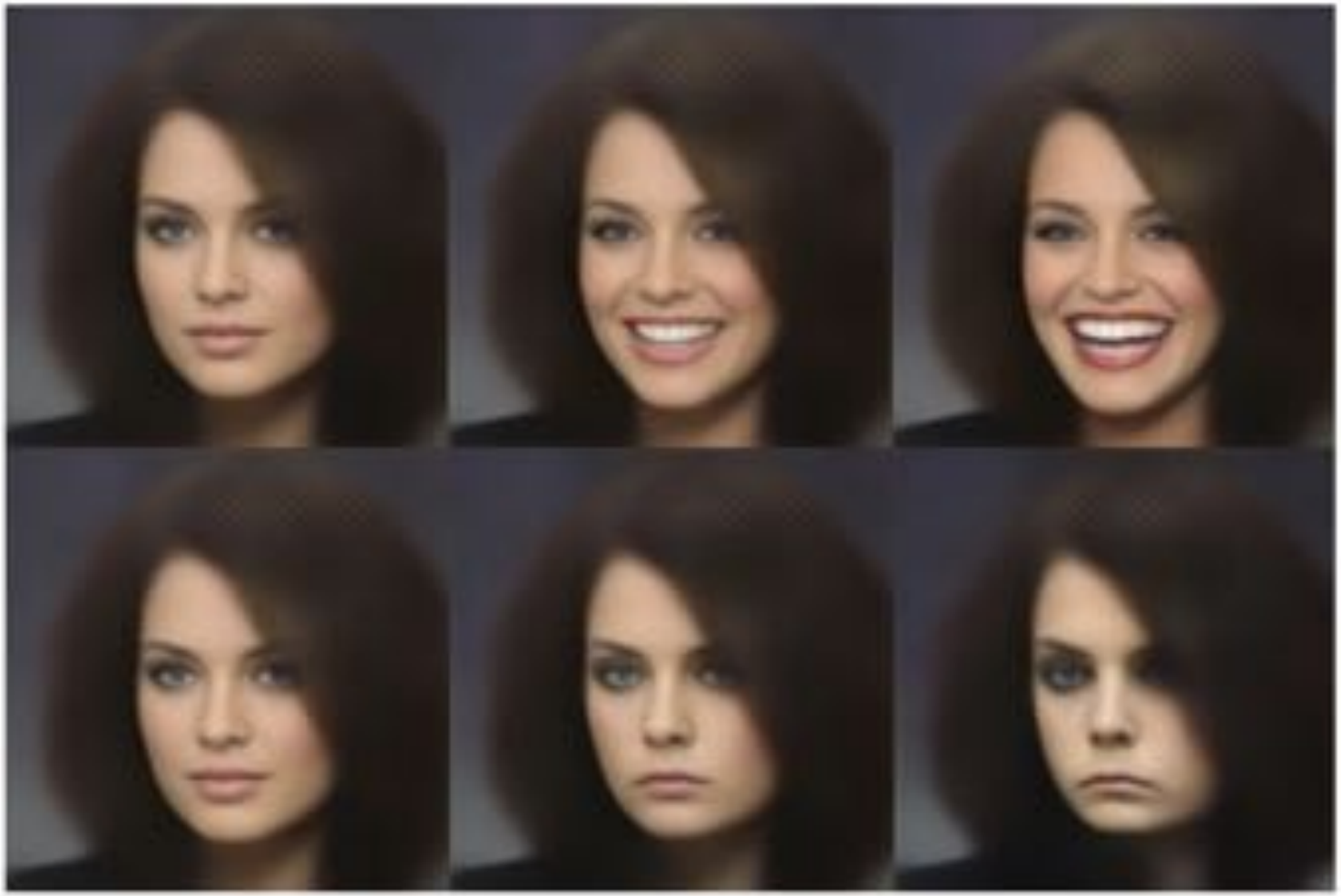


Kingma, D. P.,& Welling, M. (2019). An Introduction to Variational Autoencoders. arXiv preprint arXiv:1906.02691.



(White et al. 2016)

Exercise: Bayesian PCA in Pyro

- VAE using linear transformations.
- Applied to MNIST data set.

`Day2/BayesianPCA.ipynb`

Exercise: Bayesian PCA in Pyro

- VAE using linear transformations.
- Applied to MNIST data set.

`Day2/BayesianPCA.ipynb`

Exercise: Variational Auto-Encoder in Pyro

- VAE using simple neural network.
- Applied to MNIST data set.

`Day2/VAE.ipynb`

Conclusions

- **Probabilistic modeling is a key aspect in AI systems**
  - Confidence in model predictions/actions.
  - To know what you do not know.

Conclusions

- **Probabilistic modeling is a key aspect in AI systems**
  - Confidence in model predictions/actions.
  - To know what you do not know.
- **PPLs are the right tool for probabilistic modeling.**
  - Enormous expressibility.
  - Powerful inference engines (BlackBox Variational Inference).

End

https://inferpy.readthedocs.io

http://www.amidsttoolbox.com/

Thanks!!!!! :)