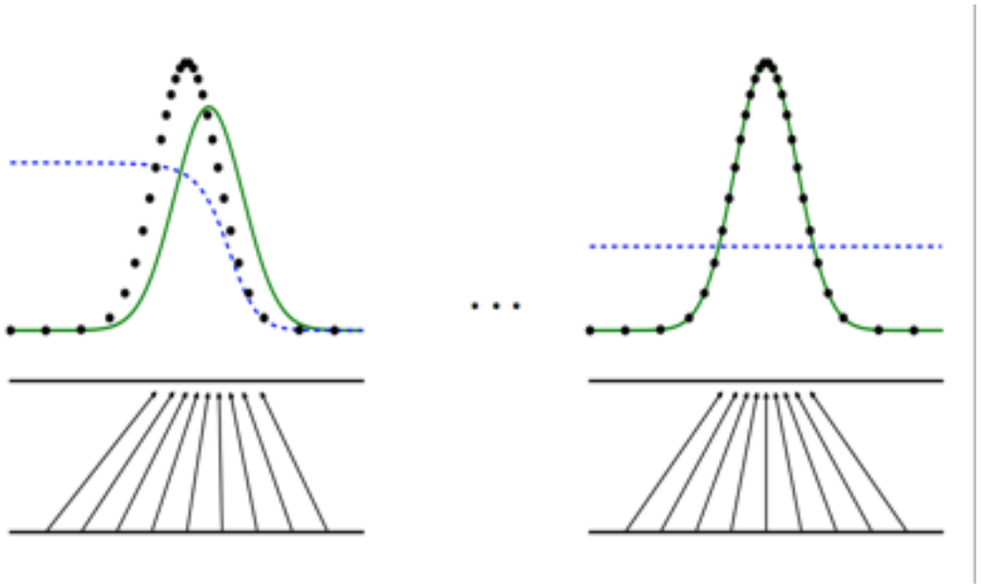
Implicit Posterior Variational Inference for Deep Gaussian Processes (IPVI DGP)



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National University of Singapore
Massachusetts Institute of Technology

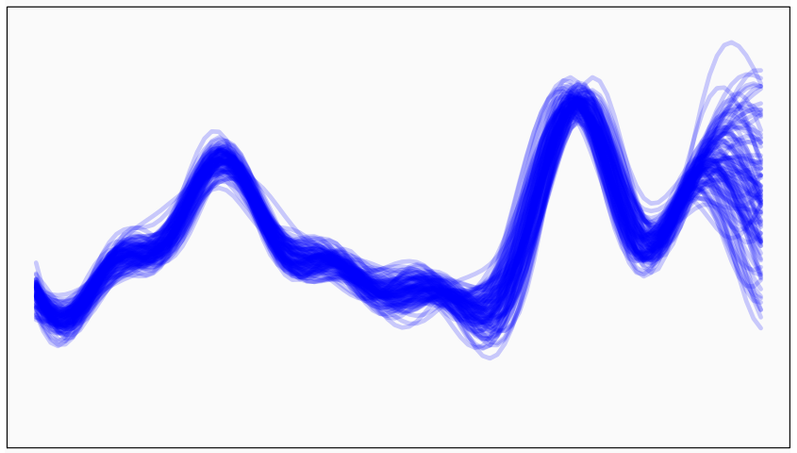
* indicates equal contribution

GP V.S. Deep GP

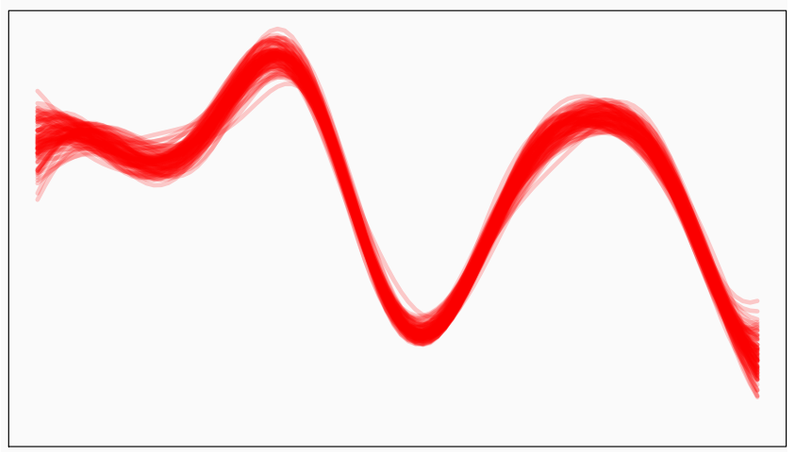
- A GP is fully specified by its kernel function
  - **RBF:** universal approximator
  - Matern
  - Brownian
  - Linear
  - Polynomial
  - ……

GP V.S. Deep GP

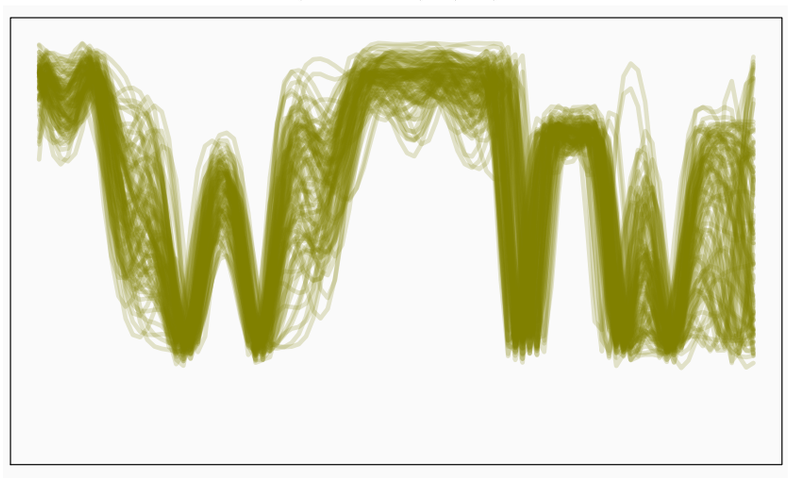
$f(x)$



$g(x)$



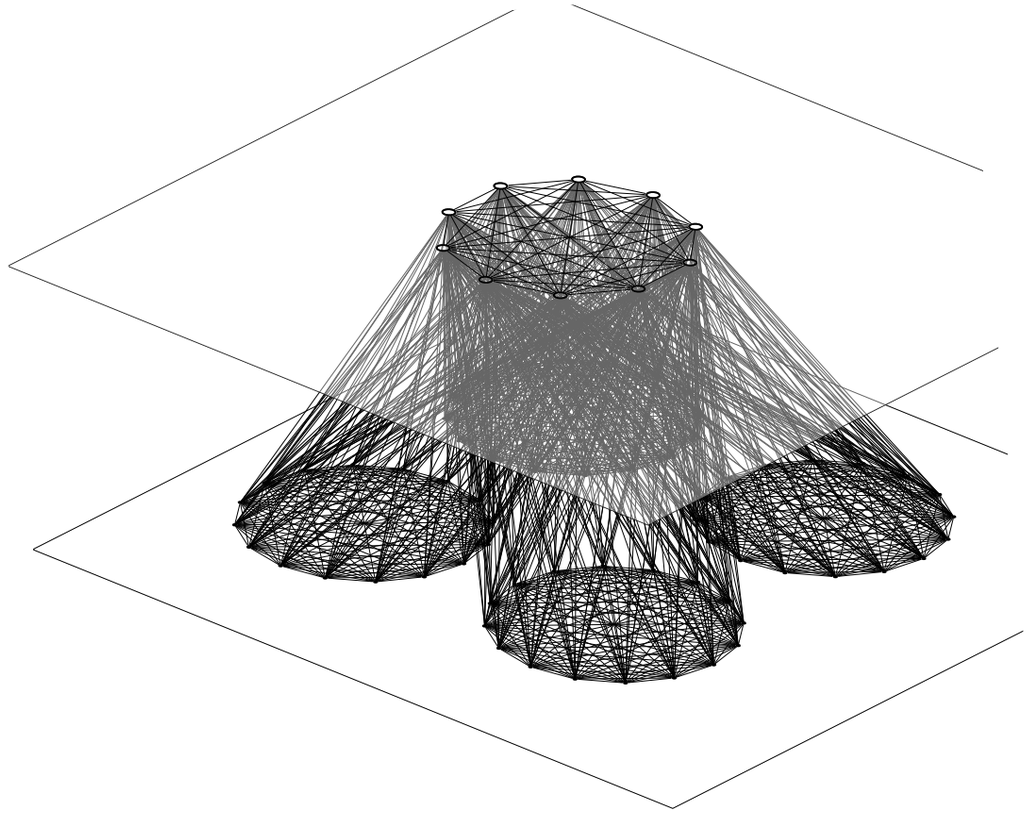
$(f \circ g)(x)$

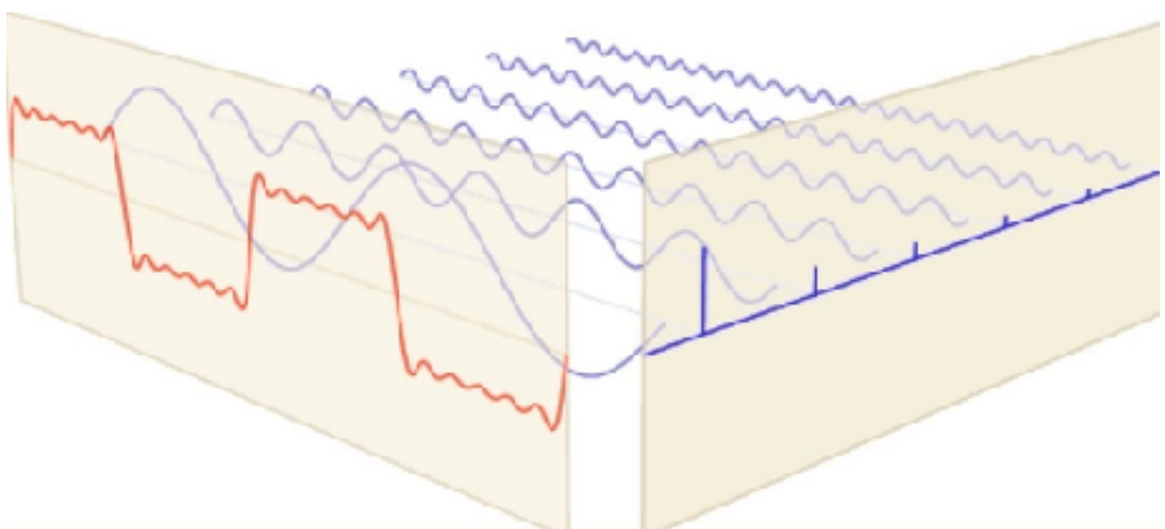


- Composition of Gaussian processes yields very complex function

Deep Gaussian Process (DGP)

- Inducing variables based approximations
  - Variational Inference
    - Damianou and Lawrence, AISTATS, 2013
    - Hensman and Lawrence, arXiv, 2014
    - Salimbeni and Deisenroth, NIPS, 2017
  - Expectation Propogation
    - Bui, ICML, 2016
  - MCMC
    - Havasi et al, NIPS 2018
- Random feature approximations
    - Cutajar et al, ICML 2017





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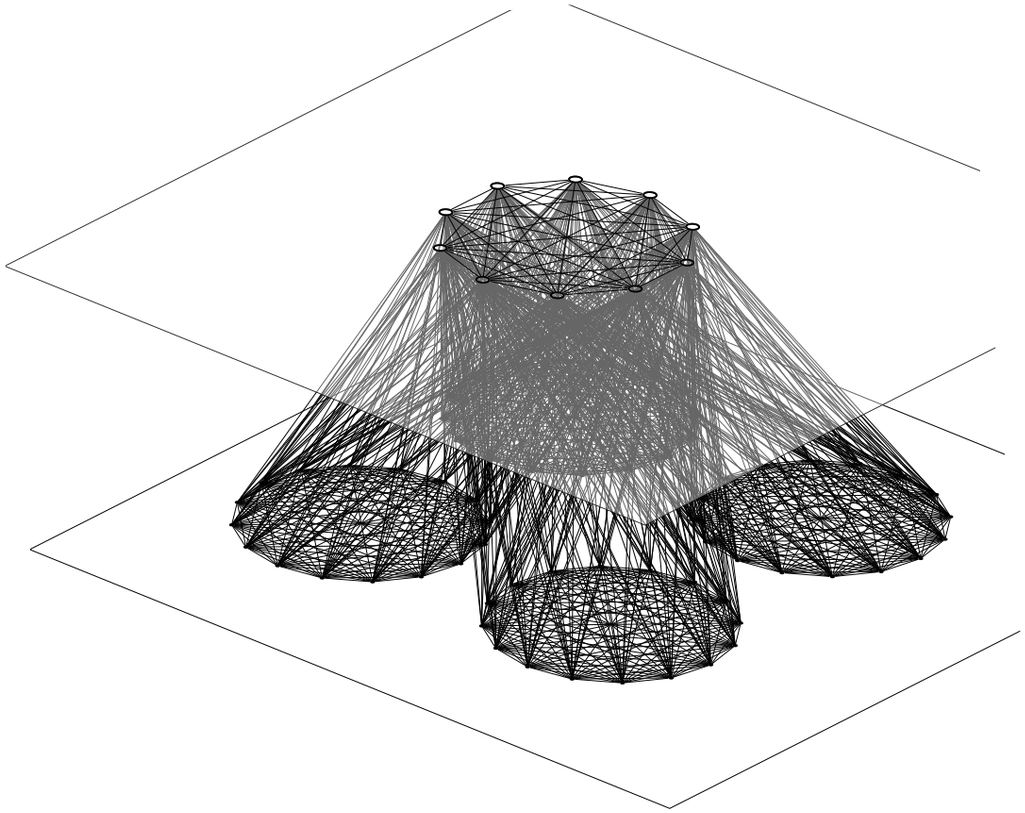
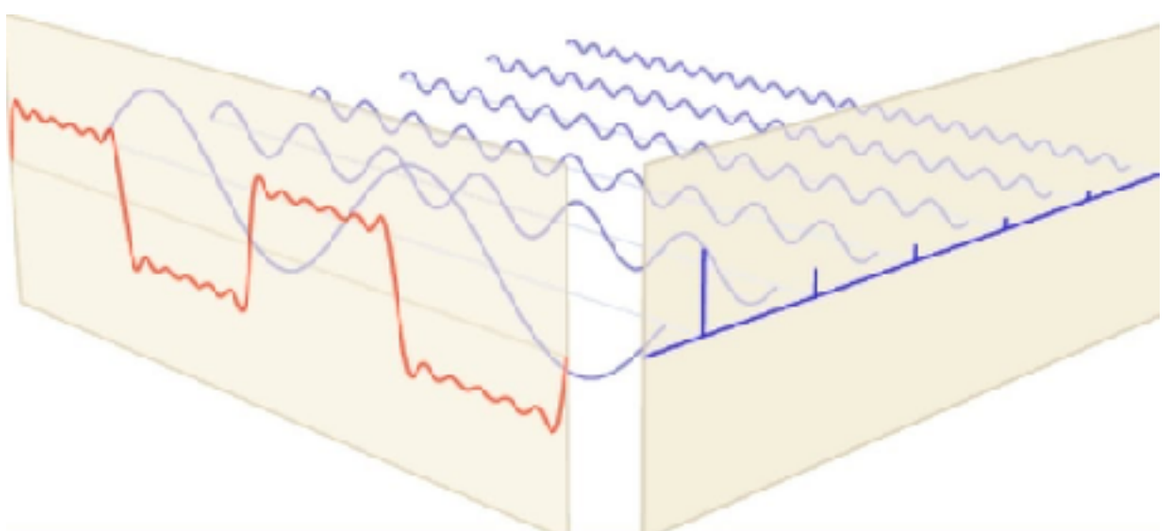
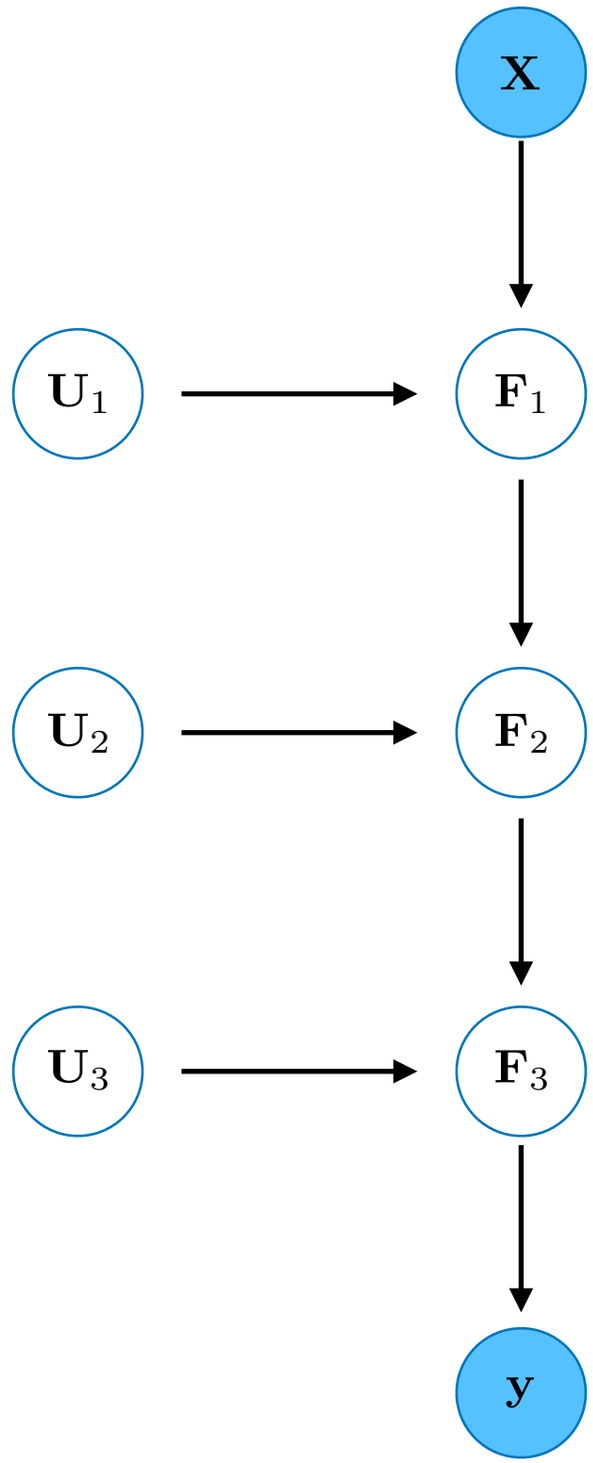




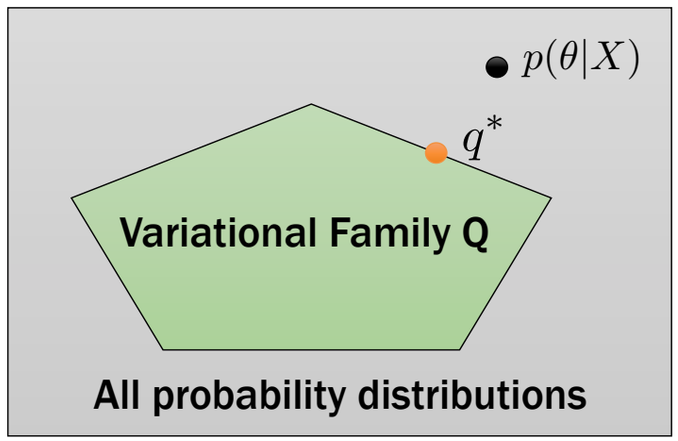
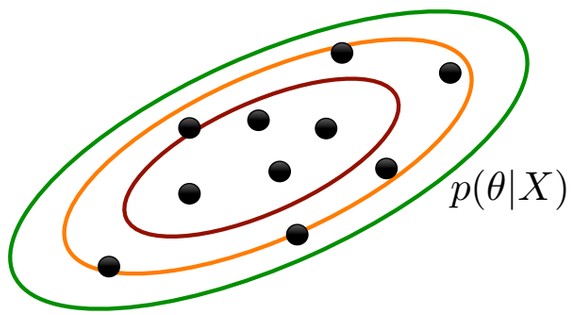
Deep GP (DGP)

- Inducing variables $\boldsymbol{\mathcal{U}} = \{\mathbf{U}_1, \ldots, \mathbf{U}_L\}$
- Posterior is intractable $p(\boldsymbol{\mathcal{U}}|\mathbf{y})$



Deep GP (DGP)

- Exact inference is intractable in DGP

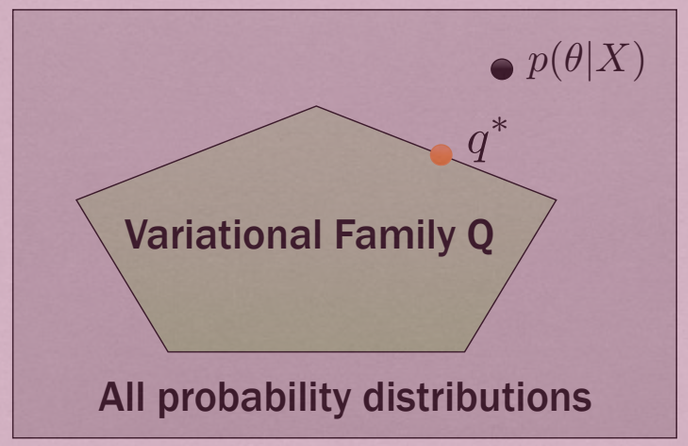
Variational Inference	Sampling
$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta) \| p(\theta \| X)]$	$\mathbb{E}_{p(\theta \| X)}[f(\theta)] \approx \frac{1}{T} \sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta \| X)$
	

Deep GP (DGP)

- Exact inference is impossible in DGP

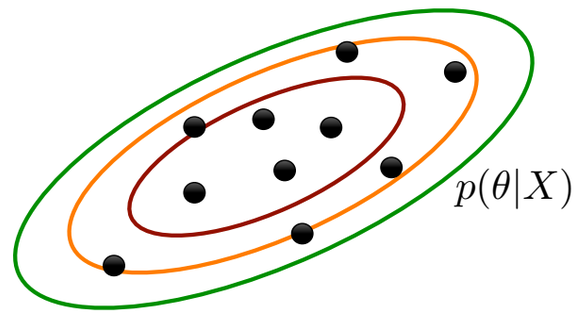
Variational Inference

$$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta)||p(\theta|X)]$$



Sampling

$$\mathbb{E}_{p(\theta|X)}[f(\theta)] \approx \frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta|X)$$



Deep GP (DGP)

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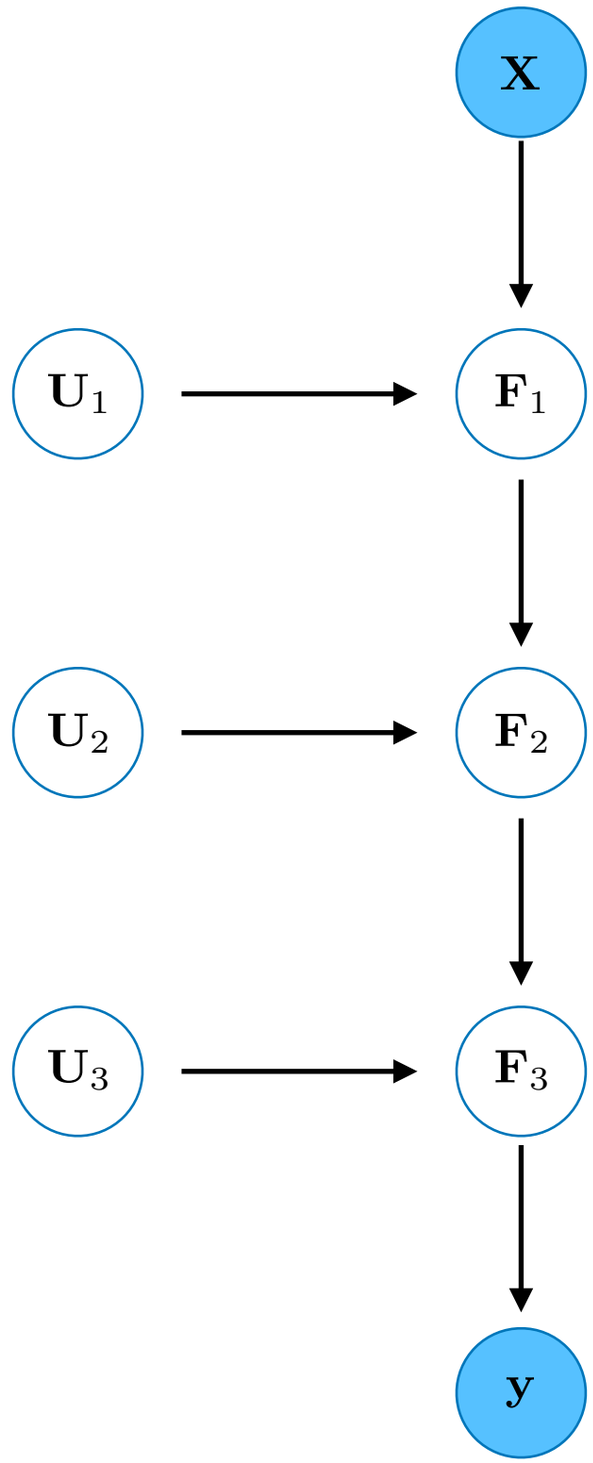


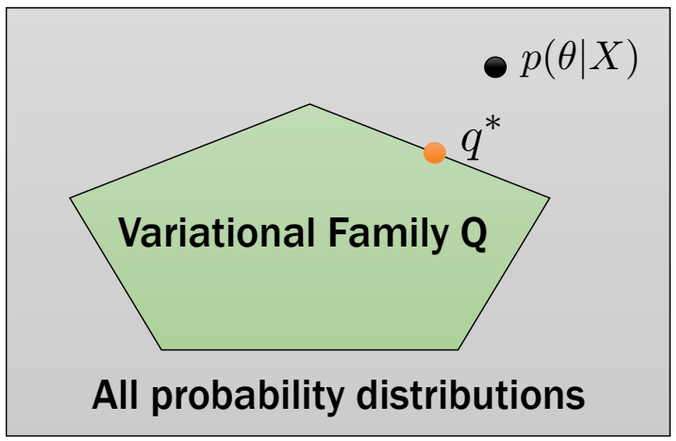
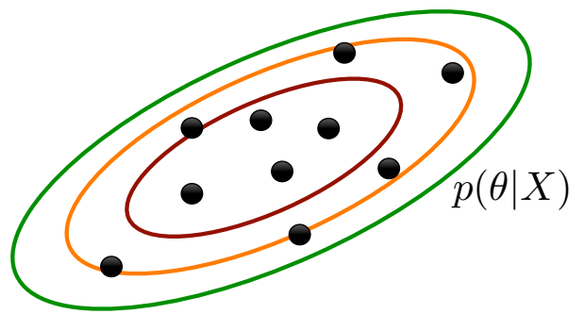
- Gaussian approximation: $q(\mathbf{U}_l)$
- mean field approximation: $q(\boldsymbol{\mathcal{U}}) = \prod_{l=1}^{L} q(\mathbf{U}_l)$

$$\text{ELBO} = \int q(\mathbf{F}_L) \log p(\mathbf{y}|\mathbf{F}_L) \mathrm{d}\mathbf{F}_L - \text{KL}[q(\boldsymbol{\mathcal{U}})||p(\boldsymbol{\mathcal{U}})]$$

$$q(\mathbf{F}_L) = \int \prod_{l=1}^{L} p(\mathbf{F}_l|\mathbf{U}_l, \mathbf{F}_{l-1}) q(\boldsymbol{\mathcal{U}}) \mathrm{d}\mathbf{F}_1 \ldots \mathrm{d}\mathbf{F}_{L-1} \mathrm{d}\boldsymbol{\mathcal{U}}$$

Deep GP (DGP)

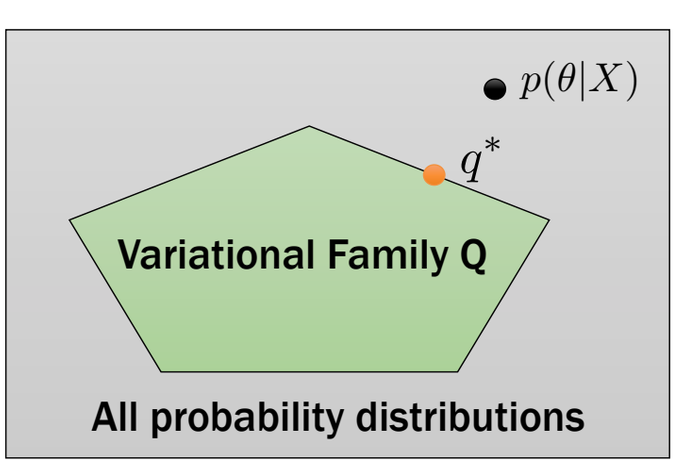
- Exact inference is impossible in DGP

Variational Inference	Sampling
$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta) \| p(\theta \| X)]$ 	$\mathbb{E}_{p(\theta\|X)}[f(\theta)] \approx \frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta\|X)$ 
1. biased 2. local minima	

Variational Inference

Variational Inference

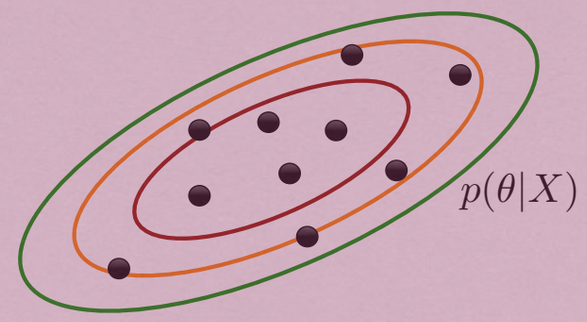
$$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta)||p(\theta|X)]$$



1. biased
2. local minima

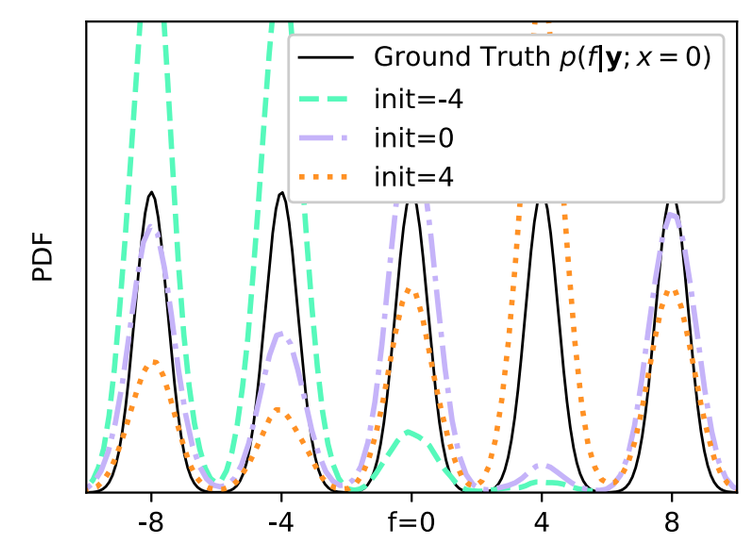
Sampling

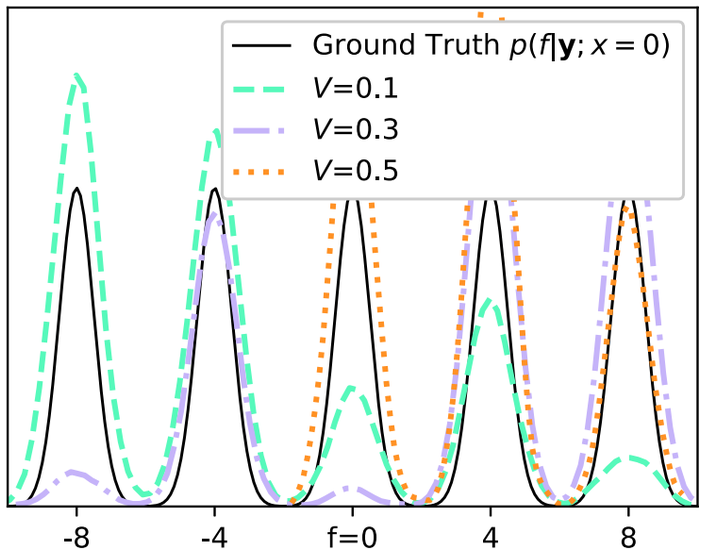
$$\mathbb{E}_{p(\theta|X)}[f(\theta)] \approx \frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta|X)$$

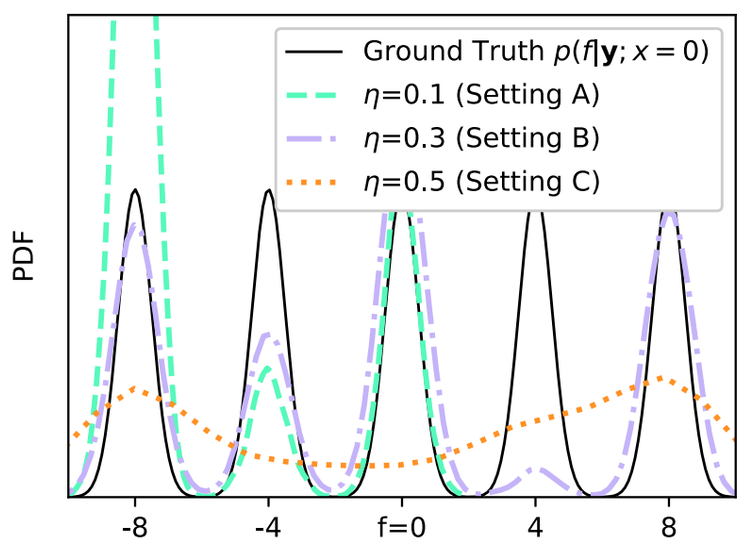


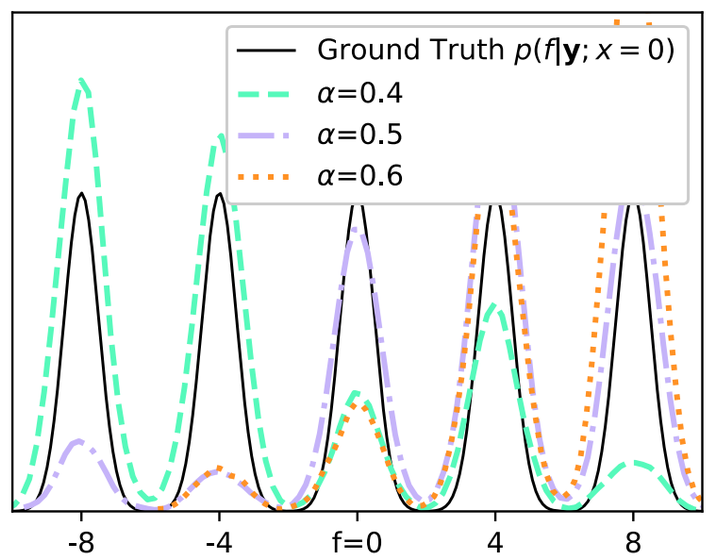
MCMC

- 5 mode posterior distribution
- Various parameter setting for MCMC method
  - init
  - V
  - η
  - α



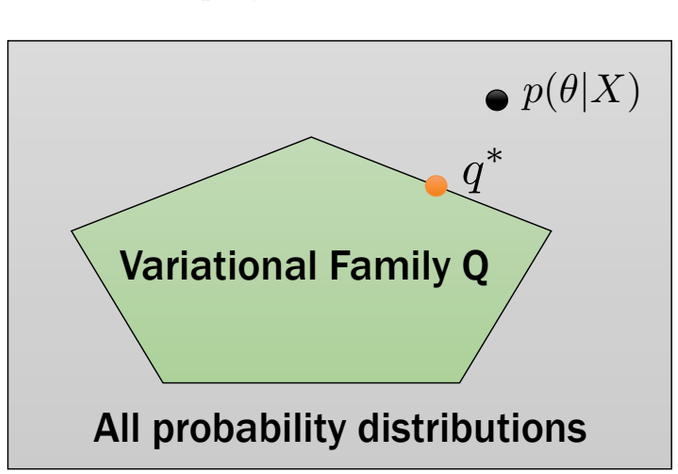
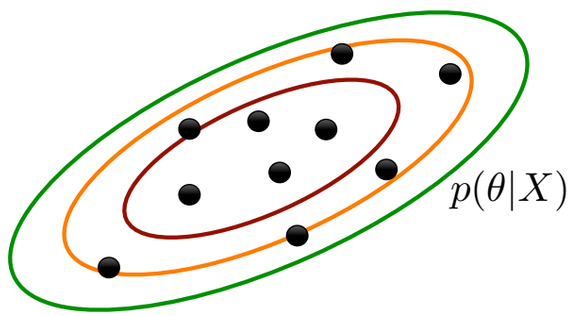






Deep GP (DGP)

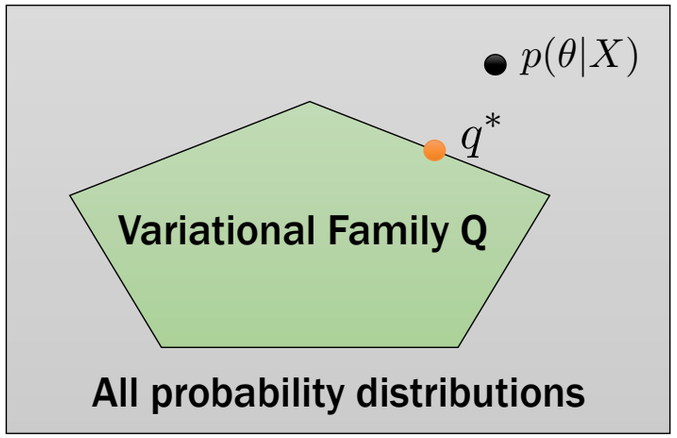
- Stochastic Gradient Markov Chain Monte Carlo

Variational Inference	Sampling
$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta) \| p(\theta \| X)]$ 	$\mathbb{E}_{p(\theta\|X)}[f(\theta)] \approx \frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta\|X)$ 
1. biased 2. local minima	1. local modes 2. efficiency

Deep GP (DGP)

Variational Inference

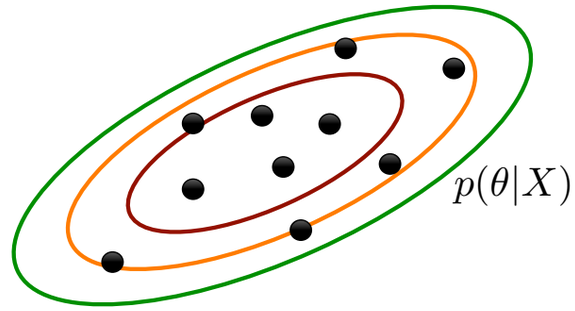
$$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta)||p(\theta|X)]$$



efficiency

Sampling

$$\mathbb{E}_{p(\theta|X)}[f(\theta)] \approx \frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta|X)$$



unbiased

Deep GP (DGP)

Variational Inference

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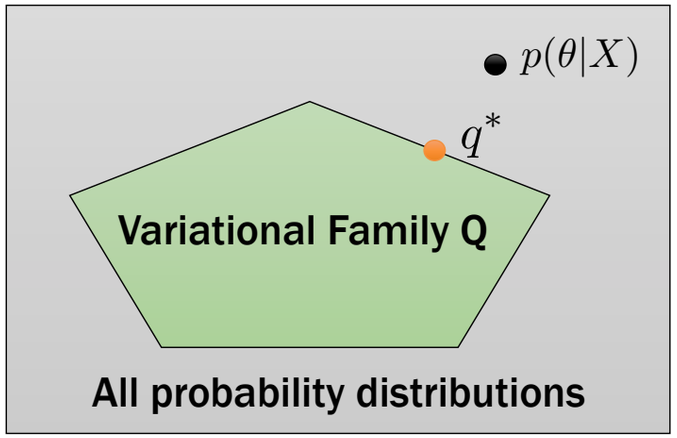

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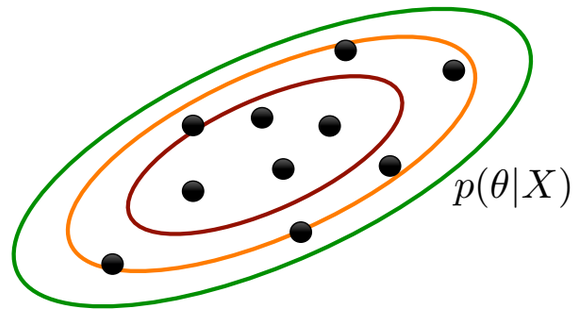
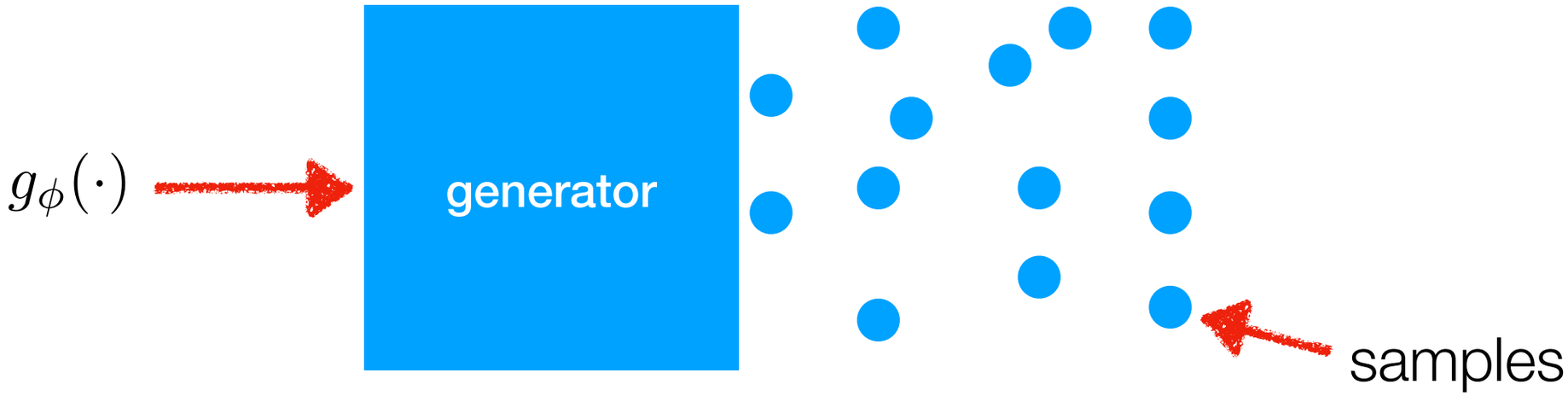


unbiased

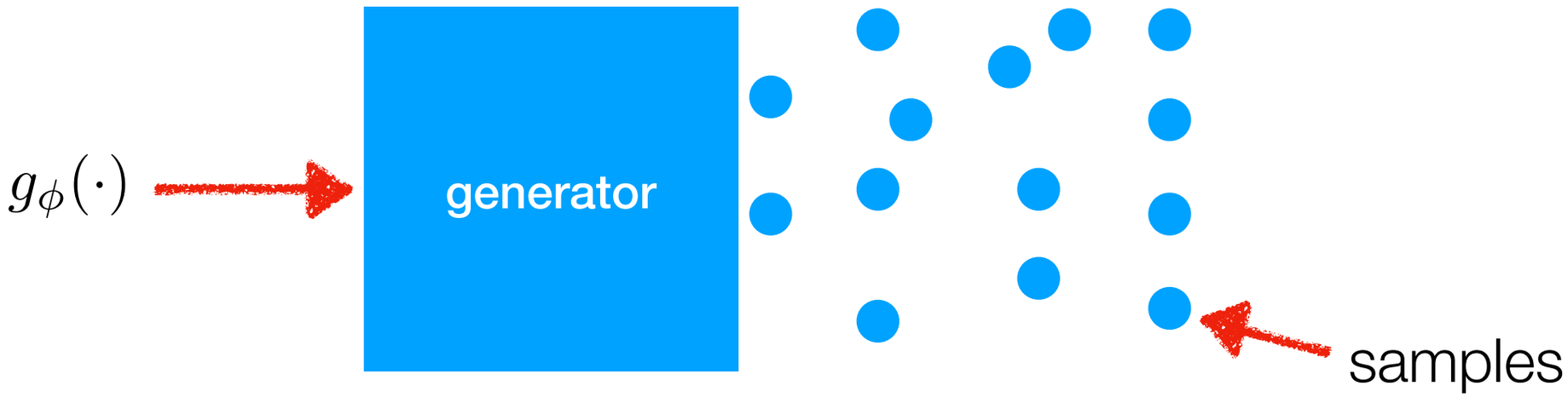
true posterior efficiently

Implicit Posterior Variational Inference



$$\text{ELBO} = \mathbb{E}_{q(\mathbf{F}_L)}[\log p(\mathbf{y}|\mathbf{F}_L)] - \text{KL}\left[q_\Phi(\boldsymbol{\mathcal{U}})||p(\boldsymbol{\mathcal{U}})\right]$$

Implicit Posterior Variational Inference



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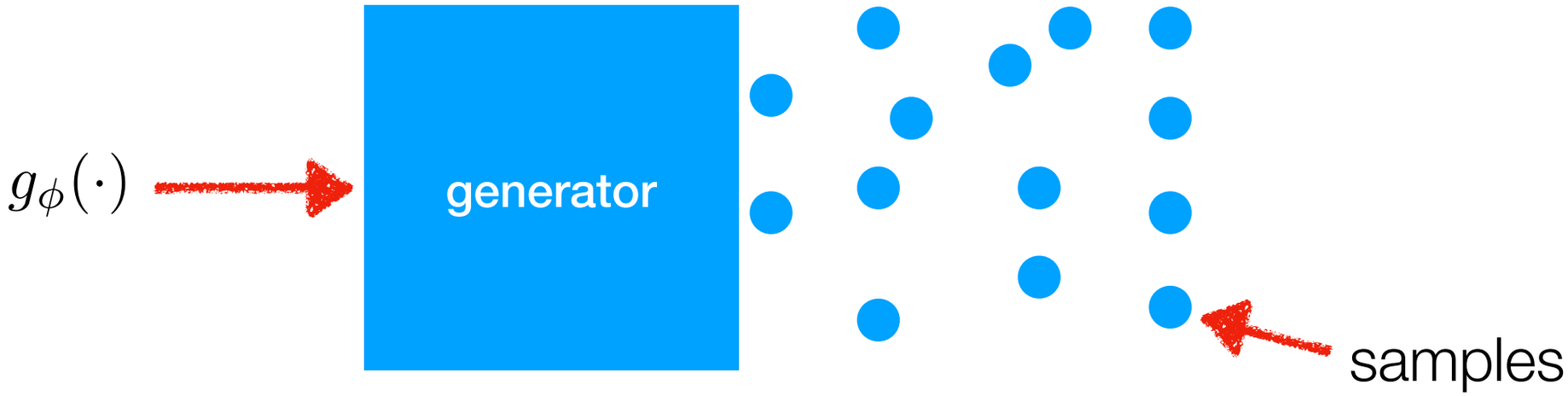
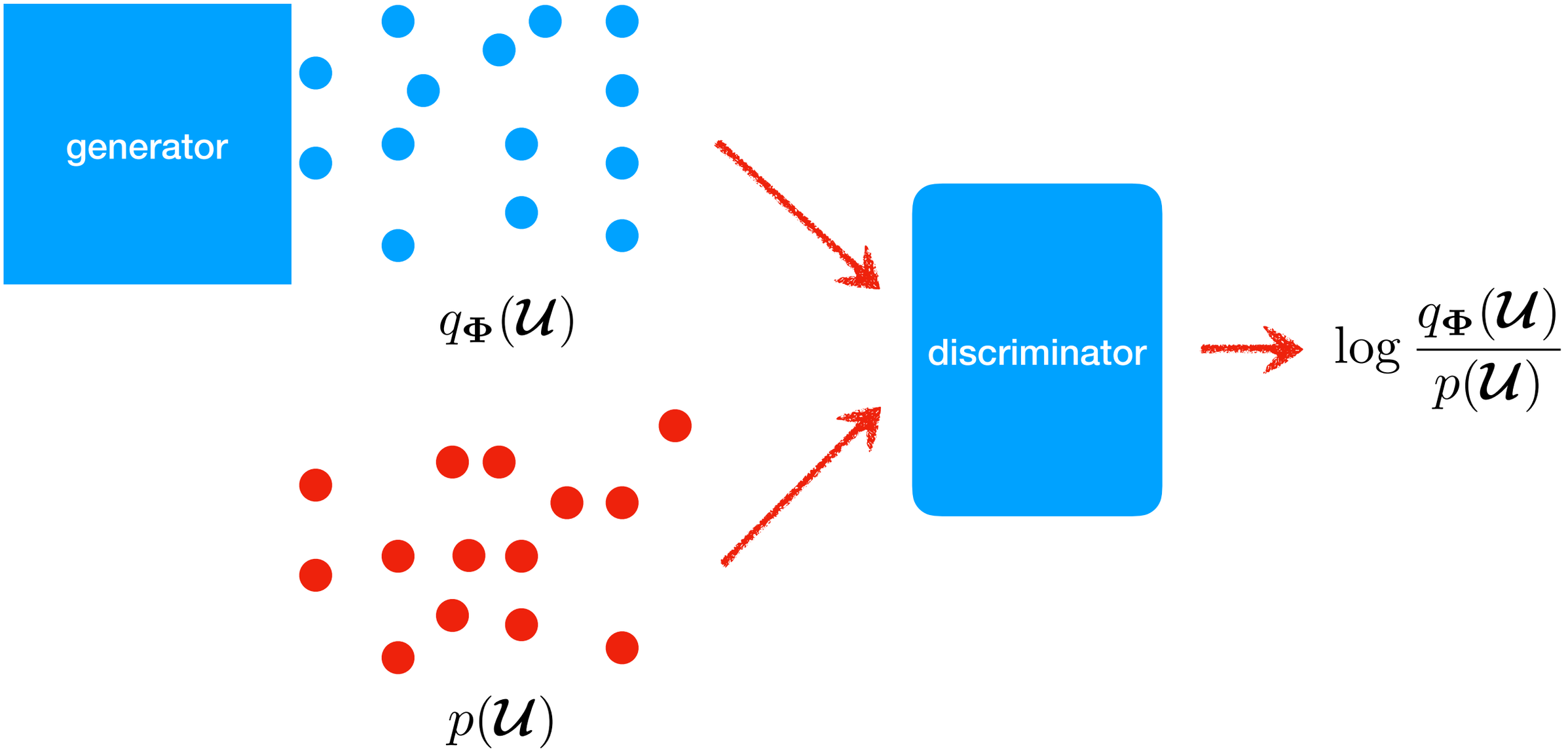
Implicit Posterior Variational Inference



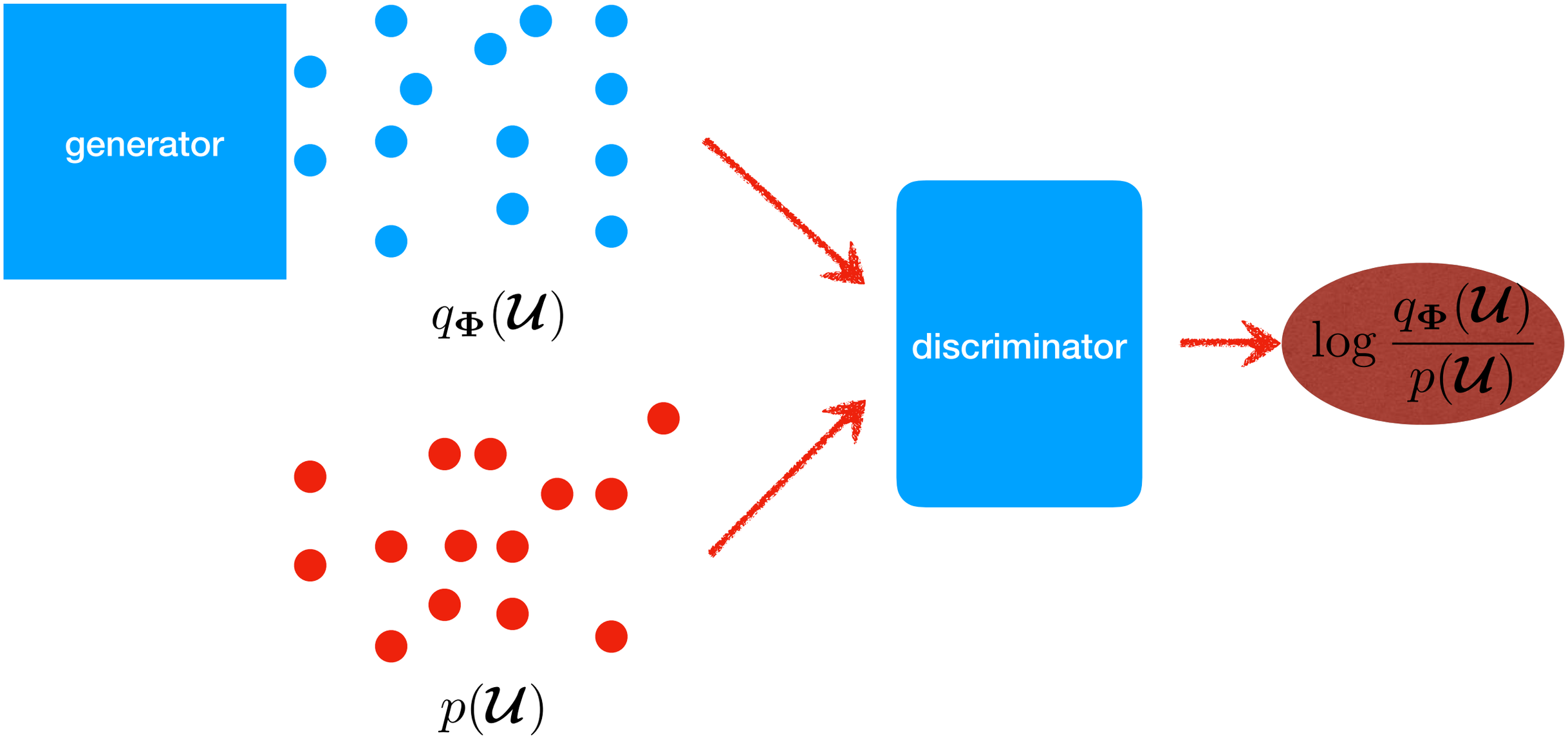
$$\text{ELBO} = \mathbb{E}_{q(\mathbf{F}_L)}[\log p(\mathbf{y}|\mathbf{F}_L)] - \text{KL}\left[q_\Phi(\boldsymbol{\mathcal{U}})||p(\boldsymbol{\mathcal{U}})\right]$$

$$\text{KL}[q_\Phi(\boldsymbol{\mathcal{U}})\|p(\boldsymbol{\mathcal{U}})] = \mathbb{E}_{q_\Phi(\boldsymbol{\mathcal{U}})}\left[\log \frac{q_\Phi(\boldsymbol{\mathcal{U}})}{p(\boldsymbol{\mathcal{U}})}\right]$$

Implicit Posterior Variational Inference



Implicit Posterior Variational Inference



Implicit Posterior Variational Inference

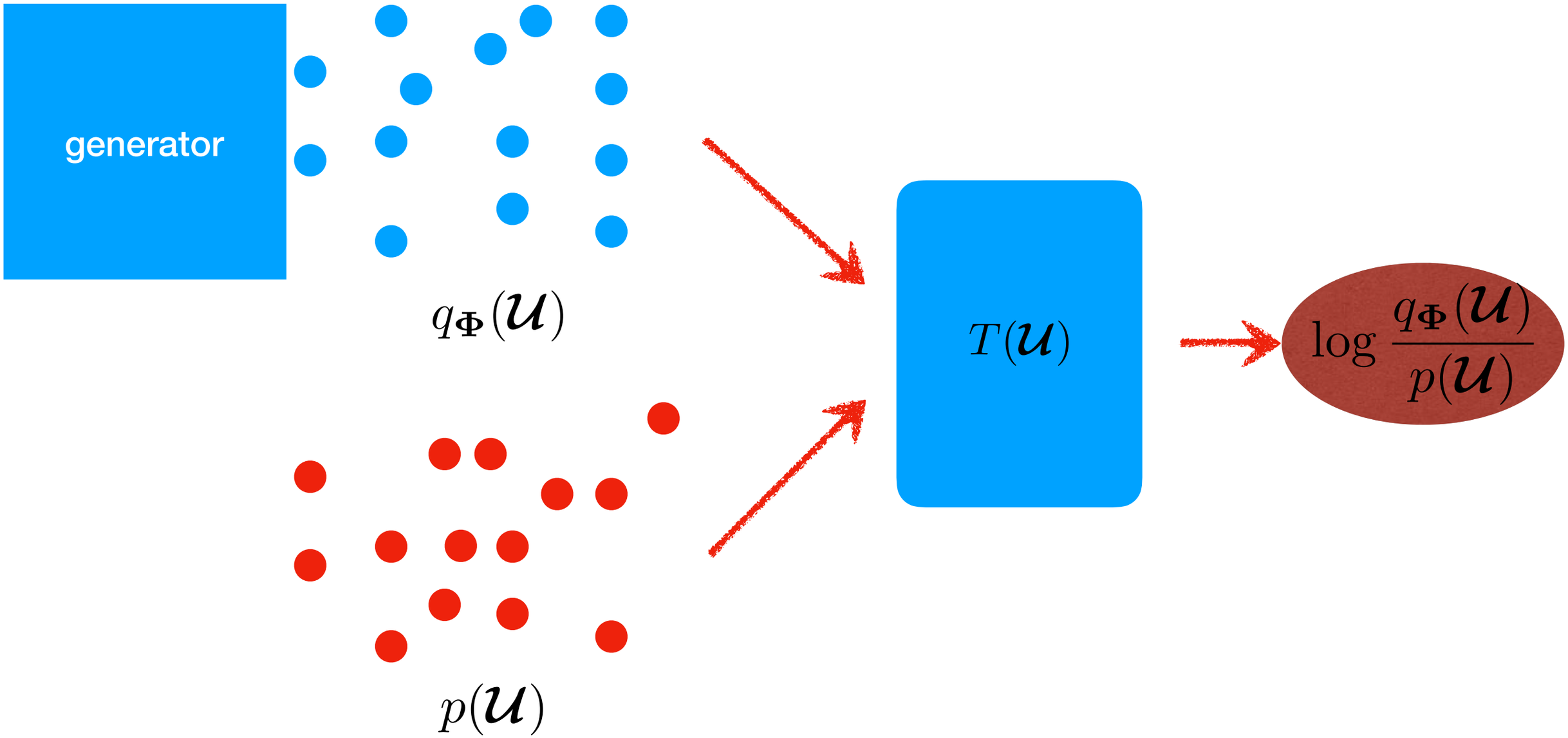
Proposition Let $\sigma(x) \triangleq 1/(1+\exp(-x))$. Consider the following maximization problem:

$$\max_{T} \ \mathbb{E}_{p(\boldsymbol{\mathcal{U}})}[\log(1-\sigma(T(\boldsymbol{\mathcal{U}}))] + \mathbb{E}_{q_\Phi(\boldsymbol{\mathcal{U}})}[\log \sigma(T(\boldsymbol{\mathcal{U}}))] \ .$$

If $p(\boldsymbol{\mathcal{U}})$ and $q_\Phi(\boldsymbol{\mathcal{U}})$ are known, then the optimal T^* is the log-density ratio:

$$T^*(\boldsymbol{\mathcal{U}}) = \log q_\Phi(\boldsymbol{\mathcal{U}}) - \log p(\boldsymbol{\mathcal{U}}) \ .$$

Implicit Posterior Variational Inference



Implicit Posterior Variational Inference

$$\textbf{Player [1]:} \quad \max_{\{\Psi\}} \mathbb{E}_{p(\boldsymbol{\mathcal{U}})} \left[\log(1 - \sigma(T_\Psi(\boldsymbol{\mathcal{U}}))\right] + \mathbb{E}_{q_\Phi(\boldsymbol{\mathcal{U}})}[\log \sigma(T_\Psi(\boldsymbol{\mathcal{U}}))],$$

$$\textbf{Player [2]:} \quad \max_{\{\theta,\Phi\}} \mathbb{E}_{q_\Phi(\boldsymbol{\mathcal{U}})} \left[\mathcal{L}(\theta, \mathbf{X}, \mathbf{y}, \boldsymbol{\mathcal{U}}) - T_\Psi(\boldsymbol{\mathcal{U}})\right]$$

IBR: Iterative Best Response

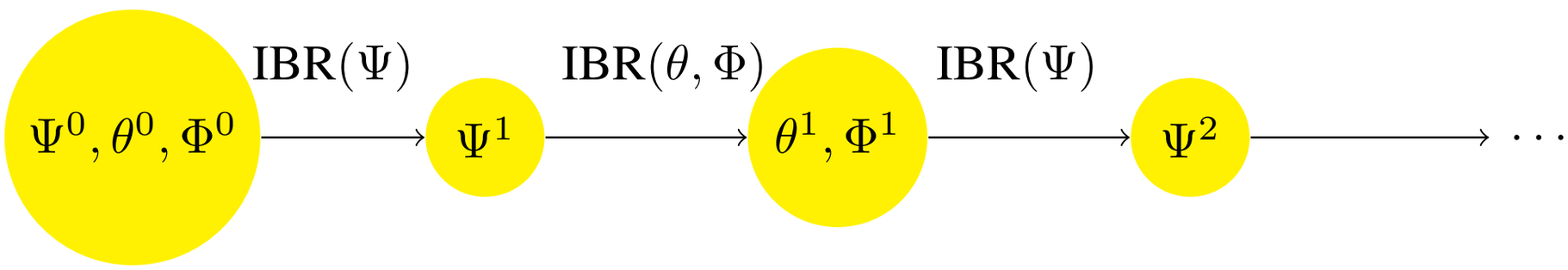


Figure 1: IBR between two players

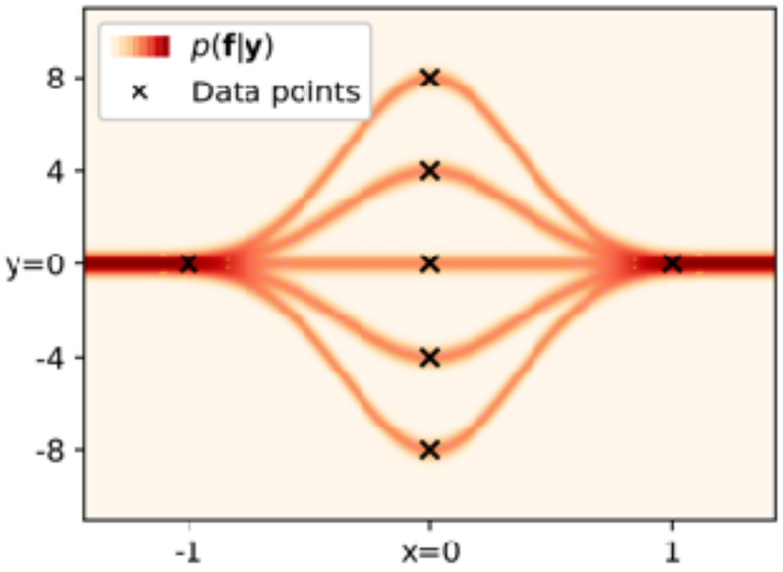
Experimental Results

- Metrics for evaluation
  - RMSE
  - MNLP
  - MLL: mean log likelihood
  - Jenson Shannon Divergence: measure the divergence between distributions

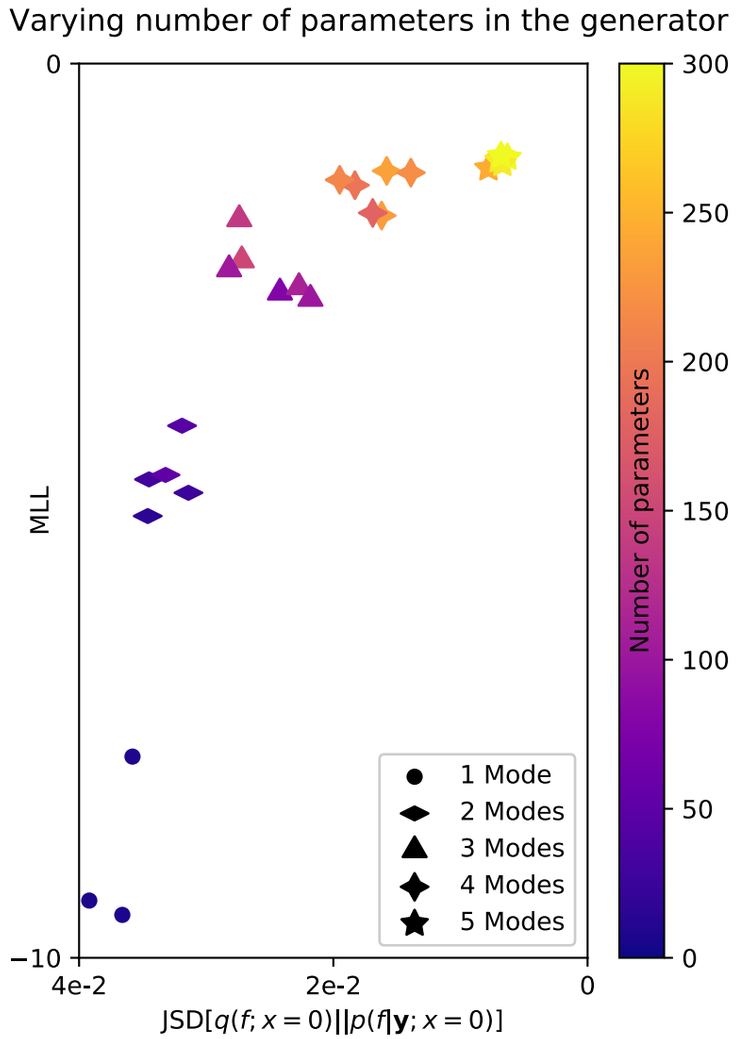
- Algorithms for comparison
  - DSVI DGP: Doubly stochastic variational inference DGP [Salimbeni and Deisenroth, 2017]
  - SGHMC DGP: Stochastic gradient Hamilton Monte Carlo DGP [Havasi et al, 2018]

Experimental Results

- Synthetic Experiment: Learning a Multi-Modal Posterior Belief



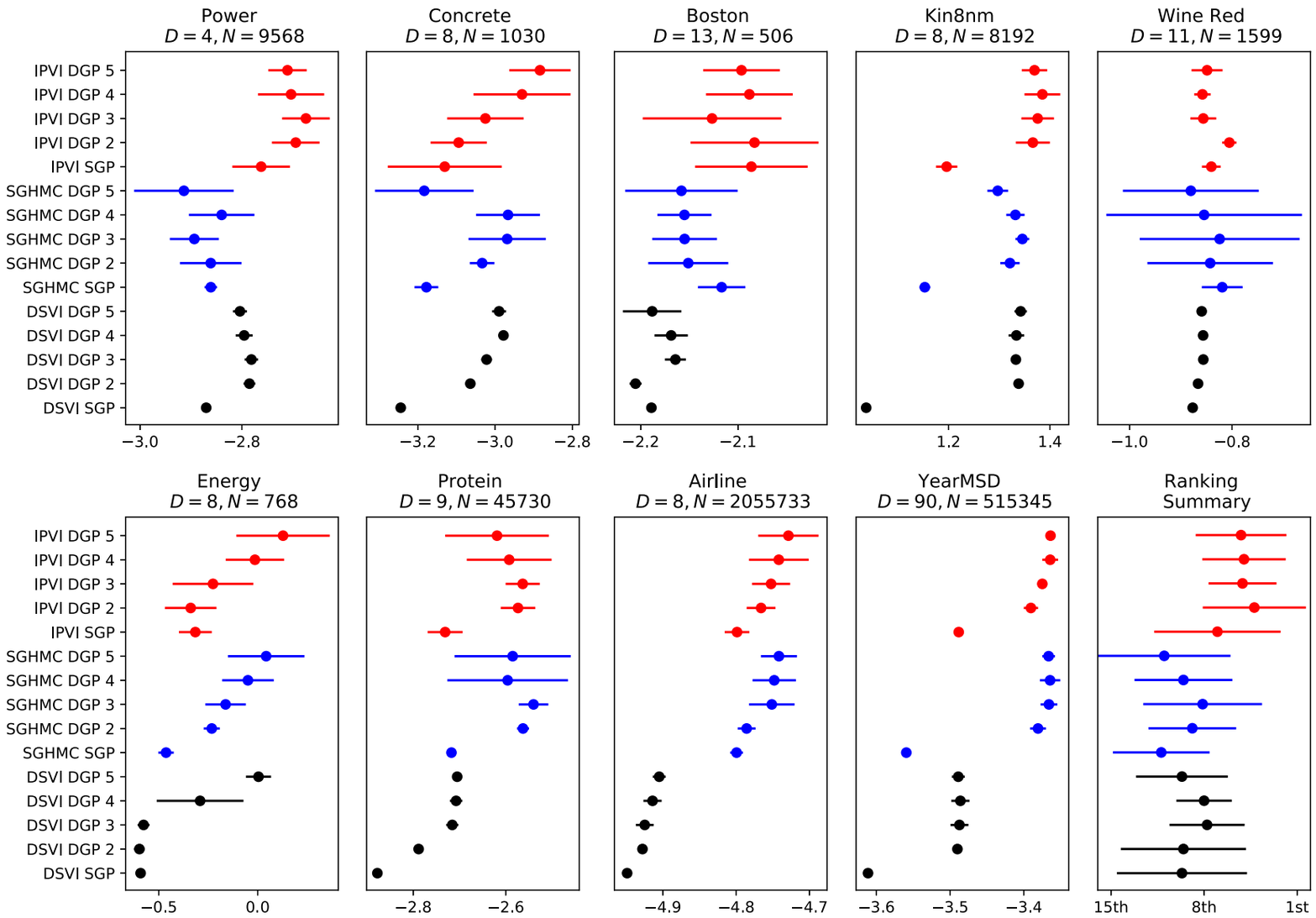
Setting	JSD	MLL
IPVI A (LR= $1e^{-4}$)	$1.0e^{-2}$	-1.15
IPVI B (LR= $1e^{-3}$)	$8.3e^{-3}$	-0.99
IPVI C (LR= $1e^{-2}$)	$8.6e^{-3}$	-1.02
SGHMC A ($\eta = 0.1$)	$2.1e^{-2}$	-2.36
SGHMC B ($\eta = 0.3$)	$1.2e^{-2}$	-1.10
SGHMC C ($\eta = 0.5$)	$7.5e^{-2}$	-2.83



- IPVI is better than SGHMC
- Expressiveness of IPVI increases w.r.t the increase of parameters.

Experimental Results

- MNLP: UCI Benchmark Regression & Real World Regression



- Our IPVI DGP
- SGHMC DGP: [Havasi et al, 2018]
- DSVI DGP:[Salimbeni and Deisenroth, 2017]
- Our IPVI DGP performs the best.

Experimental Results

- Classification

Dataset	MNIST		Fashion-MNIST		CIFAR-10	
	SGP	DGP 4	SGP	DGP 4	SGP	DGP 4
DSVI	**97.32**	97.41	86.98	87.99	47.15	51.79
SGHMC	96.41	97.55	85.84	87.08	47.32	52.81
IPVI	97.02	**97.80**	**87.29**	**88.90**	**48.07**	**53.27**

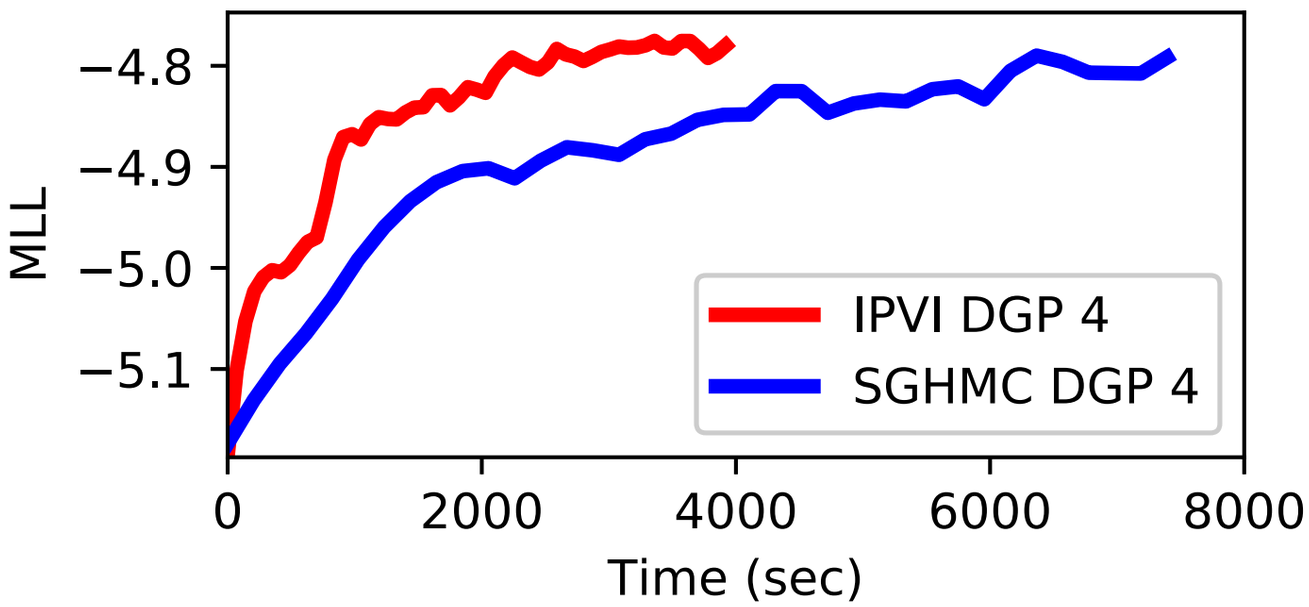
- Mean test accuracy
- DSVI DGP: Doubly stochastic variational inference DGP [Salimbeni and Deisenroth, 2017]
- SGHMC DGP: Stochastic gradient Hamilton Monte Carlo DGP [Havasi et al, 2018]

Experimental Results

- Time Efficiency

	IPVI	SGHMC
Average training time (per iter.)	0.35 sec.	3.18 sec.
$\mathcal{U}$ generation (100 samples)	0.28 sec.	143.7 sec.

- Time incurred by a 4-layer DGP model for Airline dataset.



- MLL vs. total incurred time to train a 4-layer DGP model for the Airline dataset.
- IPVI is much faster than SGHMC in terms of training as well as sampling.

Conclusion

- Present a novel IPVI DGP framework
  - Boost expressive power of GP
  - Recover unbiased posterior belief
  - Preserve time efficiency