Inference Suboptimality in Variational Autoencoders



Chris Cremer, Xuechen Li, David Duvenaud

VAE Objective

$$\log p(x) = \mathbb{E}_{z \sim q(z|x)} \left[\log \left(\frac{p(x,z)}{q(z|x)} \right) \right] + \text{KL} \left(q(z|x) || p(z|x) \right)$$

ELBO Inference Gap

Inference Gaps

- Approximation Gap
 - Inability of the variational distribution to model the true posterior
- Amortization Gap
 - Limited capacity of the recognition network to generalize inference over all datapoints



Posterior Visualizations



Amortization Approximation Gap Gap

Flexible Approximations

Flow Transformation



 $v' = v \circ \sigma_1(z) + \mu_1(z)$ $z' = z \circ \sigma_2(v') + \mu_2(v')$

 $q\downarrow Flow(z|x)$

Auxiliary Variable



Inference Model

 $q\downarrow AF(z|x)$

Posterior Visualizations



Estimating the Gaps

max (*L↓IWAE* [*q*1*],*L↓AIS*)

Lower bound with optimal q within its variational family For every datapoint, optimize its variational parameters

Lower bound with the amortized q



Amortization vs Approximation

	MNIST		Fashion-MNIST		3-BIT CIFAR	
	q_{FFG}	q_{AF}	q_{FFG}	q_{AF}	q_{FFG}	q_{AF}
$\log \hat{p}(x)$	-89.80	-88.94	-97.47	-97.41	-816.9	-820.56
$\mathcal{L}_{ ext{VAE}}[q^*_{AF}]$	-90.80	-90.38	-98.92	-99.10	-820.19	-822.16
$\mathcal{L}_{ ext{VAE}}[q^*_{FFG}]$	-91.23	-113.54	-100.53	-132.46	-831.65	-861.62
$\mathcal{L}_{ ext{VAE}}[q]$	-92.57	-91.79	-104.75	-103.76	-869.12	-864.28
Approximation	1.43	1.44	3.06	1.69	14.75	1.60
Amortization	1.34	1.41	4.22	4.66	37.47	42.12
Inference	2.77	2.85	7.28	6.35	52.22	43.72

For these model choices:

• Amortization is generally larger than approximation gap

Can we reduce the amortization gap by increasing encoder capacity?

Larger Encoder Reduces Amortization Error

	MNIST		Fashior	ו-MNIST
	q↓FFG	q↓AF	q↓FFG	q↓AF
Regular Encoder	1.34	1.41	4.22	4.66
Larger Encoder	1.11	0.75	3.09	3.76

Parameters of Flow Reduce Amortization Gap

- Common reasoning for flow: reduce approximation gap
 - Could improvements also be due to reduction in amortization gap?
- Experiment:
 - Trained a VAE on MNIST
 - Retrained new encoders on the fixed decoder
 - Encoders differ only in their variational distribution

	q↓FFG	q↓Flow
Approximation	1.91	0.43
Amortization	43.22	12.86

Generator Learns to Accommodate the Approximation

How much does pz x fit to q(z|x)? How Gaussian is pz x when trained with $q\downarrow FFG$ vs $q\downarrow AF$?

Generator Trained With

	q↓FFG	$q \downarrow AF$
$KL(q\downarrow FFG\uparrow x x p(z x))$	1.43	24.60
$KL(q\downarrow AF\uparrow x x p(z x))$	1.00	1.44

Larger Decoder Capacity Reduces Approximation Gap

- Does increasing decoder capacity decrease the approximation gap?
 - Does a more powerful decoder make the true posterior easier to model with the choice of approximation?
- Experiment:
 - Train VAEs with decoders that have 0, 2, 4 hidden layers
 - Compute the approximation gaps (ie. How Gaussian is $pz \ x$?)

Generator Hidden Layers	0	2	4
Approximation Gap	3.90	1.83	1.63

Inference Generalization

Approximation GapAmortization Gap



- From training to validation set:
 - amortization gap increases
 - approximation gap constant

- Increased capacity: more prone to overfitting but better inference
- Flow improves model while overfitting less

Summary

- Inference Gap: Amortization vs Approximation
- Amortization > Approximation
- Generator accommodates approximation
- Inform model design choices

Poster: Hall B #176

Thanks

Experiments

Dataset Models

- Encoder Capacity
- Decoder Capacity
- Variational Distribution

MNIST/Fashion	3-BIT CIFAR-10
784-200-200-50	Conv-Conv-Conv-FC
50-200-200-784	FC-ConvT-ConvT-ConvT

VAE

- Latent Variable Model
- Amortized Inference



• Inference Suboptimality

 $p \downarrow \theta x \ z \ p(z)$ Generator (Decoder)

 $q \downarrow \phi(z|x)$ Recognition Net (Encoder)

$$\log p(x) = \mathbb{E}_{z \sim q(z|x)} \left[\log \left(\frac{p(x,z)}{q(z|x)} \right) \right] + \mathrm{KL} \left(q(z|x) || p(z|x) \right)$$