Deep Generative Models and a Probabilistic Programming Library

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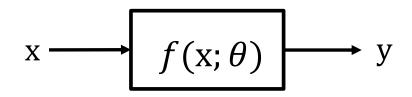
Department of Computer Science and Technology

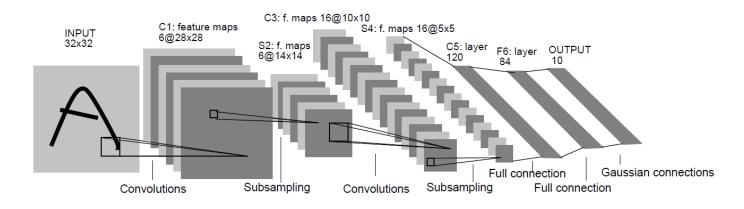
Tsinghua University

VALSE, Dalian, 2018

Discriminative (Deep) Learning

Learn a (differentiable) function mapping from input to output





Gradient back-propagation

Generative Modeling

Have training examples

$$x \sim p_{data}(x)$$

Want a model that can draw samples:

$$x' \sim p_{\text{model}}(x)$$

• where $p_{\text{model}}(x) \approx p_{\text{data}}(x)$

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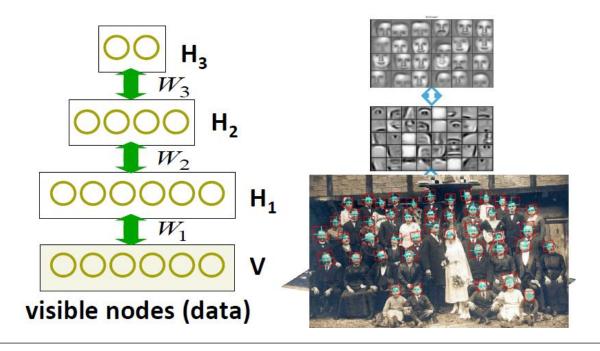
Why generative models?

- Leverage unlabeled datasets, which are often much larger than labeled ones
 - Unsupervised learning
 - e.g., clustering, density estimation, feature extraction, dimension reduction, data generation
 - Semi-supervised learning
 - e.g., classification, information extraction, learning-to-rank, network analysis, opinion mining
- Conditional generative models
 - □ Speech synthesis: Text ⇒ Speech

 - □ Image captioning: Image \Rightarrow Text

Generative models are everywhere ...

- (hierarchical) Language models for text
- Gaussian mixture models for clustering/density estimation
- Probabilistic PCA/FA/ICA for dimension reduction
- Probabilistic matrix factorization (PMF) for recommendation
- Deep belief networks (Hinton et al., 2016)

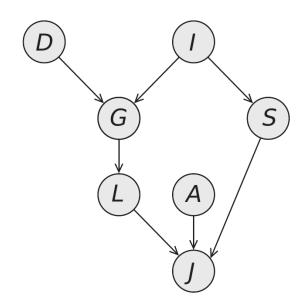


Two ways to build deep generative models

- Traditional one
 - Hierarchical Bayesian methods
- More modern one
 - Deep generative models

Hierarchical Bayesian Modeling

Build a hierarchy throng distributions in analytical forms



$$P(D, I, G, S, L, A, J) = P(D)P(I)P(G|D, I)P(S|I) \cdot P(A)P(L|G)P(J|L, A, S)$$

Simple, Local Factors: a conditional probability distribution

Deep Generative Models

- More flexible by using differential function mapping between random variables
- If z is uniformly distributed over (0, 1), then y = f(z) has the distribution

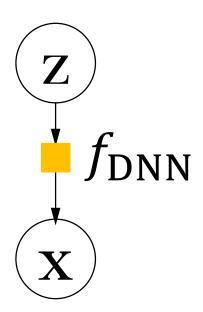
$$p(y) = p(z) \left| \frac{dz}{dy} \right|$$

- where p(z) = 1
- This trick is widely used to draw samples from exponential family distributions (e.g., Gaussian, Exponential)

Deep Generative Models

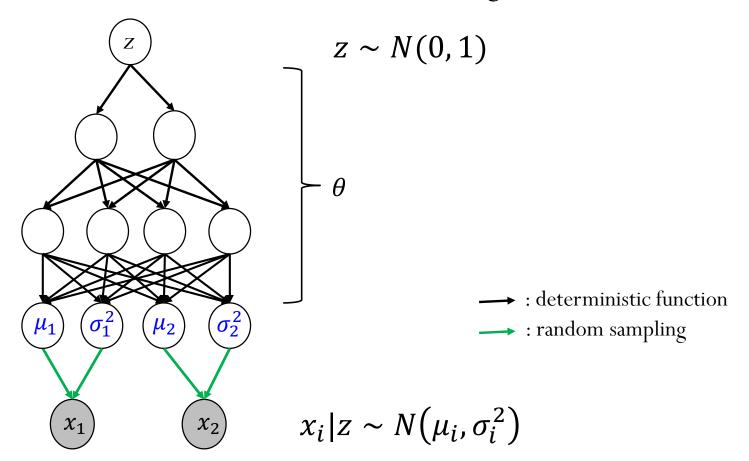
More flexible by using differential function mapping between random variables

DGMs learn a function transform with deep neural networks



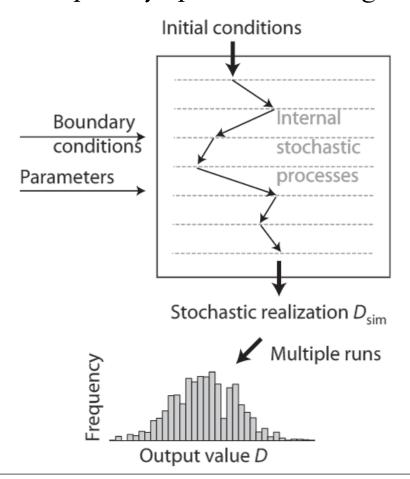
An example with MLP

- ♦ 1D latent variable z; 2D observation x
- ♦ Idea: NN + Gaussian (or Bernoulli) with a diagonal covariance



Implicit Deep Generative Models

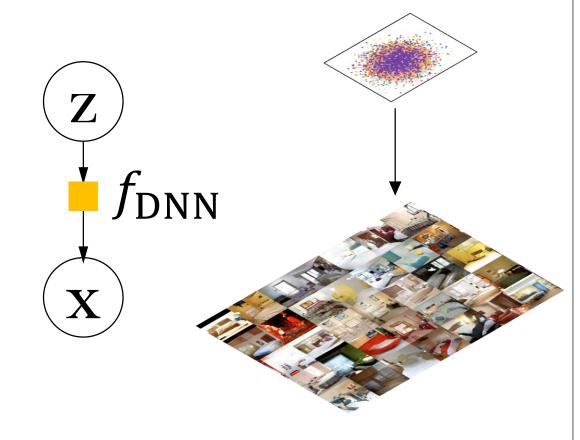
• Generate data with a stochastic process whose likelihood function is not explicitly specified (Hartig et al., 2011)



Deep Generative Models

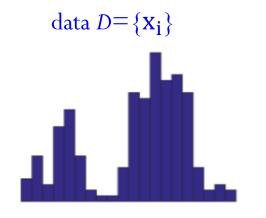
[Image Generation: Generative Adversarial Nets, Goodfellow13 & Radford15]

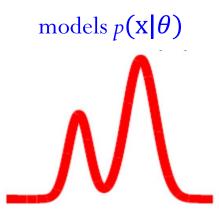




Learning Deep Generative Models

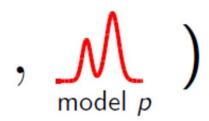
◆ Given a set D of unlabeled samples, learn the unknown parameters (or a distribution)





Find a model that minimizes





Learning Deep Generative Models

Maximum likelihood estimation (MLE):

$$\hat{\theta} = \operatorname{argmax} p(D|\theta)$$

- has an explicit likelihood model
- Minimax objective (e.g., GAN)
 - a two-player game to reach equilibrium
- Moment-matching:
 - □ draw samples from p: $\widehat{D} = \{y_i\}_{i=1}^M$, where $y_i \sim p(x|\theta)$
 - - rich enough to distinguish any two distributions in certain RKHS

Related Work at VALSE 2018

- Duplex GAN for Domain Adaptation (DGM)
 - Hu, Kan, Shan, Chen
- Multimodal Possion Gamma Belief Networks (DGM)
 - Wang, Chen, Zhou
- WHAI: Weibull Hybrid Autoencoding Inference for Deep Topic Models (DGM)
 - Zhang, Chen, Guo, Zhou
- The Assumed Parameter Filter (probabilistic programming)
 - Erol, Wu, Li, Russell
- ...

Our work on DGMs

Learning algorithms and theories

- Max-margin variational auto-encoder (Li et al., NIPS 2015)
- Learning to generate with memory (Li et al., ICML 2016)
- Conditional moment-matching generative networks (Ren et al., NIPS 2016)
- Population matching discrepancy (Chen et al., NIPS 2017)
- Implicit variational inference (Shi et al., ICLR 2018)

Semi-supervised learning & Style transfer

- Max-margin variational auto-encoder for SSL (Li et al., PAMI 2017)
- □ Triple generative adversarial networks (Li et al., NIPS 2017)
- Structured generative adversarial networks (Deng et al., NIPS 2017)
- Learning to write styled Chinese characters by reading a handful of examples (Sun et al., IJCAI 2018)
- Smooth neighbors for SSL (Luo et al., CVPR 2018)

Programming library

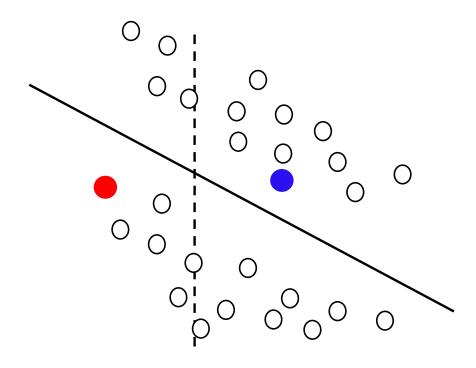
□ ZhuSuan (Shi et al., arXiv 2017)

Outline

- Deep Generative Models
- Semi-supervised Learning & Style transfer
- ◆ ZhuSuan: a Probabilistic Programming library
- ♦ Conclusions & QA

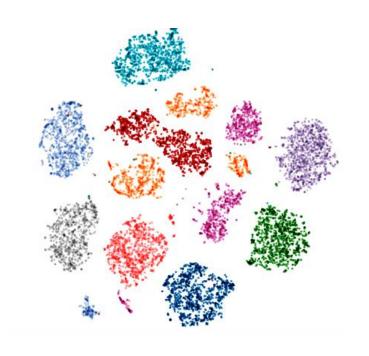
Semi-supervised Learning

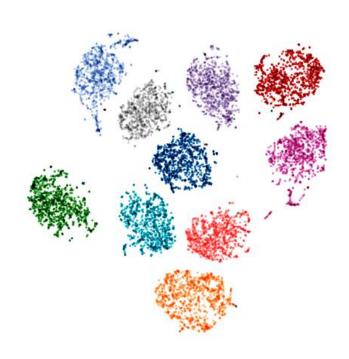
A toy example



Representation Matters

◆ t-SNE embedding of learned representations by different DGM models on CIFAR10



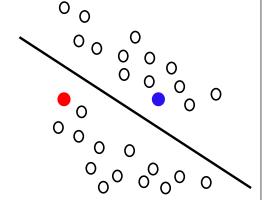


Triple Generative Adversarial Nets

- ♦ A minimax game for semi-supervised learning
 - □ GAN is for unsupervised learning $p_{\text{model}}(x) = p_{\text{data}}(x)$
 - We aim to learn the joint distribution $p_{\text{model}}(x, y) = p_{\text{data}}(x, y)$
- A simple insight
 - factorization form with conditionals

$$p(x,y) = p(x)p(y|x)$$
 A classifier
= $p(y)p(x|y)$

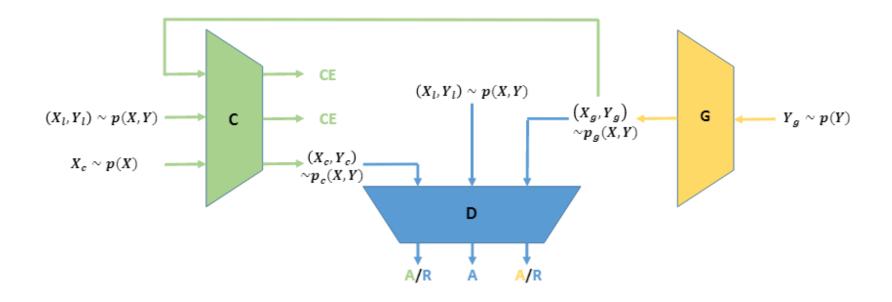
A class-conditional generator



- We need three players
 - \Box Two generators to generate (x,y)
 - $lue{}$ A discriminator to distinguish fake (x,y)

Triple-GAN

♦ The network architecture



- Both C and G are generators
- D is the discriminator
- CE: cross-entropy loss for learning classifier

[Li et al., NIPS 2017]

A minimax game

The optimization problem

$$\min_{C,G} \max_{D} U(C,G,D) = E_{p}[\log D(x,y)] + \alpha E_{p_{c}}[\log(1-D(x,y))] + (1-\alpha)E_{p_{g}}[\log(1-D(x,y))]$$

- \Box The hyper-parameter *a* is often set at 1/2
- The standard supervised loss can be incorporated

$$\min_{C,G} \max_{D} \tilde{U}(C,G,D) = U(C,G,D) + E_{\rho}[-\log p_{c}(y|x)]$$

Major theoretical results

Theorem

The equilibrium of $\tilde{U}(C,G,D)$ is achieved if and only if $p(x,y)=p_g(x,y)=p_c(x,y)$ with $D_{C,G}^*(x,y)=\frac{1}{2}$ and the optimum value is $-\log 4$.

Lemma

For any fixed C and G, the optimal discriminator D is:

$$D_{C,G}^*(x,y) = \frac{p(x,y)}{p(x,y) + p_{\alpha}(x,y)},$$

where $p_{\alpha}(x, y) := (1 - \alpha)p_{g}(x, y) + \alpha p_{c}(x, y)$.

Some Practical Tricks for SSL

- Pseudo discriminative loss: using $(x, y) \sim p_g(x, y)$ as labeled data to train C
 - Explicit loss, equivalent to $KL(p_g(x,y)||p_c(x,y))$
 - Complementary to the implicit regularization by D
- Collapsing to the empirical distribution p(x, y)
 - Sample $(x, y) \sim p_c(x, y)$ as true data for D
 - Biased solution: target shifting towards $p_c(x, y)$
- Unlabeled data loss on C
 - Confidence (Springenberg [2015])
 - Consistence (Laine and Aila [2016])

Semi-supervised classification

Table 1: Error rates (%) on partially labeled MNIST, SHVN and CIFAR10 datasets. The results with † are trained with more than 500,000 extra unlabeled data on SVHN.

Algorithm	MNIST $n = 100$	SVHN $n = 1000$	CIFAR10 $n = 4000$
M1+M2 [11]	$3.33 (\pm 0.14)$	$36.02 (\pm 0.10)$	
<i>VAT</i> [18]	2.33		24.63
Ladder [23]	$1.06 (\pm 0.37)$		$20.40 (\pm 0.47)$
Conv-Ladder [23]	$0.89 \ (\pm 0.50)$		
ADGM [17]	$0.96 (\pm 0.02)$	22.86 [†]	
SDGM [17]	$1.32 (\pm 0.07)$	$16.61(\pm 0.24)^{\dagger}$	
MMCVA [15]	$1.24~(\pm 0.54)$	4.95 (±0.18) [†]	
CatGAN [26]	$1.39 (\pm 0.28)$		19.58 (±0.58)
Improved-GAN [25]	$0.93 (\pm 0.07)$	$8.11 (\pm 1.3)$	$18.63 \ (\pm 2.32)$
<i>ALI</i> [5]		7.3	18.3
Triple-GAN (ours)	0.91 (±0.58)	$5.77(\pm 0.17)$	16.99 (±0.36)

Class-conditional generation



Disentangle class and style

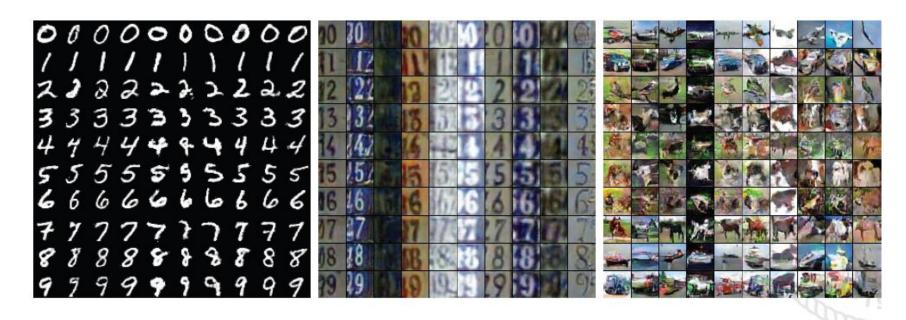


Figure: Same y for each row. Same z for each column.

Latent space interpolation on MNIST

Latent space interpolation on SVHN

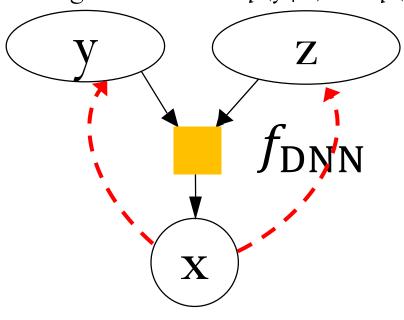


Latent space interpolation on CIFAR10



Structured GAN

- Structural extensions to Triple-GAN
 - Learn joint distribution p(x, y, z)
 - □ Ability to infer the posterior p(y, z | x), p(y | x), p(z | x)
 - Structural bias to disentangle latent factors y and z by information regularization on p(y | x) and p(x | x)



[Deng et al., NIPS 2017]

Structured GAN

Produces even better results than Triple-GAN

Method	MNIST			SVHN	CIFAR-10
	n = 20	n = 50	n = 100	n = 1000	n = 4000
Ladder [22]	-	-	$0.89(\pm 0.50)$	-	$20.40(\pm 0.47)$
VAE [12]	-	-	$3.33(\pm 0.14)$	$36.02(\pm 0.10)$	-
CatGAN [28]	-	-	$1.39(\pm 0.28)$	-	$19.58(\pm 0.58)$
ALI [5]	-	-	-	7.3	18.3
ImprovedGAN [27]	$16.77(\pm 4.52)$	$2.21(\pm 1.36)$	$0.93 (\pm 0.07)$	$8.11(\pm 1.3)$	$18.63(\pm 2.32)$
TripleGAN [15]	$5.40(\pm 6.53)$	$1.59(\pm 0.69)$	$0.92(\pm 0.58)$	$5.83(\pm 0.20)$	$18.82(\pm 0.32)$
SGAN	4.0 (± 4.14)	$1.29(\pm 0.47)$	$0.89(\pm 0.11)$	$5.73(\pm 0.12)$	$17.26(\pm 0.69)$

• inception score: $6.91(\pm 0.07)$

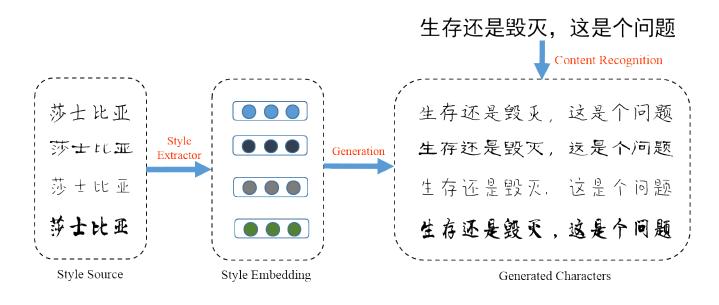
□ TripleGAN: $5.08(\pm 0.09)$

□ Improved-GAN: $3.87(\pm 0.03)$



Style Transfer for Chinese Characters

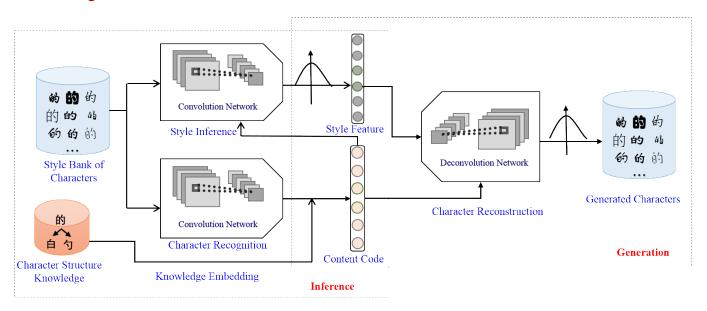
 Build a generative model for Chinese characters generation and writing style transfer tasks

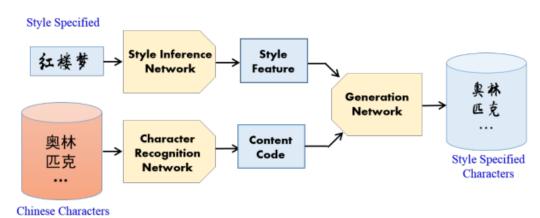


One-shot Generalization

Disentanglement

Style-Transfer VAE





Structural Information

- Content Code (Knowledge)
 - Instead one-hot label to identify unique Chinese characters with human knowledge.
 - Reuse the structure information sharing in all Chinese characters.

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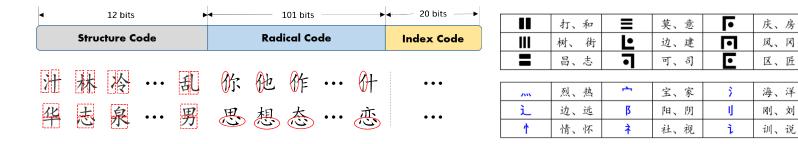
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国、四

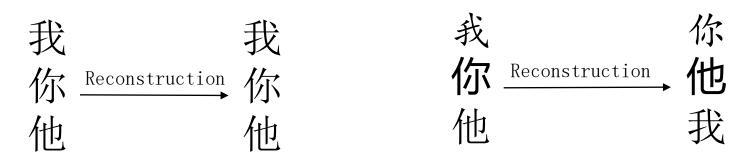
不、大

形、杉

提、打

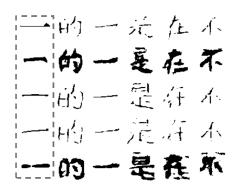


Pairwise Training:



One-Shot Generation

寨的一是在不了有和人这 却的一是在不了有和人这 命的一是在不了有和人这 欺的一是在不了有和人这 努的一是在不了有和人这 康的一是在不了有和人这 **刨的一是在不了有和人这** 劝的一是在不了有和人这 丑的一是在不了有和人这 具的一是在不了有和人这 渥的一是在不了有和人这 拿的一是在不了有和人这 税的一是在不了有和人这 劫的一是在不了有和人这 娃的一是在不了有和人这 贱的一是在不了有和人这 腿的一定在不了有和人这 退的一是在不了有和人这 茂的一是在不了有和人这 练的一星石みで有利人这



Too simple characters can't provide sufficient style information.

Low-Shot Generation

刘禹锡山不在高有仙则鸣水不在深有龙则灵刘禹锡山不在高有仙则鸣水不在深有龙则灵刘禹锡山不在高有仙则鸣水不在深有龙则灵刘禹锡山不在高有仙则鸣水不在深有龙则灵

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十一是卫甲

十王井口一是卫甲

Sometimes low-shot can capture more detailed style information.

Style Generation

Interpolation

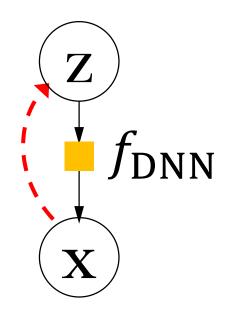
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Outline

- ♦ Deep Generative Models
- ♦ Semi-supervised Learning
- ZhuSuan: a Probabilistic Programming library
- ♦ Conclusions & QA

Bayesian inference

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



Given Disease, what is the Cause?
Given Object, what are the Components?
Given Docs, what are the Topics?

Find Cause of Disease
Extract Topics from Docs
Identify Objects from Images
Recognize Words in Speeches

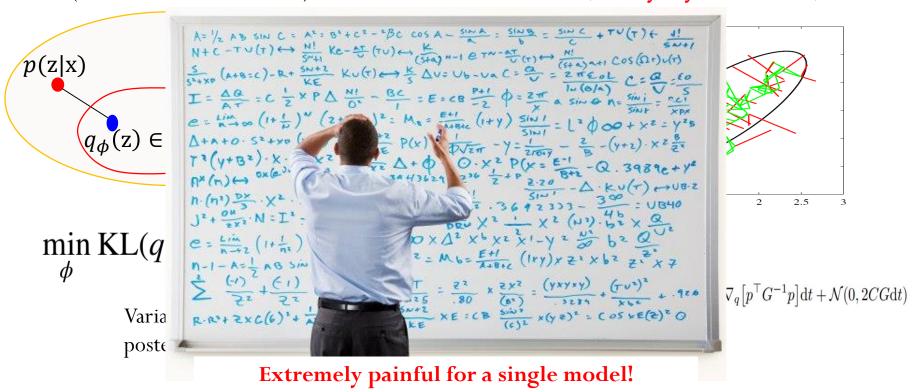
Inference in Old Days

Variational Inference

MCMC

(Too much math!!!)

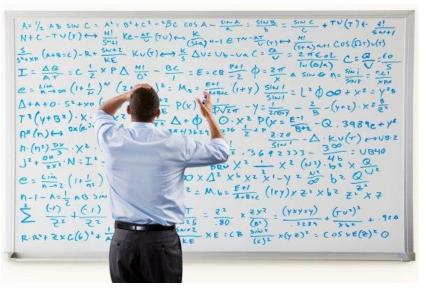
(Many dynamics!!!)





Inference in ZhuSuan

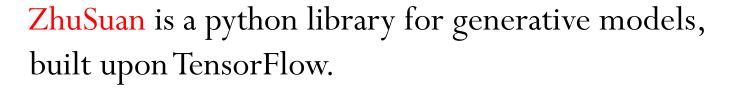
Turn painful math deviations into Easy and Intuitive (Probabilistic) Programming

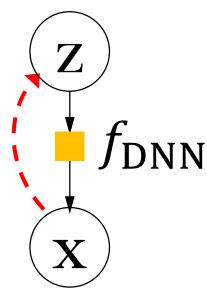






ZhuSuan



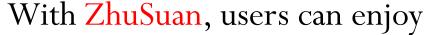


Unlike existing DL libraries, which are mainly for supervised tasks, ZhuSuan is featured for:

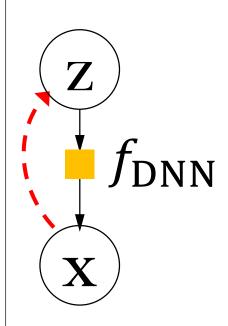
- its deep root into Bayesian Inference
- supporting various kinds of generative models: traditional hierarchical Bayesian models & recent deep generative models.



ZhuSuan



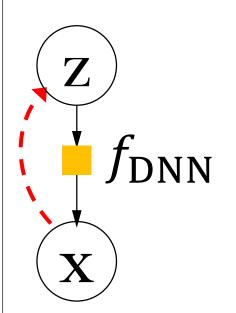
- powerful fitting and multi-GPU training of deep learning
- while at the same time they can use generative models to
 - ✓ model the complex world
 - exploit unlabeled data
 - ✓ deal with uncertainty by performing principled Bayesian inference
 - ✓ generate new samples





Model Primitives: BayesianNet

- A DAG representing a Bayesian Network
- Two types of nodes:
 - Deterministic nodes: Can be composed of any Tensorflow operations.
 - Stochastic nodes: Use Stochastic Tensor's from ZhuSuan's library.
 - Start a BayesianNet environment

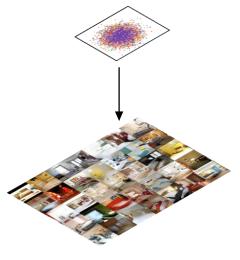


```
import zhusuan as zs
with zs.BayesianNet() as model:
    # build the model
```



Example: Variational Autoencoders





```
Z
f_{DNN}: 2L MLP
```

```
egin{aligned} z &\sim 	ext{N}(z|0,I) \ x_{logits} &= f_{NN}(z) \ x &\sim 	ext{Bernoulli}(x|	ext{sigmoid}(x_{logits})) \end{aligned}
```

import tensorflow as tf
from tensorflow.contrib import layers
import zhusuan as zs

```
with zs.BayesianNet() as model:
    z_mean = tf.zeros([n, n_z])
    z_logstd = tf.zeros([n, n_z])
    z = zs.Normal('z', z_mean, z_logstd)
    h = layers.fully_connected(z, 500)
    x_logits = layers.fully_connected(
        h, n_x, activation_fn=None)
    x = zs.Bernoulli('x', x_logits)
```



Variational Inference in ZhuSuan

```
with zs.BayesianNet() as variational:
    # build variational ...
qz_samples, log_qz = variational.query(
    'z', outputs=True, local_log_prob=True)
```

Build variational posterior as BayesianNet

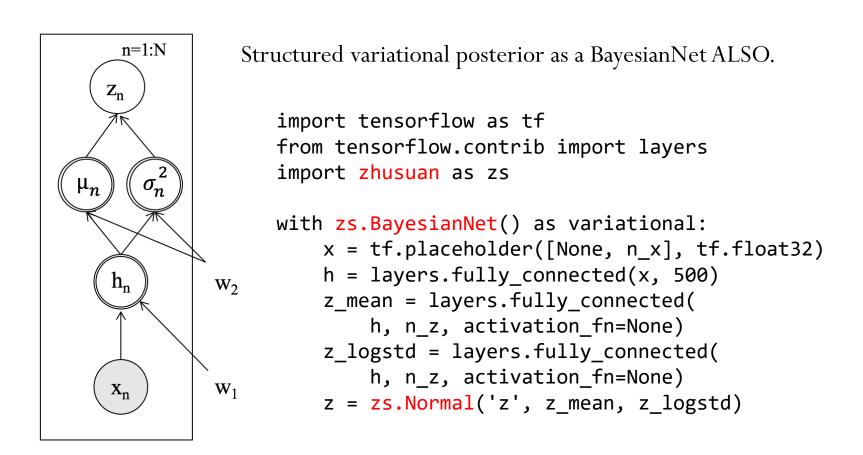
Call variational objectives

```
optimizer = tf.train.AdamOptimizer(learning_rate=0.001)
run_op = optimizer.minimize(-lower_bound)
With tf.Session() as sess:
    for iter in range(iters):
        sess.run(run_op)
```

Run gradient descent!



Example: Variational Autoencoders ZHUSUAN





Variational Inference Algorithms

ZhuSuan supports a broad class of variational objectives, ranging from widely used evidence lower bounds to recent state-of-arts.

Works for continuous latent variables

- ZS.Sgvb: Stochastic gradient variational Bayes.
- **ZS.iwae**: Importance weighted lower bounds.

Works for both continuous and discrete latent variables

- **zs.nvil**: Variance reduced score function estimator/REINFORCE.
- **ZS.Vimco**: Variance reduced multi-sample score function estimator.

*This is like optimization algorithms (SGD, momentum, Adam, etc.) in deep learning software. Users need not dive into the technical details of these algorithms because ZhuSuan provides easy-to-use APIs for users to directly try on their generative models.



like an optimizer!

HMC like a TensorFlow optimizer

```
# like creating the variable to optimize over.
                                                     Create the variable to store
z = tf.Variable(0.)
                                                     samples
# like optimizer = tf.train.AdamOptimizer(...)
                                                     Initialize HMC
hmc = zs.HMC(step size=1e-3, n leapfrogs=10)
# like optimize op = optimizer.minimize(...)
                                                     Call sample() method to
sample op, hmc info = hmc.sample(
                                                     return a sample operation
  log joint, observed={'x': x}, latent={'z': z})
with tf.Session() as sess:
    for iter in range(iters):
        # like sess.run(optimize op)
                                                     Run the sample operation
```

= sess.run(sample op)

Applications: ZhuSuan as a Research Platform



ZhuSuan is featured for both Bayesian Statistics and Deep Learning. State-of-the-Art models can be found in ZhuSuan's examples.

- Bayesian Logistic Regression
- Bayesian Neural Nets for Multivariate Regression
- ♦ (Convolutional) Variational Autoencoders (VAE)
- Semi-supervised learning for images with VAEs
- Deep Sigmoid Belief Networks
- ♦ Generative Adversarial Networks (GAN)
- Gaussian processes (GPs)
- Topic Models
- More to come ...



ZhuSuan: GitHub Page

ZHUSUAN

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86 lines (63 sloc) 2.49 KB	mainly designed for supervised tasks, ZhuSuan is featured for its deep root into Bayesian Inference, thus supporting kinds of generative models: both the traditional hierarchical Bayesian models and recent deep generative models.							
	With ZhuSuan, users can enjoy powerful fitting and multi-GPU training of deep learning, while at the same time th							

Welcome to ZhuSuan

ZhuSuan is a python probabilistic programming library for advantages of Bayesian methods and deep learning. ZhuSu which are mainly designed for deterministic neural network primitives and algorithms for building probabilistic models algorithms include:

- Variational inference with programmable variational po (SGVB, REINFORCE, VIMCO, etc.).
- Importance sampling for learning and evaluating models, with programmable proposals.
- Hamiltonian Monte Carlo (HMC) with parallel chains, and optional automatic parameter tuning.

flow. Unlike existing deep learning libraries, which are root into Bayesian Inference, thus supporting various models and recent deep generative models.

g of deep learning, while at the same time they can use generative models to model the complex world, exploit unlabeled data and deal with uncertainty by performing principled Bayesian inference.

[™] Supported Inference

(Stochastic) Variational Inference (VI & SVI)

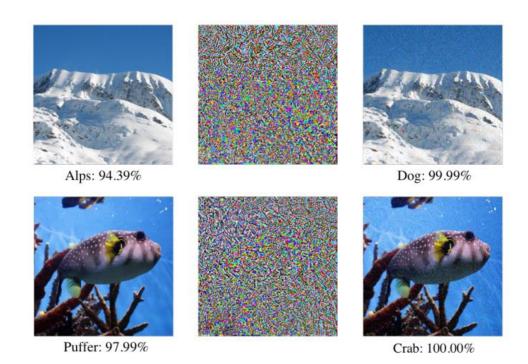
- Kinds of variational posteriors we support:
 - · Mean-field posterior: Fully-factorized.
 - o Structured posterior: With user specified dependencies.
- Variational objectives we support:
 - o SGVB: Stochastic gradient variational Bayes
 - IWAE: Importance weighted objectives
 - o NVIL: Score function estimator with variance reduction
 - VIMCO: Multi-sample score function estimator with variance



Summary

- Deep Generative models are powerful tools
 - hierarchical Bayesian models
 - deep generative models
 - semi-supervised learning & style transfer
- ZhuSuan provides a Python programming library
 - deep root into Bayesian inference
 - support deep generative models

DL still long way to go ...



- Y. Dong, F. Liao, T. Pang, H. Su, J. Zhu, X. Hu, et al., Boosting Adversarail Attacks with Momentum, CVPR 2018.
- F. Liao, M. Liang, Y. Dong, T. Pang, J. Zhu, X. Hu. Defense against Adversarial Attack using High-level Representation Guided Denoiser, CVPR 2018.
- NIPS 2017 Adversarial Attack & Defense, first-places in all three tasks.

What VALSE taught me?





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The 10th Asian Conference on Machine Learning, Beijing

Beijing Jiaotong University November 14 - 16, 2018







ACML 2018

Welcome to the 10th Asian Conference on Machine Learning (ACML 2018). The conference will take place on November 14 - 16, 2018 at Beijing Jiaotong University, Beijing, China. The conference aims to provide a leading international forum for researchers in machine learning and related fields to share their new ideas, progresses and achievements. Submissions from regions other than the Asia-Pacific are also highly encouraged.

Thanks!





ZhuSuan: A Library for Bayesian Deep Learning. J. Shi, J. Chen, J. Zhu, S. Sun, Y. Luo, Y. Gu, Y. Zhou. arXiv preprint, arXiv:1709.05870, 2017

Online Documents: http://zhusuan.readthedocs.io/