

Semi-Supervised Learning: Generative Models

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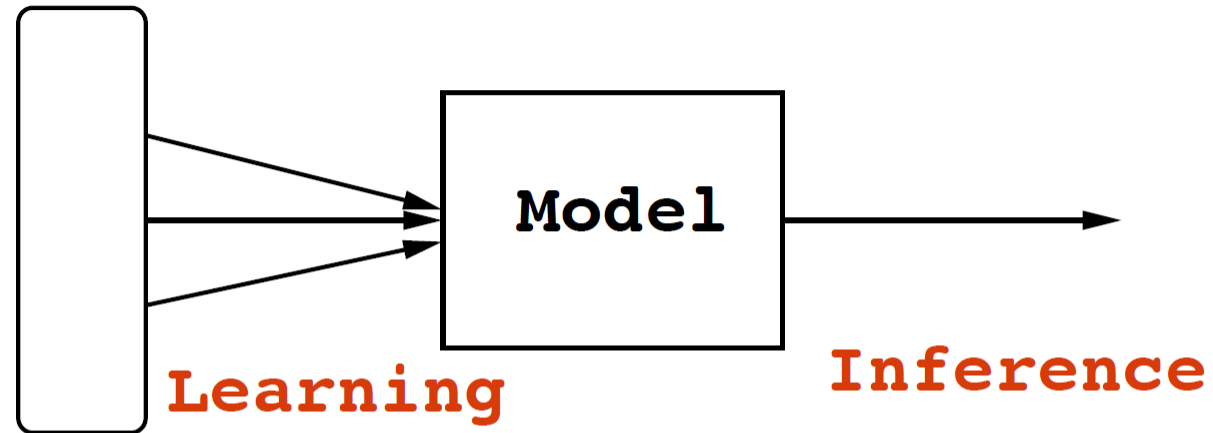
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Discriminative vs. Generative

Choi (2015)

Environments



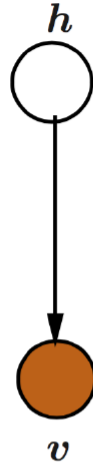
Data sources

Machine Learning: A scientific discipline that is concerned with the design and development of **algorithms** that allow computers to **learn from empirical data** (sensor data or database) and to make **predictions**.

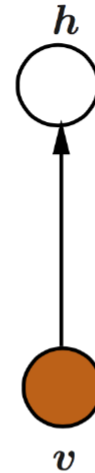
Discriminative vs. Generative

Choi (2015)

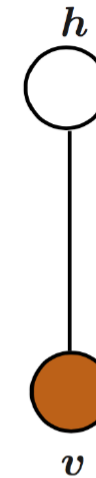
Generative model



Discriminative model



Undirected model



- ▶ Generative model: Joint distribution $p(\mathbf{v}, \mathbf{h}) = p(\mathbf{v}|\mathbf{h})p(\mathbf{h})$
- ▶ Discriminative model: Directly model $p(\mathbf{h}|\mathbf{v})$
- ▶ Undirected model: Energy-based model

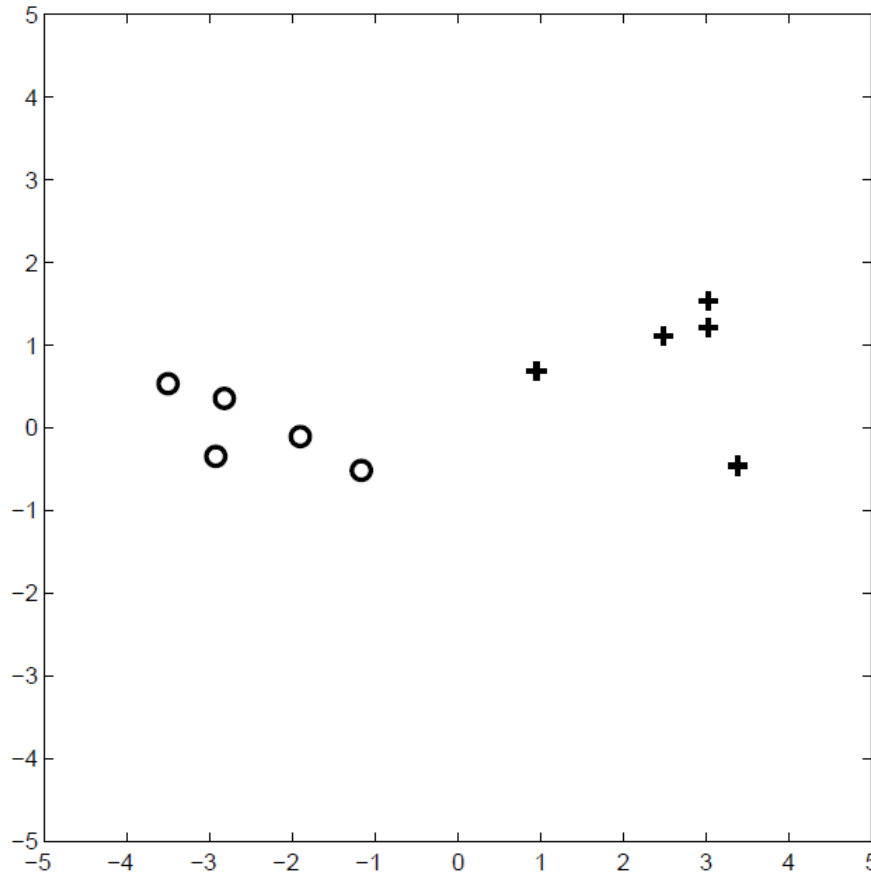
$$p(\mathbf{v}, \mathbf{h}) = \frac{\exp \{-E(\mathbf{v}, \mathbf{h})\}}{\sum_{\mathbf{v}', \mathbf{h}'} \exp \{-E(\mathbf{v}', \mathbf{h}')\}}$$

Generative Models

Zhu (2007)

- Example

✓ Assuming each class has a Gaussian distribution, what is the decision boundary?



Model parameters :

$$\theta = \{w_1, w_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2\}$$

$$\begin{aligned} p(x, y|\theta) &= p(y|\theta)p(x|y, \theta) \\ &= w_y \mathcal{N}(x; \mu_y, \Sigma_y) \end{aligned}$$

Classification :

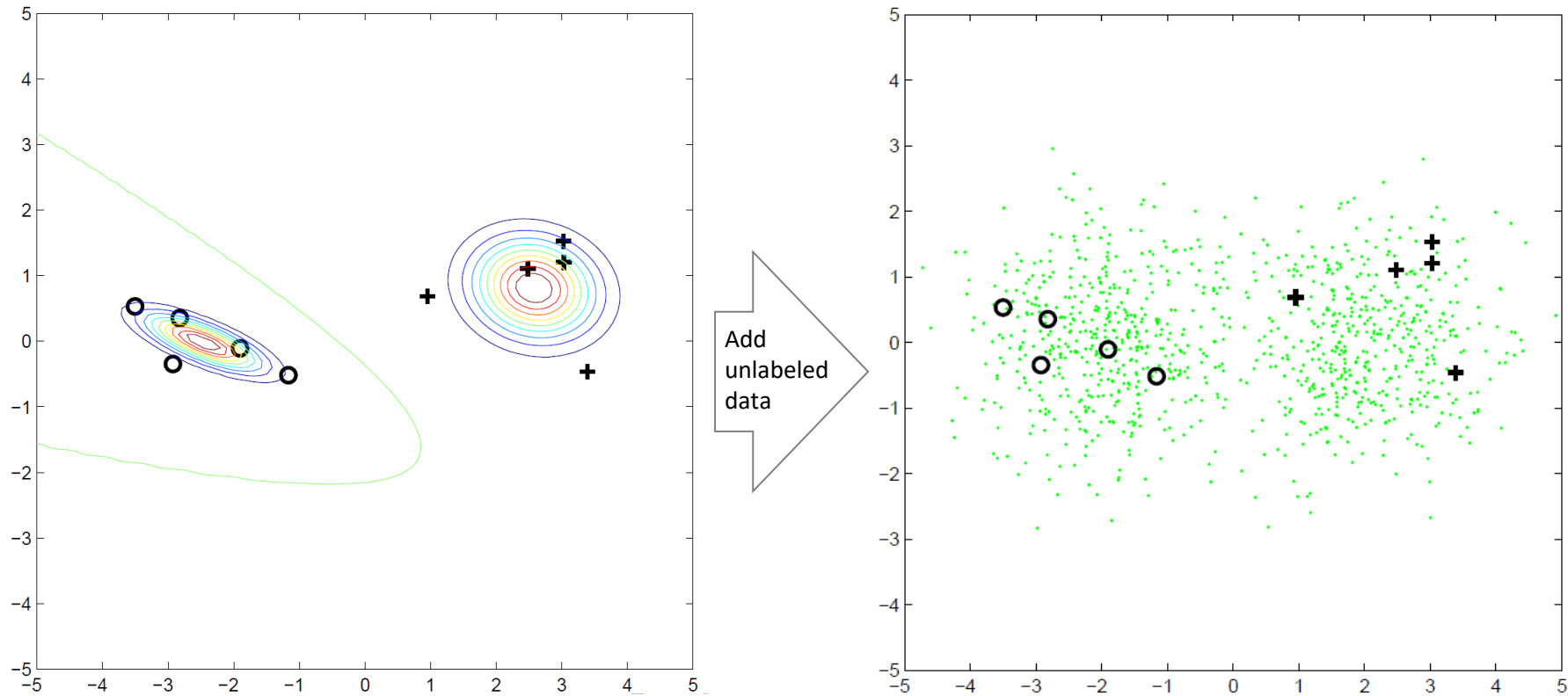
$$p(y|x, \theta) = \frac{p(x, y|\theta)}{\sum_{y'} p(x, y'|\theta)}$$

Generative Models

Zhu (2007)

- Example

✓ The most likely model, and its decision boundary:

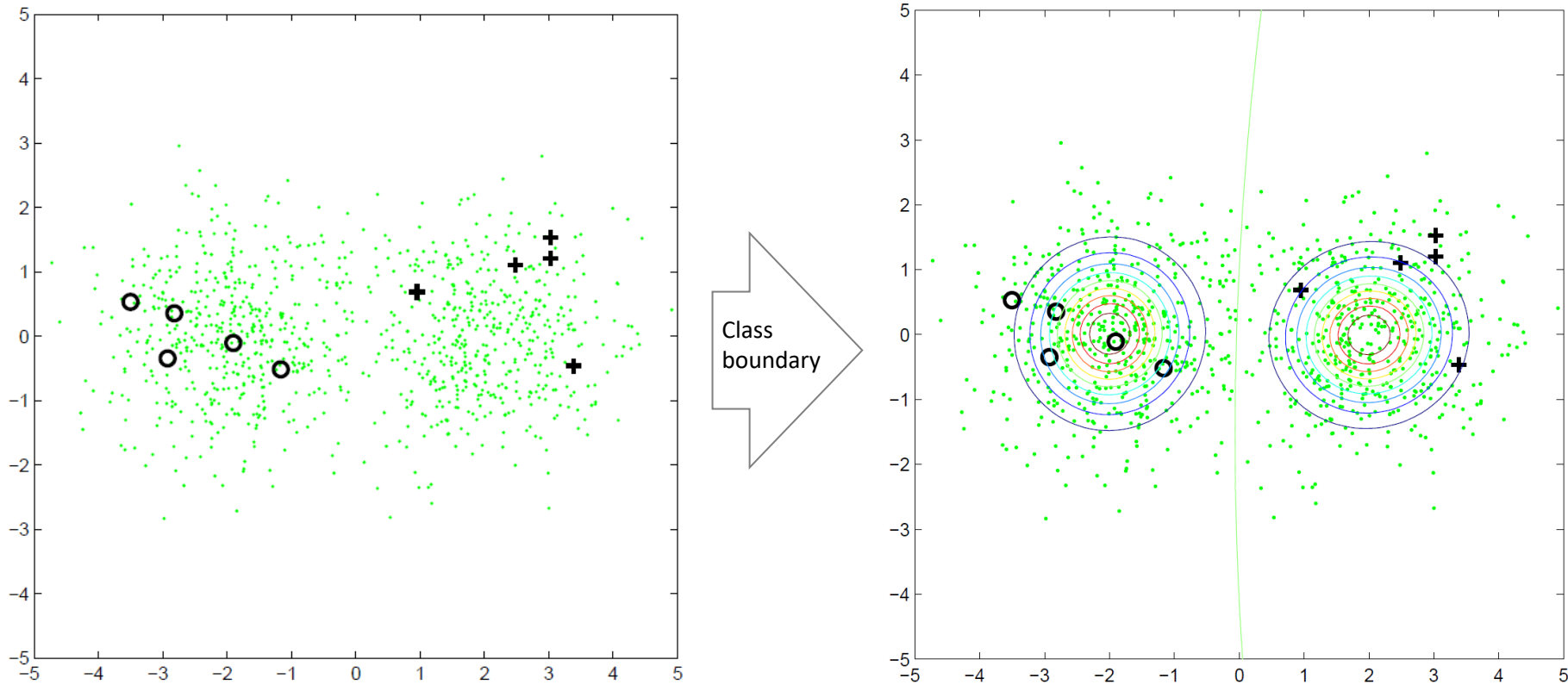


Generative Models

Zhu (2007)

- Example

✓ The most likely model, and its decision boundary:

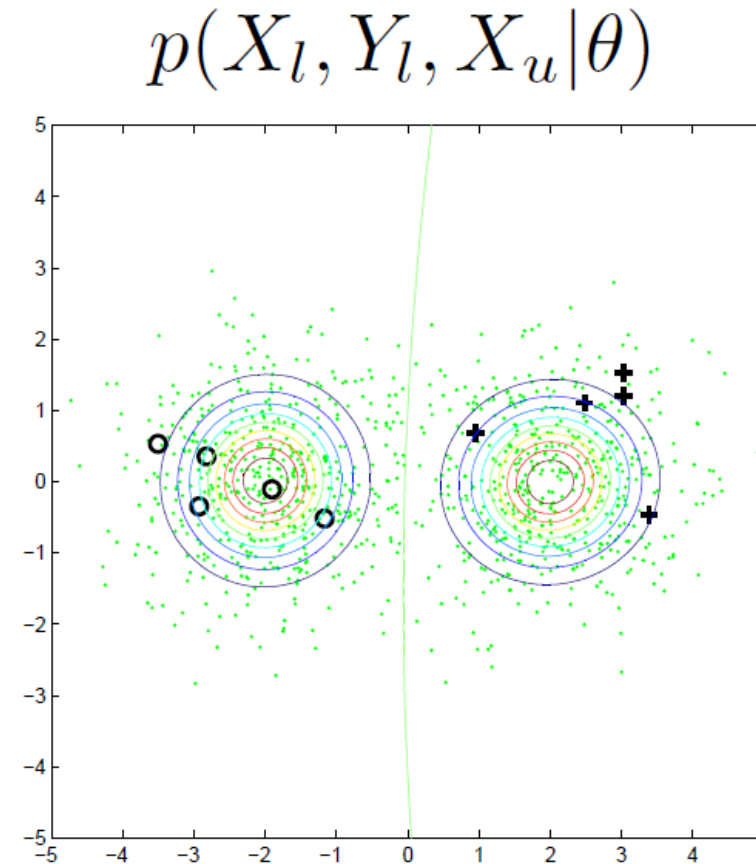
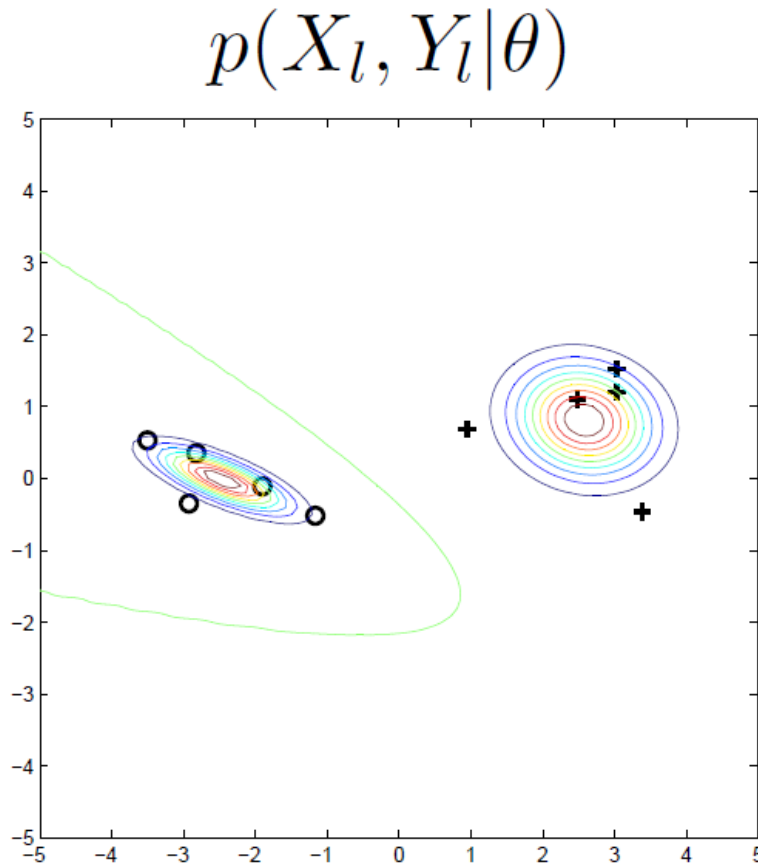


Generative Models

Zhu (2007)

- Example

- ✓ They are different because they maximize different quantities



Generative Models

Fox-Roberts and Rosten (2014), Kingma et al. (2014)

- Assumption: The full generative model $p(\mathbf{X}, \mathbf{y}|\theta)$

✓ Generative model for semi-supervised learning:

- Quantity of interests:

$$p(\mathbf{X}_l, \mathbf{y}_l, \mathbf{X}_u|\theta) = \sum_{\mathbf{y}_u} p(\mathbf{X}_l, \mathbf{y}_l, \mathbf{X}_u, \mathbf{y}_u|\theta)$$

- Find the maximum likelihood estimate (MLE) of θ , the maximum a posteriori (MAP) estimate, or be Bayesian

✓ Examples of some generative models

- Mixture of Gaussian distribution (GMM): Image classification (EM algorithm)
- Mixture of multinomial distribution (Naïve Bayes): Text categorization (EM algorithm)
- Hidden Markov Models (HMM): Speech recognition (Baum-Welch algorithm)

Generative Models: Gaussian Mixture Model

Zhu (2007)

- Gaussian Mixture Model

- ✓ For simplicity, consider binary classification with GMM using MLE

- Labeled data only

$$p(\mathbf{X}_l, \mathbf{y}_l | \theta) = \sum_{i=1}^l \log p(y_i | \theta) p(\mathbf{x}_i | y_i, \theta)$$

- MLE for θ is trivial (frequency, sample mean, sample covariance)

- Labeled and unlabeled data

$$p(\mathbf{X}_l, \mathbf{y}_l, \mathbf{X}_u | \theta) = \sum_{i=1}^l \log p(y_i | \theta) p(\mathbf{x}_i | y_i, \theta) + \sum_{i=l+1}^{l+u} \log \left(\sum_{y=1}^2 p(y | \theta) p(\mathbf{x}_i | y, \theta) \right)$$

- MLE is difficult because of hidden variables
- The Expectation-Maximization (EM) algorithm is used to find a local optimum

Generative Models: Gaussian Mixture Model

Zhu (2007)

- The EM algorithm for GMM

- ✓ Step 0: Start from MLE $\theta = \{w, \mu, \Sigma\}_{1,2}$ on $(\mathbf{X}_l, \mathbf{y}_l)$, repeat

- ✓ Step 1: The **E-Step**: compute the expected label for all $\mathbf{x} \in \mathbf{X}_u$

$$p(y|\mathbf{x}, \theta) = \frac{p(\mathbf{x}, y|\theta)}{\sum_{y'} p(\mathbf{x}, y'|\theta)}$$

- label $p(y = 1|\mathbf{x}, \theta)$ -fraction of \mathbf{x} with class 1

- label $p(y = 2|\mathbf{x}, \theta)$ -fraction of \mathbf{x} with class 2

- ✓ Step 2: The **M-Step**: update MLE θ with (now labeled) \mathbf{X}_u

- w_c : proportion of class c

- μ_c : sample mean of class c

- Σ_c : sample covariance of class c

- Can be viewed as a special form of self-training

Generative Models: Gaussian Mixture Model

Zhu (2007)

- The EM algorithm in general

- ✓ Set up:

- Obtain data $\mathcal{D} = (\mathbf{X}_l, \mathbf{y}_l, \mathbf{X}_u)$
 - hidden data $\mathcal{H} = \mathbf{y}_u$

$$p(\mathcal{D}|\theta) = \sum_{\mathcal{H}} p(\mathcal{D}, \mathcal{H}|\theta)$$

- ✓ Goal: find θ to maximize $p(\mathcal{D}|\theta)$

- ✓ Properties

- EM starts from an arbitrary θ_0
 - The E-step: $q(\mathcal{H}) = p(\mathcal{H}|\mathcal{D}, \theta)$
 - The M-step: maximize $\sum_{q(\mathcal{H})} \log p(\mathcal{D}, \mathcal{H}|\theta)$
 - EM iteratively improves $p(\mathcal{D}|\theta)$
 - EM converges to a local maximum of θ

Generative Models: Gaussian Mixture Model

Zhu (2007)

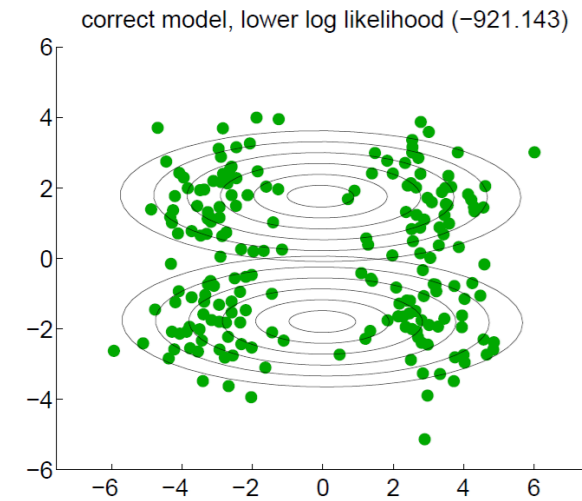
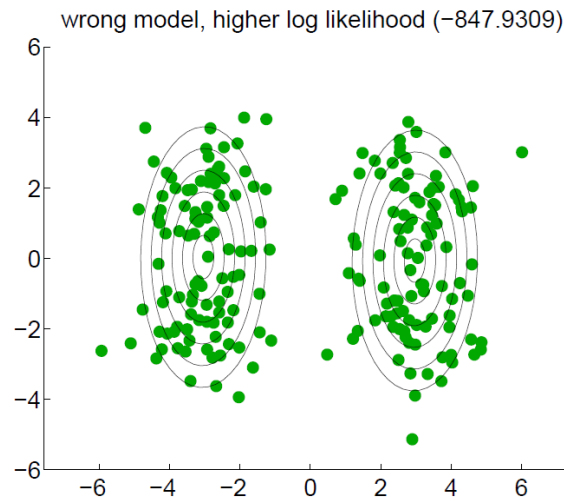
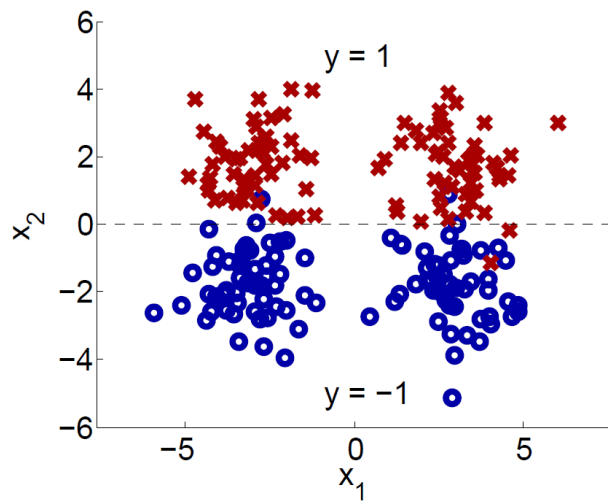
- The EM algorithm in general
 - ✓ Key is to maximize the posterior probability
 - ✓ EM is just one way to maximize it; other ways to find parameters are possible (variational approximation, direct optimization, etc.)
- Advantages
 - ✓ Clear, well-studied probabilistic framework
 - ✓ Can be extremely effective, if the model is close to correct

Generative Models: Gaussian Mixture Model

Zhu (2007)

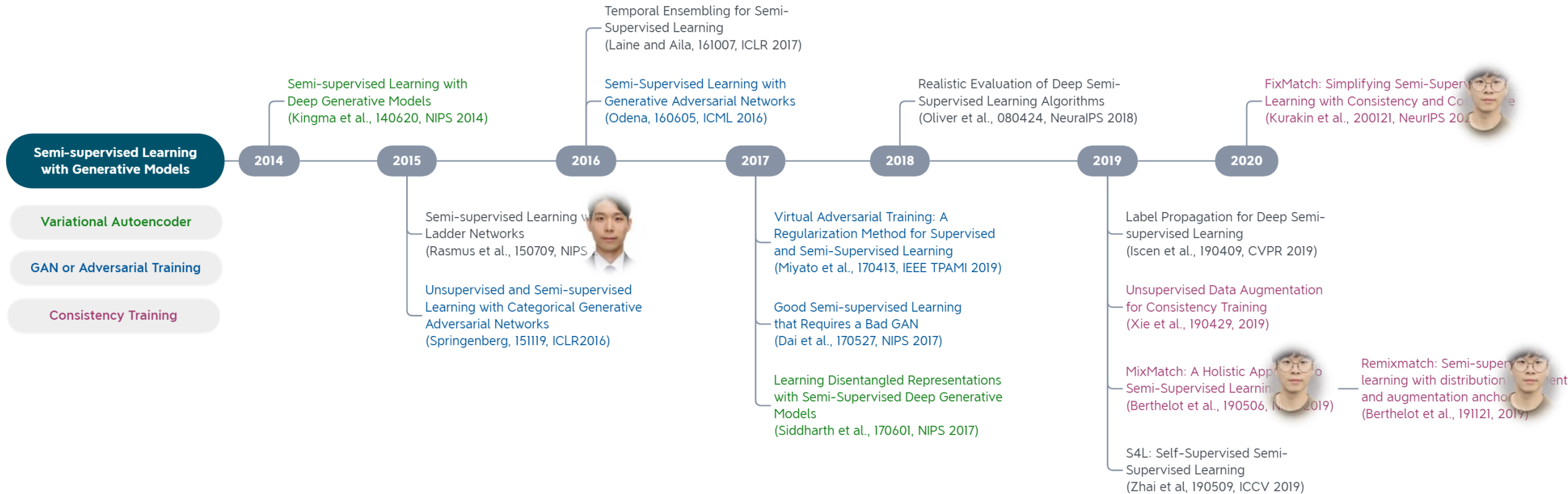
- Disadvantages

- ✓ Often difficult to verify the correctness of the model
- ✓ Model identifiability, local optima of the EM algorithm
- ✓ Unlabeled data may hurt if generative model is wrong



Semi-supervised Learning with Generative Models

Recent Advances



Deep Generative Models

Kingma et al. (2014)

- Variational Inference

- ✓ David Blei, Variational Inference: Foundations and Modern Methods (NIPS 2016 tutorial)

- https://youtu.be/ogdv_6dbvVQ

The probabilistic pipeline

```
graph TD; A[KNOWLEDGE & QUESTION] --> B[Make assumptions]; C[DATA] --> D[Discover patterns]; B --> D; D --> E[Predict & Explore]
```

- **Inference** is the key algorithmic problem.
- Answers the question: What does this model say about this data?
- Our goal: **General** and **scalable** approaches to inference

Variational Inference: Foundations and Modern Methods (NIPS 2016 tutorial)
조회수 18,614회 • 2018. 1. 18.

289 4 공유 저장 ...

Deep Generative Models

Kingma et al. (2014)

- Variational Lower Bound

- ✓ We have some data X , a generative probability model $P(X|\theta)$ that shows us how to randomly sample (e.g., generate) data points that follow distribution of X , assuming we know the “magic values” of the θ parameters

$$p(\theta|\mathbf{X}) = \frac{p(\mathbf{x}|\theta)p(\theta)}{p(\mathbf{X})} = \frac{p(\mathbf{x}|\theta)p(\theta)}{\int_{-\infty}^{\infty} p(\mathbf{x}|\theta)p(\theta)d\theta}$$

$$\text{posterior} = \frac{\text{likelihood} \cdot \text{prior}}{\text{evidence}}$$

- ✓ The goal is to find the posterior $P(\theta|X)$, that tells us the distribution of the θ parameters
 - Sometimes is the end goal
 - Sometimes we want the parameters to generate some new data points using $P(X|\theta)$
- ✓ The problem is intractable because of its denominator

Deep Generative Models

Kingma et al. (2014)

- The solution: Approximation

- ✓ Approximate $P(\theta|X)$ by another function $Q(\theta|X)$

- Solving for Q is relatively fast because we can assume a particular shape for $Q(\theta|X)$ and turn the inference problem (finding $P(\theta|X)$) into an optimization problem (finding Q)
- $Q(\theta|X)$ should be as close as possible to $P(\theta|X)$

- ✓ In terms of “closeness”, the standard way of measuring it is to use KL divergence

$$\begin{aligned} D_{KL}(Q||P) &= \int_{-\infty}^{\infty} q(\theta|\mathbf{X}) \log \frac{q(\theta|\mathbf{X})}{p(\theta|\mathbf{X})} d\theta \\ &= \int_{-\infty}^{\infty} q(\theta|\mathbf{X}) \log \frac{q(\theta|\mathbf{X})}{p(\theta, \mathbf{X})} d\theta + \int_{-\infty}^{\infty} q(\theta|\mathbf{X}) \log p(\mathbf{X}) d\theta \\ &= \int_{-\infty}^{\infty} q(\theta|\mathbf{X}) \log \frac{q(\theta|\mathbf{X})}{p(\theta, \mathbf{X})} d\theta + \log p(\mathbf{X}) \\ &= E_q \left[\log \frac{q(\theta|\mathbf{X})}{p(\theta, \mathbf{X})} \right] + \log p(\mathbf{X}) \end{aligned}$$

Deep Generative Models

Kingma et al. (2014)

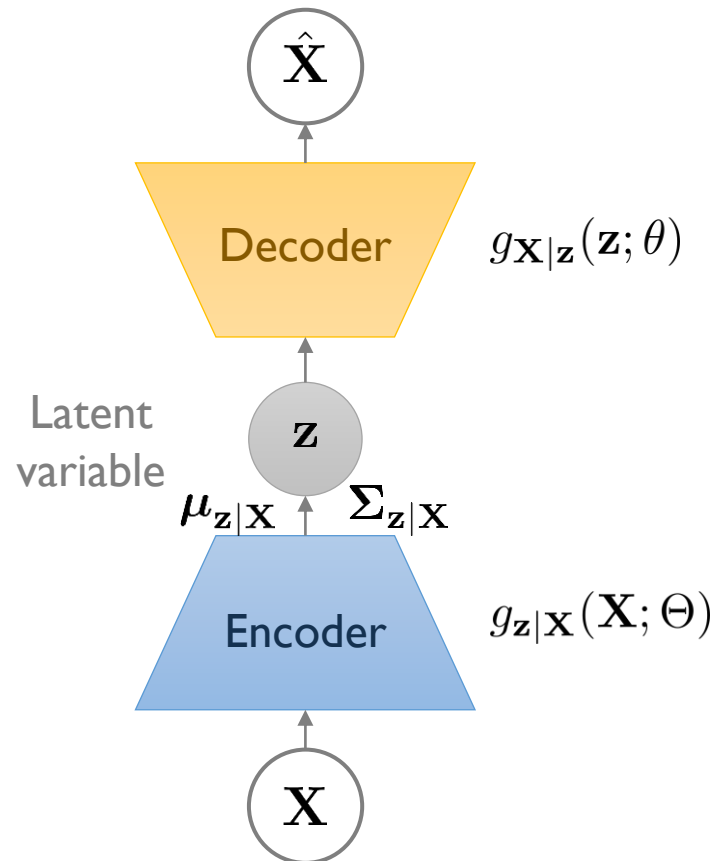
- Evidence Lower Bound (ELBO):
 - ✓ For multiple data points, we can sum over them
 - ✓ ELBO is a lower bound on the evidence, i.e., a lower bound on the probability of our data occurring given our model
 - ✓ Maximizing the ELBO is equivalent to minimizing the KL divergence
 - ✓ The first two terms try to maximize the MAP estimate (likelihood + prior)
 - ✓ The last term tries to ensure Q is diffuse

$$\begin{aligned}\log p(\mathbf{X}) &= -E_q \left[\log \frac{q(\theta|\mathbf{X})}{p(\theta, \mathbf{X})} \right] + D_{KL}(Q||P) \\ \log p(\mathbf{X}) &\geq -E_q \left[\log \frac{q(\theta|\mathbf{X})}{p(\theta, \mathbf{X})} \right] \\ &= E_q [\log p(\theta, \mathbf{X}) - \log q(\theta|\mathbf{X})] \\ &= E_q [\log p(\mathbf{X}|\theta) + \log p(\theta) - \log q(\theta|\mathbf{X})] \\ &= E_q [\text{likelihood} + \text{prior} - \text{approx.posterior}]\end{aligned}$$

Deep Generative Models

Kingma et al. (2014)

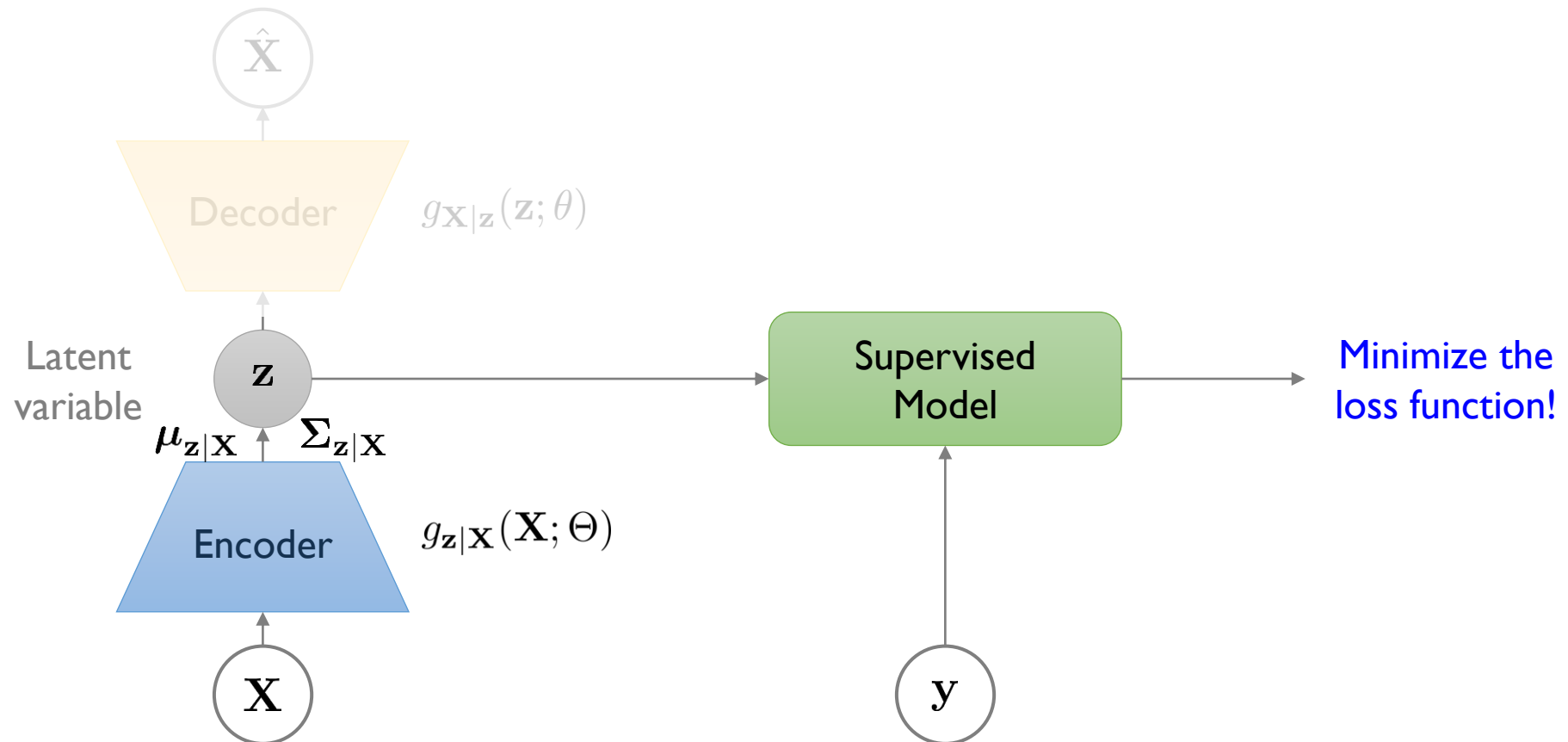
- A Vanilla VAE for Semi-supervised Learning (MI Model)
 - ✓ Phase I: train a variational auto-encoder (VAE) based on both labeled and unlabeled data



Deep Generative Models

Kingma et al. (2014)

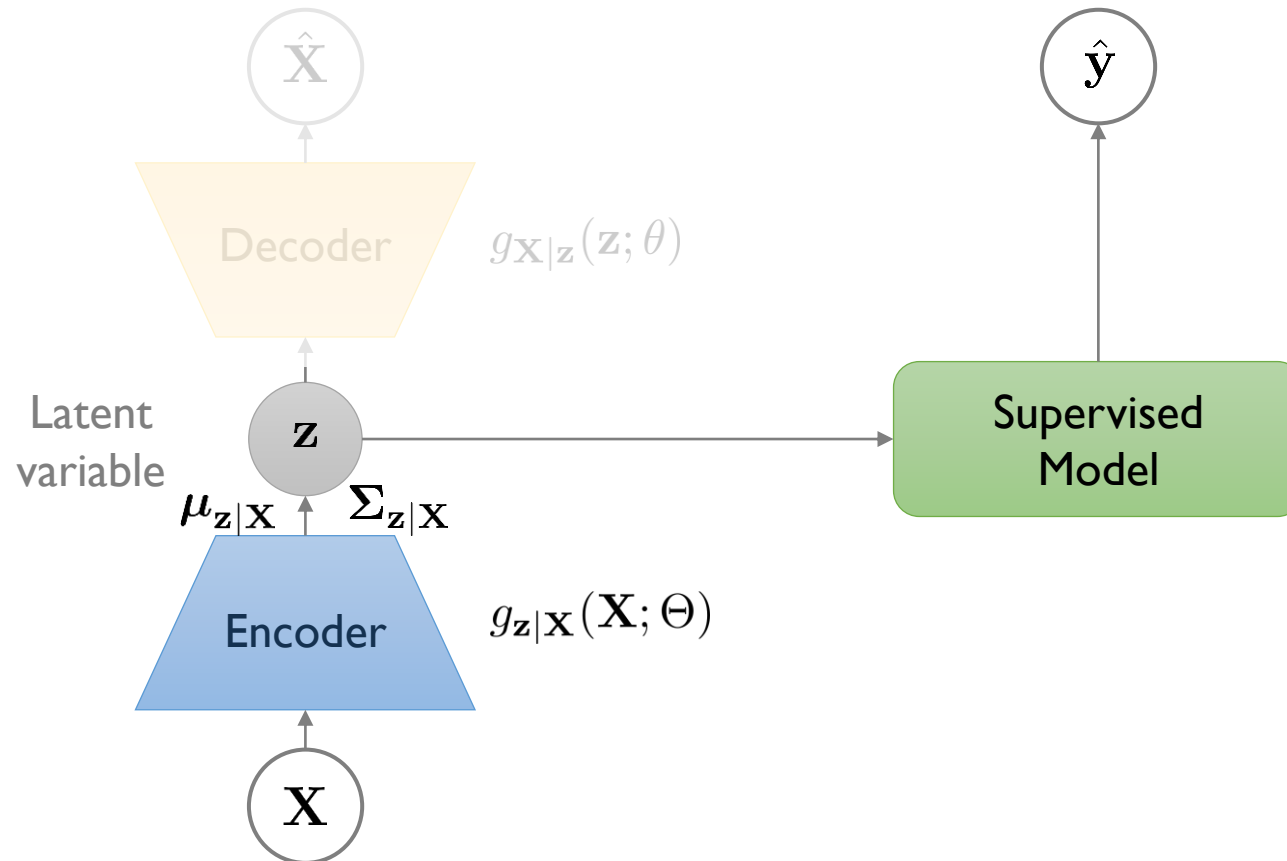
- A Vanilla VAE for Semi-supervised Learning (MI Model)
 - ✓ Phase 2: Solve a standard supervised learning problem on the labeled data using (\mathbf{Z}, \mathbf{y}) pairs



Deep Generative Models

Kingma et al. (2014)

- A Vanilla VAE for Semi-supervised Learning (MI Model)
 - ✓ Phase 3: Inference for unlabeled data or new test data

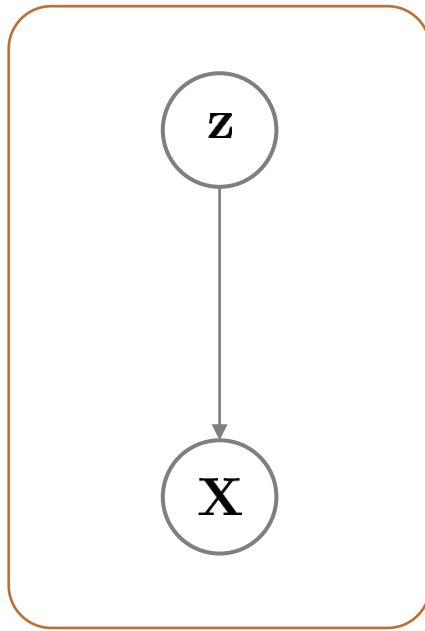


Deep Generative Models

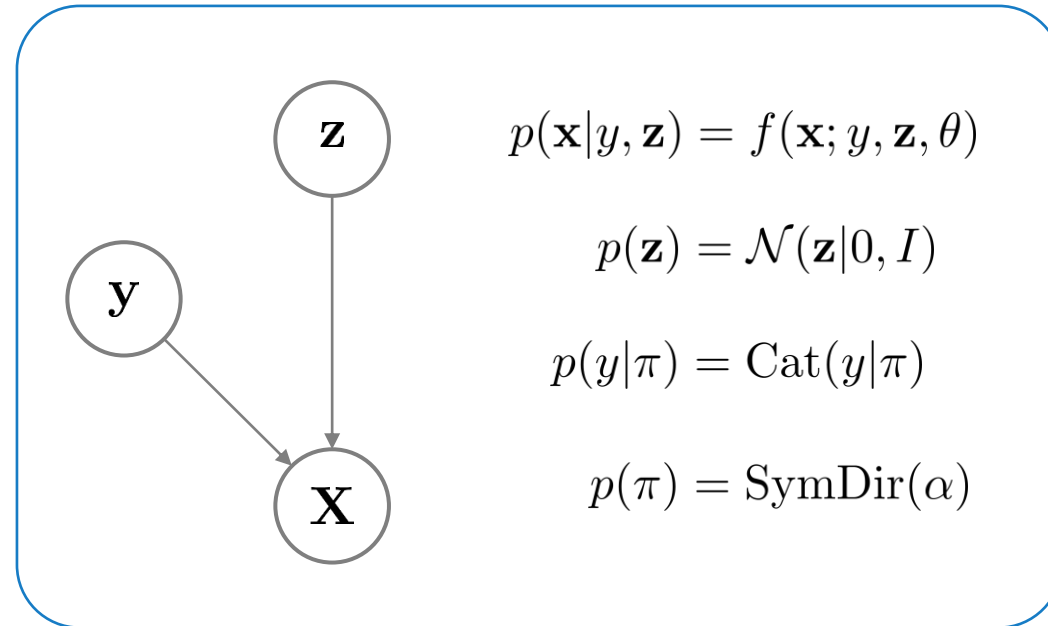
Kingma et al. (2014)

- Extending the VAE for Semi-supervised Learning (M2 Model)
 - ✓ M1 model basically ignored the labeled data when training the VAE model
 - ✓ M2 model explicitly takes in into account

M1 Model



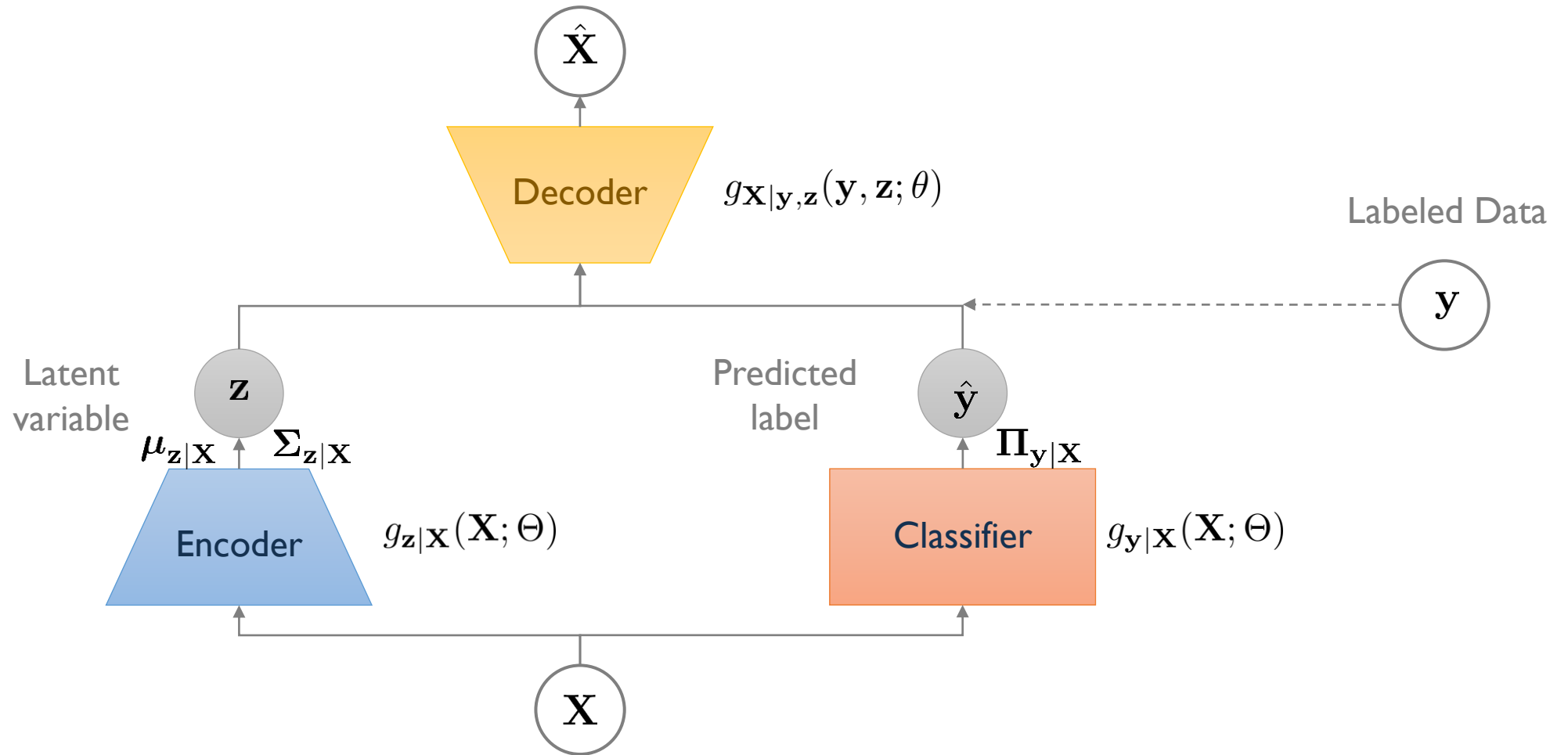
M2 Model



Deep Generative Models

Kingma et al. (2014)

- Extending the VAE for Semi-supervised Learning (M2 Model)



Deep Generative Models

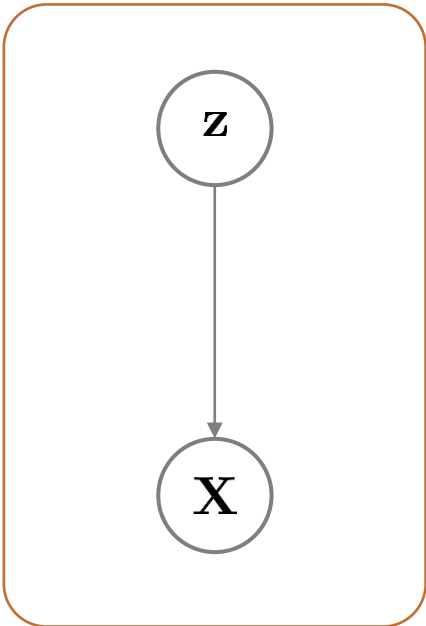
Kingma et al. (2014)

- Stack of M1 and M2

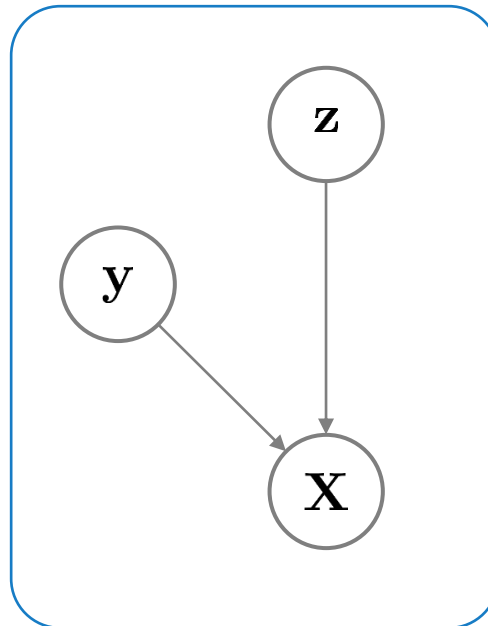
- ✓ Train generative semi-supervised model (M2) on unsupervised features z_1 from latent feature model (M1)

$$p_{\theta}(\mathbf{x}, y, \mathbf{z}_1, \mathbf{z}_2) = p(y)p(\mathbf{z}_2)p_{\theta}(\mathbf{z}_1|y, \mathbf{z}_2)p_{\theta}(\mathbf{x}|\mathbf{z}_1)$$

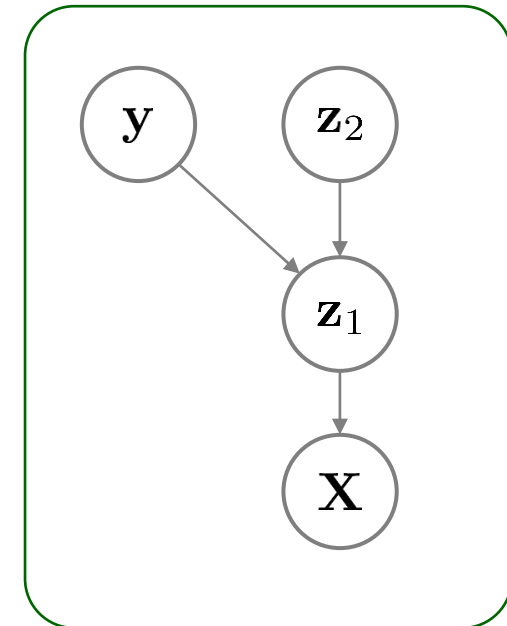
M1 Model

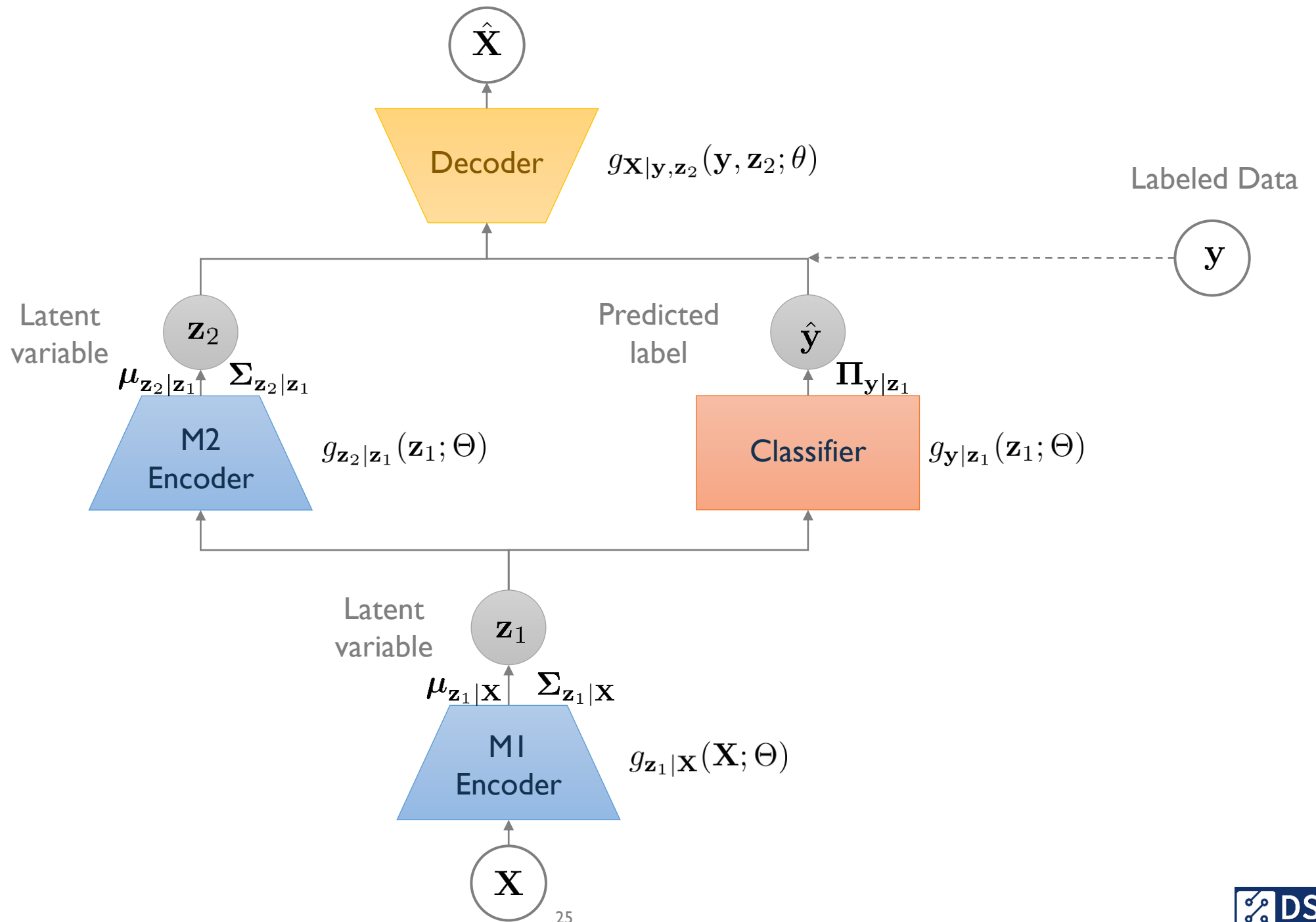


M2 Model



M1+M2 Model





Deep Generative Models

Kingma et al. (2014)

- Performance (from paper)

Table 1: Benchmark results of semi-supervised classification on MNIST with few labels.

N	NN	CNN	TSVM	CAE	MTC	AtlasRBF	M1+TSVM	M2	M1+M2
100	25.81	22.98	16.81	13.47	12.03	8.10 (\pm 0.95)	11.82 (\pm 0.25)	11.97 (\pm 1.71)	3.33 (\pm 0.14)
600	11.44	7.68	6.16	6.3	5.13	–	5.72 (\pm 0.049)	4.94 (\pm 0.13)	2.59 (\pm 0.05)
1000	10.7	6.45	5.38	4.77	3.64	3.68 (\pm 0.12)	4.24 (\pm 0.07)	3.60 (\pm 0.56)	2.40 (\pm 0.02)
3000	6.04	3.35	3.45	3.22	2.57	–	3.49 (\pm 0.04)	3.92 (\pm 0.63)	2.18 (\pm 0.04)

- Performance (implemented, <https://bjlkeng.github.io/posts/semi-supervised-learning-with-variational-autoencoders/>)

Model	N=100	N=500	N=1000	N=2000	N=5000	Model	N=1000	N=2000	N=5000	N=10000	N=25000
PCA + SVM	0.692	0.871	0.891	0.911	0.929	CNN	0.433	0.4844	0.610	0.673	0.767
CNN	0.262	0.921	0.934	0.955	0.978	Inception	0.661	0.684	0.728	0.751	0.773
M1	0.628	0.885	0.905	0.921	0.933	PCA + SVM	0.356	0.384	0.420	0.446	0.482
M2	•	•	0.975	•	•	M1	0.321	0.362	0.375	0.389	0.409
						M2	0.420	•	•	•	•

Table 1: MNIST Results

Table 2: CIFAR10 Results

Deep Generative Models

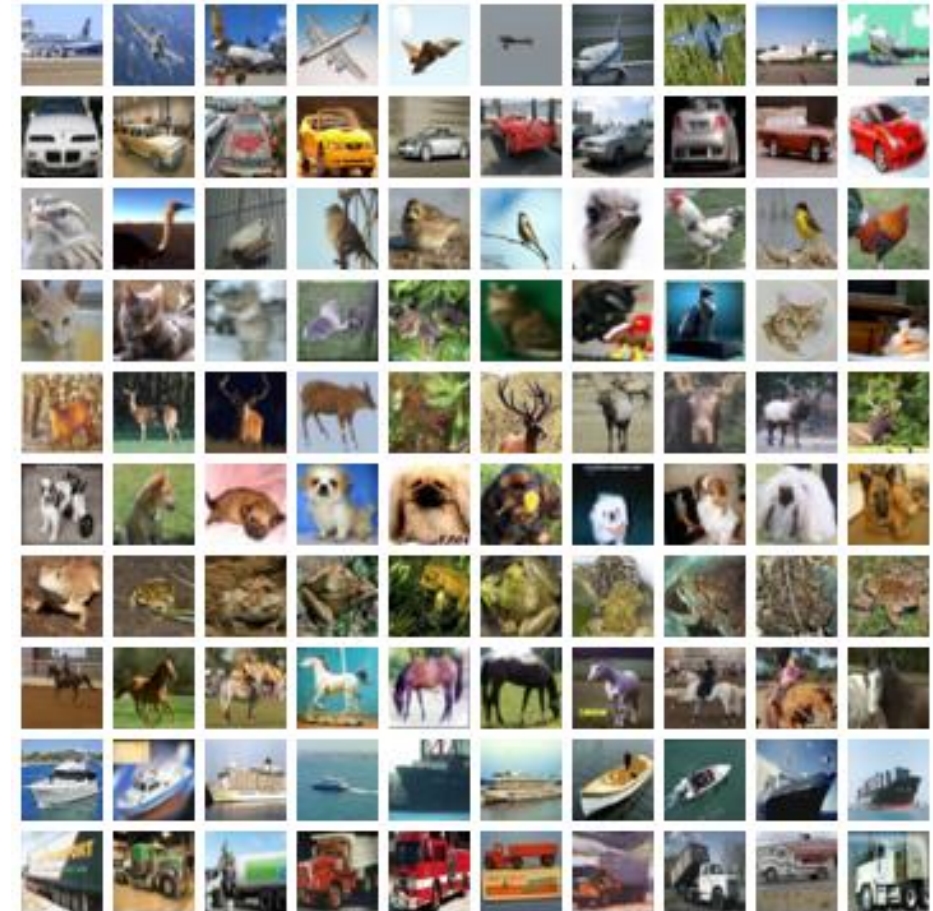
Kingma et al. (2014)

- Images generated from M2 VAE model trained on CIFAR data

Generated images



Original images



Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

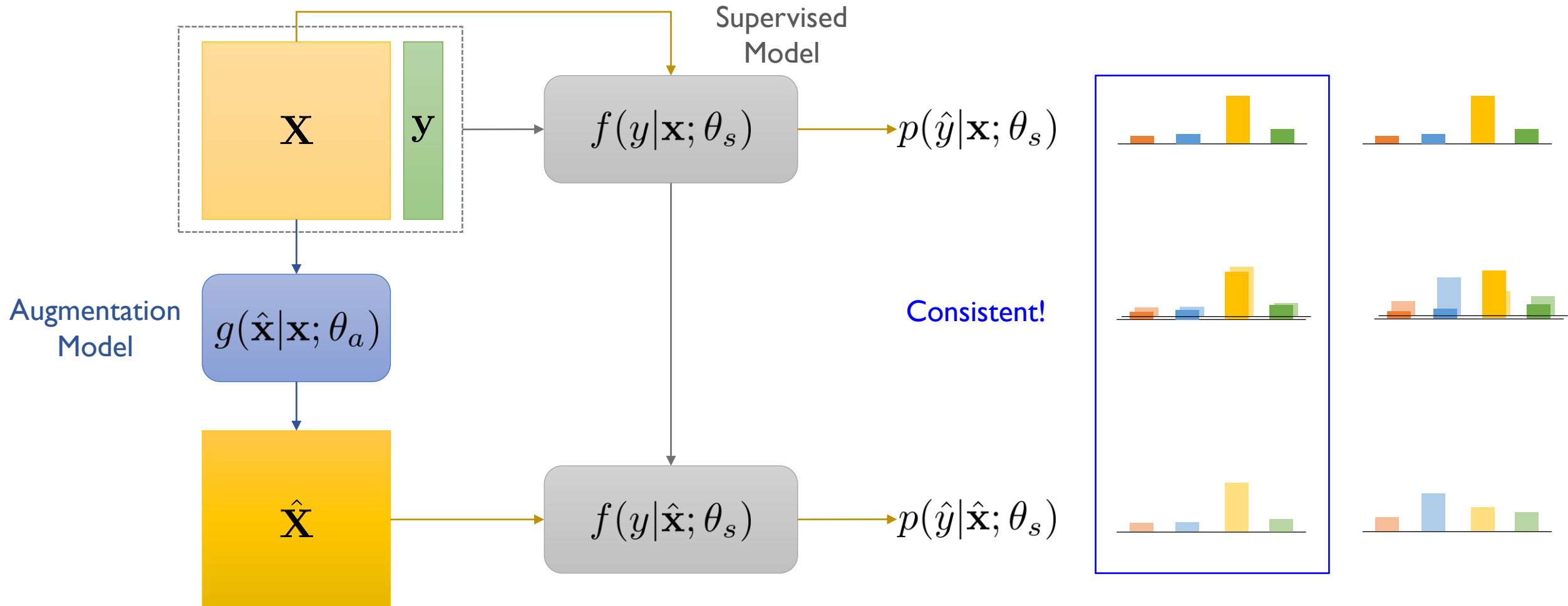
- A good model should be robust to any small change in an input example or hidden states



- Consistency training: Simply regularize model predictions to be invariant to small noise applied to either input examples or hidden states
- UDA investigate the role of noise injection in consistency training and observe that advanced data augmentation methods perform well in SSL.

Unsupervised Data Augmentation for Consistency Training

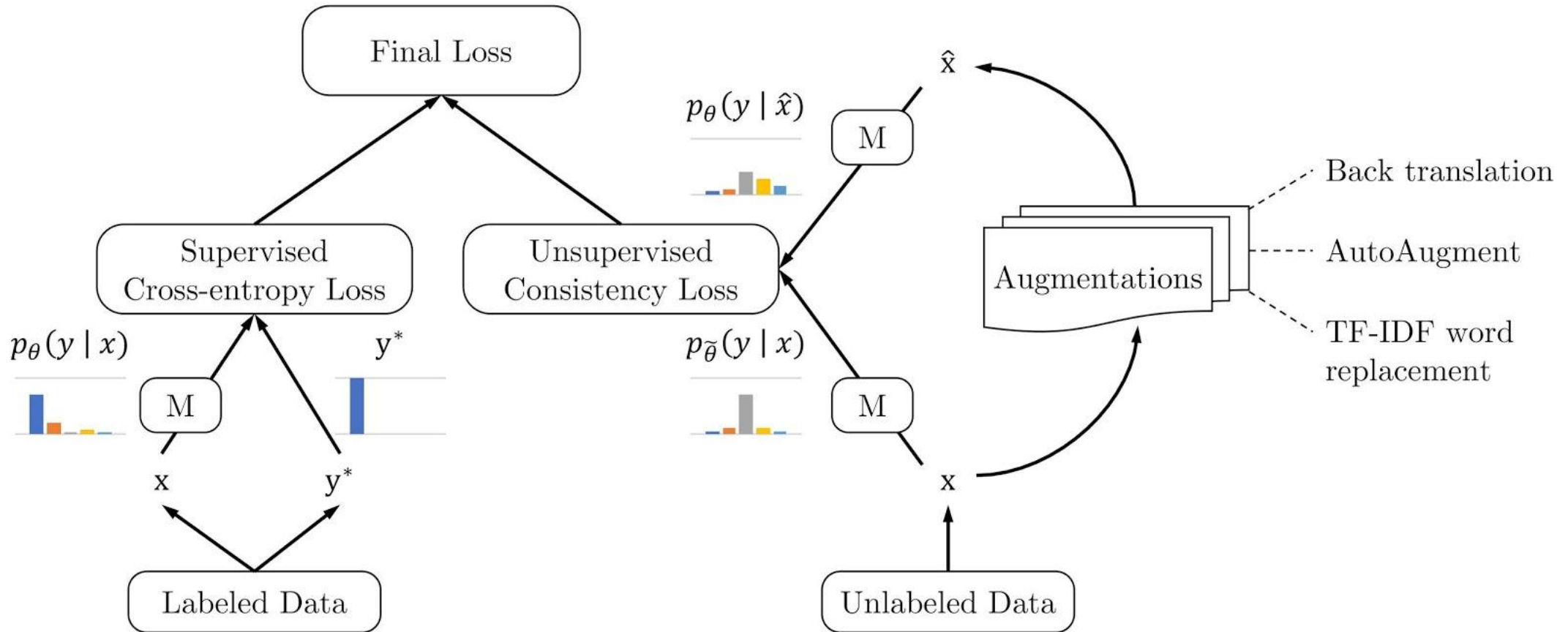
- Consistency Training



Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

- UDA at a glance

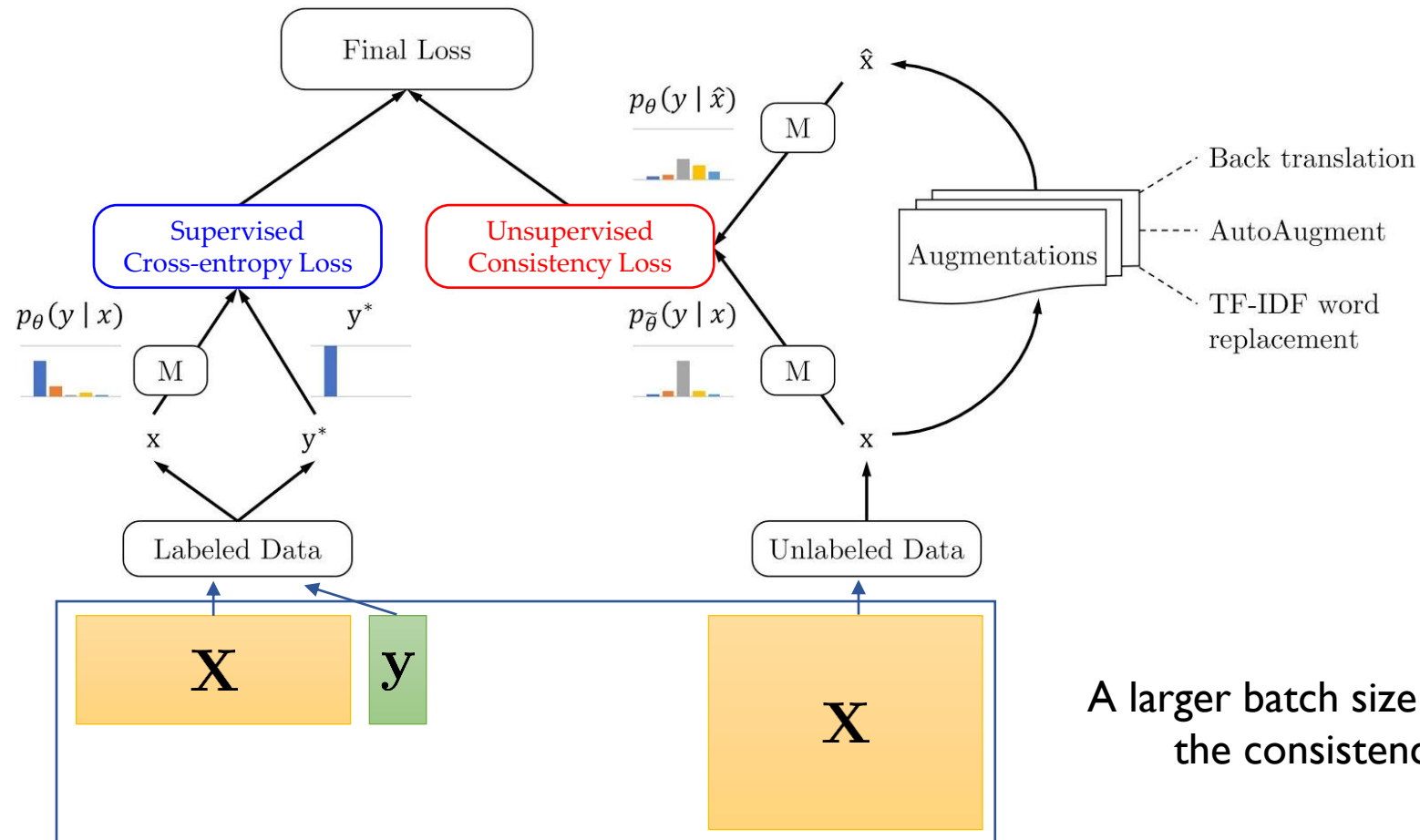


Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

- Training Objective

$$\min_{\theta} \mathcal{J}(\theta) = \mathbb{E}_{x_1 \sim p_L(x)} [-\log p_{\theta}(f^*(x_1) | x_1)] + \lambda \times \mathbb{E}_{x_2 \sim p_U(x)} \mathbb{E}_{\hat{x} \sim q(\hat{x} | x_2)} [\text{CE}(p_{\tilde{\theta}}(y | x_2) || p_{\theta}(y | \hat{x}))]$$



A larger batch size is used for the consistency loss

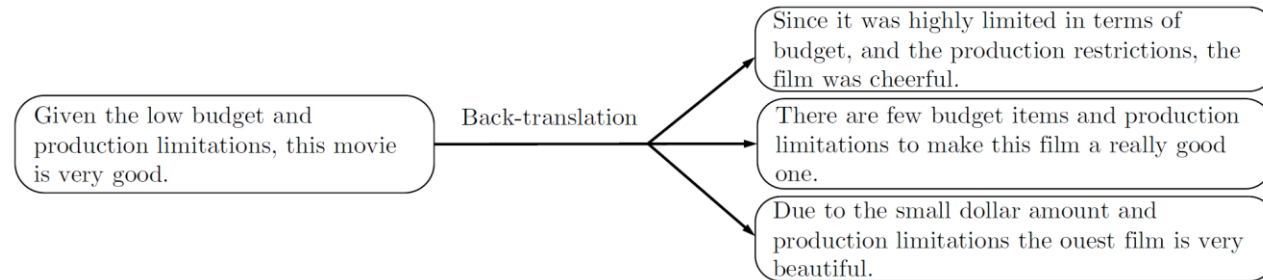
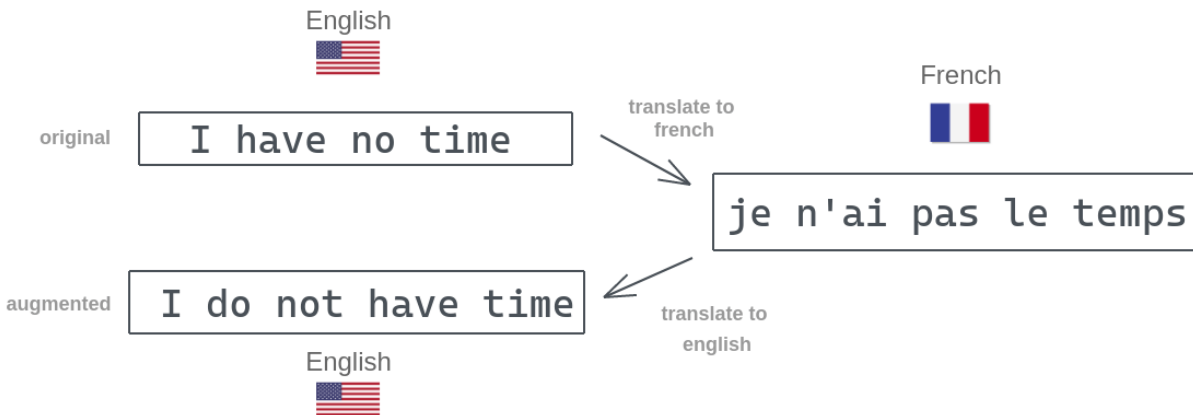
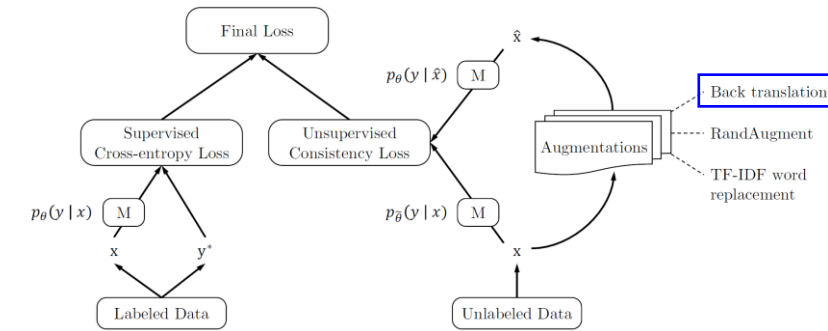
Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

- Augmentation Methods

- ✓ Back-translation for NLP

- Train the Model 1 that translates Language A to Language B
 - Train the Model 2 that translates Language B to Language A
 - Augment the Data by applying the source text to Model A and Model B sequentially



<https://amitniss.com/2020/02/back-translation-in-google-sheets/>

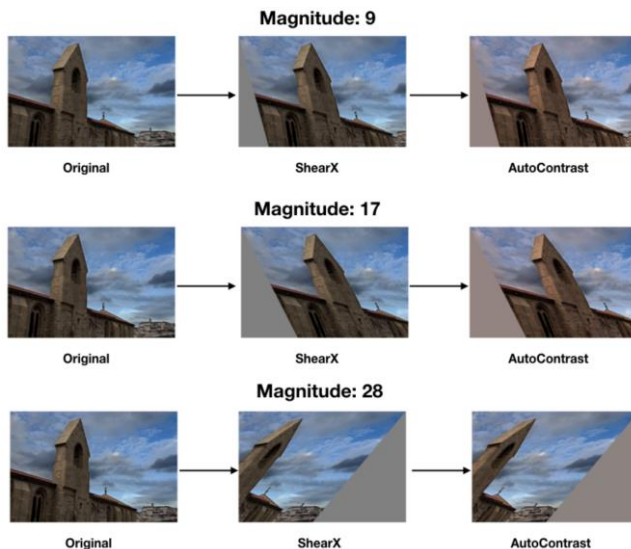
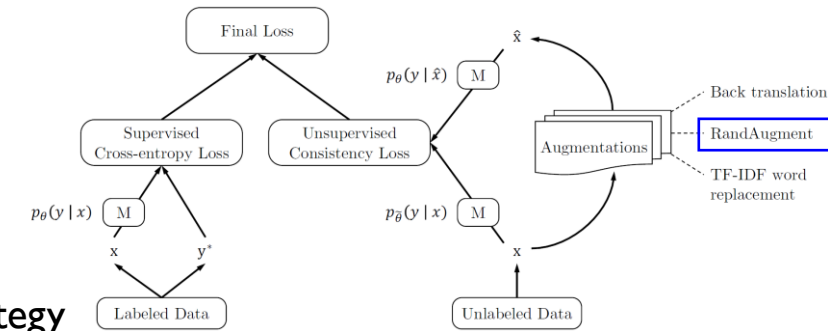
Unsupervised Data Augmentation for Consistency Training

Cubuk et al. (2020)

• Augmentation Methods

✓ RandAugment for Image Classification

- **AutoAugment**: uses a search method to combine all image processing transformations in the Python Image Library (PIL) to find a good augmentation strategy
- **RandAugment**: does not use search but instead uniformly sample from the same set of augmentation transformations in PIL (Simpler and requires no labeled data as there is no need to search for optimal policies)



```
transforms = [
    'Identity', 'AutoContrast', 'Equalize',
    'Rotate', 'Solarize', 'Color', 'Posterize',
    'Contrast', 'Brightness', 'Sharpness',
    'ShearX', 'ShearY', 'TranslateX', 'TranslateY']

def randaugment(N, M):
    """Generate a set of distortions.

    Args:
        N: Number of augmentation transformations to
            apply sequentially.
        M: Magnitude for all the transformations.
    """

    sampled_ops = np.random.choice(transforms, N)
    return [(op, M) for op in sampled_ops]
```

	baseline	PBA	Fast AA	AA	RA
CIFAR-10					
Wide-ResNet-28-2	94.9	-	-	95.9	95.8
Wide-ResNet-28-10	96.1	97.4	97.3	97.4	97.3
Shake-Shake	97.1	98.0	98.0	98.0	98.0
PyramidNet	97.3	98.5	98.3	98.5	98.5
CIFAR-100					
Wide-ResNet-28-2	75.4	-	-	78.5	78.3
Wide-ResNet-28-10	81.2	83.3	82.7	82.9	83.3
SVHN (core set)					
Wide-ResNet-28-2	96.7	-	-	98.0	98.3
Wide-ResNet-28-10	96.9	-	-	98.1	98.3
SVHN					
Wide-ResNet-28-2	98.2	-	-	98.7	98.7
Wide-ResNet-28-10	98.5	98.9	98.8	98.9	99.0

Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

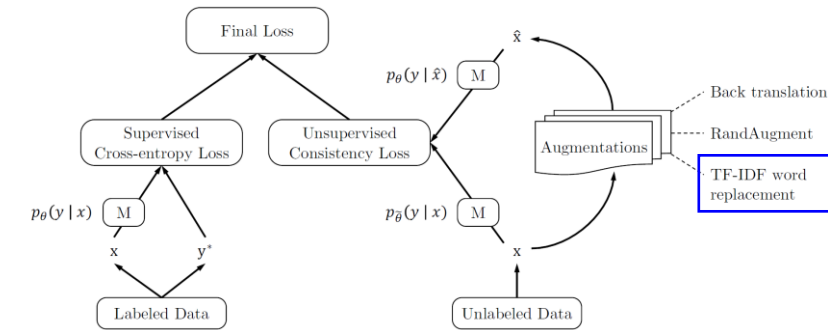
• Augmentation Methods

✓ Word replacing with TF-IDF for Text Classification

- Replaces uninformative words with low TF-IDF scores
- While keeping those with high TF-IDF values

This virus has spread worldwide
↓
A virus has spread worldwide

- For more text augmentation methods, refer to Junghee Kim's presentation at DSBA seminar



연구배경

Data Augmentation in NLP

Text Augmentation 방법 분류

Text Augmentation	Text Modification	Text Generation	특징
Random Noise Injection	문장에서 무작위로 단어를 삭제, 추가, 변경, 교체하는 방법		간단하게 문장 내에 있는 단어를 변경.
TF-IDF based word replacement	TF-IDF를 이용하여 문장의 주요 정보를 추출하고 주요성분 이외의 단어를 변경		외부 사전(WordNet)을 이용하여 단어를 변경.
Word-Embedding Substitution	Embedding 벡터를 이용하여 가까운 단어로 변경하는 방법		원문에서 사용하지 않은 단어로 변경 가능.
Masked Language Model	BERT 모델을 이용하여 무작위로 단어를 <MASK> 하고 추측한 단어로 변경		외부데이터로부터 학습한 모델을 이용.
Back Translation	번역기를 이용하여 문장을 생성하는 방법		원문으로부터 문장 전체를 새롭게 생성.
Generative Methods	GPT2와 같은 생성모델을 학습하여 새로운 문장을 생성하는 방법		원문과 문법적 구조가 다른 문장 생성이 가능.



<https://youtu.be/UVtMqh3agQY>

Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

- Performance

Image Classification

Method	Model	# Param	CIFAR-10 (4k)	SVHN (1k)
PI-Model [32]	Conv-Large	3.1M	12.36 ± 0.31	4.82 ± 0.17
Mean Teacher [58]	Conv-Large	3.1M	12.31 ± 0.28	3.95 ± 0.19
VAT + EntMin [41]	Conv-Large	3.1M	10.55 ± 0.05	3.86 ± 0.11
SNTG [35]	Conv-Large	3.1M	10.93 ± 0.14	3.86 ± 0.27
ICT [60]	Conv-Large	3.1M	7.29 ± 0.02	3.89 ± 0.04
Pseudo-Label [33]	WRN-28-2	1.5M	16.21 ± 0.11	7.62 ± 0.29
LGA + VAT [25]	WRN-28-2	1.5M	12.06 ± 0.19	6.58 ± 0.36
ICT [60]	WRN-28-2	1.5M	7.66 ± 0.17	3.53 ± 0.07
MixMatch [3]	WRN-28-2	1.5M	6.24 ± 0.06	2.89 ± 0.06
Mean Teacher [58]	Shake-Shake	26M	6.28 ± 0.15	-
Fast-SWA [1]	Shake-Shake	26M	5.0	-
MixMatch [3]	WRN	26M	4.95 ± 0.08	-
UDA (RandAugment)	WRN-28-2	1.5M	4.32 ± 0.08	2.23 ± 0.07
UDA (RandAugment)	Shake-Shake	26M	3.7	-
UDA (RandAugment)	PyramidNet	26M	2.7	-

Text Classification

Fully supervised baseline							
Datasets (# Sup examples)		IMDb (25k)	Yelp-2 (560k)	Yelp-5 (650k)	Amazon-2 (3.6m)	Amazon-5 (3m)	DBpedia (560k)
Pre-BERT SOTA		4.32	2.16	29.98	3.32	34.81	0.70
BERT _{LARGE}		4.51	1.89	29.32	2.63	34.17	0.64
Semi-supervised setting							
Initialization	UDA	IMDb (20)	Yelp-2 (20)	Yelp-5 (2.5k)	Amazon-2 (20)	Amazon-5 (2.5k)	DBpedia (140)
Random	✗	43.27	40.25	50.80	45.39	55.70	41.14
	✓	25.23	8.33	41.35	16.16	44.19	7.24
BERT _{BASE}	✗	18.40	13.60	41.00	26.75	44.09	2.58
	✓	5.45	2.61	33.80	3.96	38.40	1.33
BERT _{LARGE}	✗	11.72	10.55	38.90	15.54	42.30	1.68
	✓	4.78	2.50	33.54	3.93	37.80	1.09
BERT _{FINETUNE}	✗	6.50	2.94	32.39	12.17	37.32	-
	✓	4.20	2.05	32.08	3.50	37.12	-

Unsupervised Data Augmentation for Consistency Training

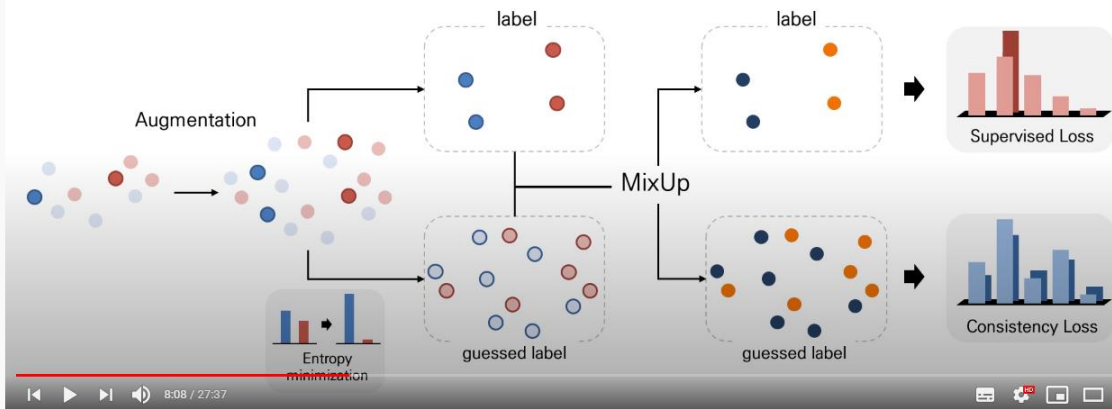
Xie et al. (2019)

- For MixMatch, Remixmatch, and FixMatch, refer to Junghoon Lee's presentations at DSBA seminar

1. Introduction

▪ MixMatch : A Holistic Approach to Semi-Supervised Learning

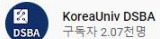
앞서 소개한 SSL 방법론들을 모두 아우르는 새로운 방법론인 MixMatch 제시



[Paper Review] MixMatch: A Holistic Approach to Semi-Supervised Learning

조회수 1,189회 · 2020. 2. 19.

👍 22 🗨 0 ➡ 공유 📌 저장 ...



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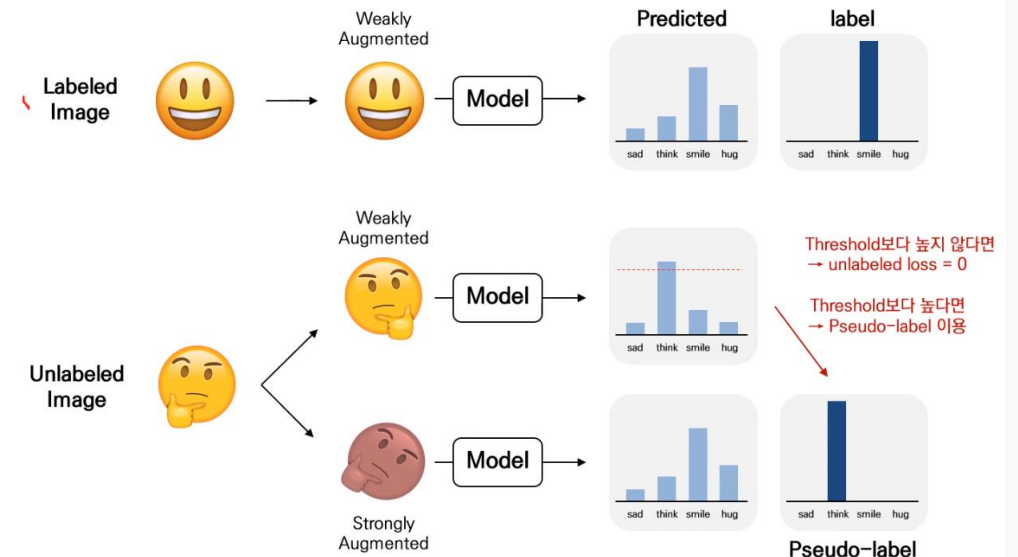
발표자: 이정훈
MixMatch: A Holistic Approach to Semi-Supervised Learning



<https://youtu.be/nSJp7bn2DIU>

3. FixMatch

▪ FixMatch



[Paper Review] ReMixMatch & FixMatch : Consistency-based Semi-supervised Learning Methods

조회수 648회 · 2020. 6. 11.

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발표자: 이정훈
consistency-based semi-supervised learning에서 RandAugment, CTAugment, Augmentation Anchoring, Pseudo-labeling 등의 방법을 도입해 높은 성능을 기록한 논문인 ReMixMatch와 FixMatch 대해 리뷰합니다.

33



<https://youtu.be/mXiPbkyGJ9g>



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Other materials

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