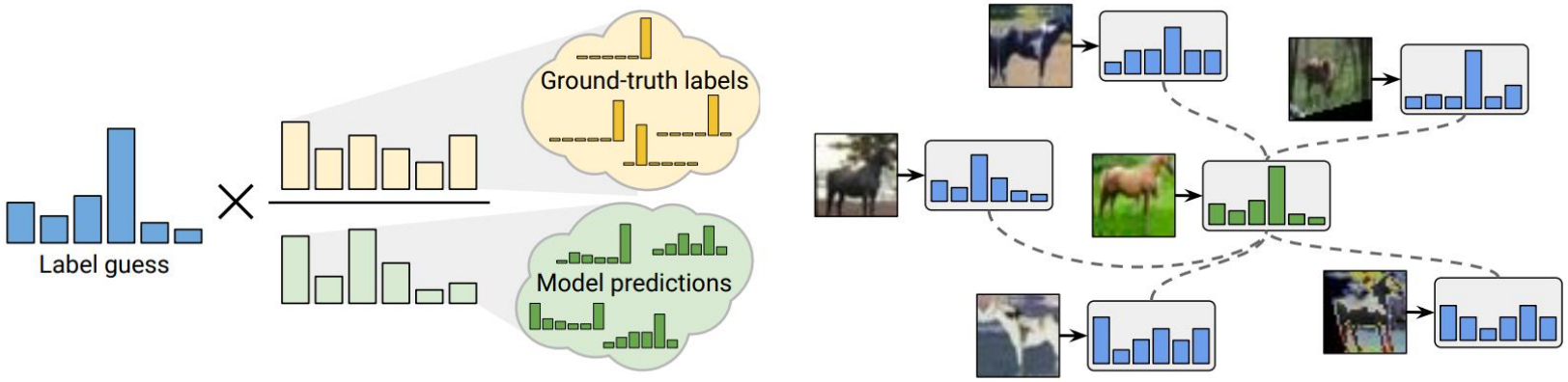
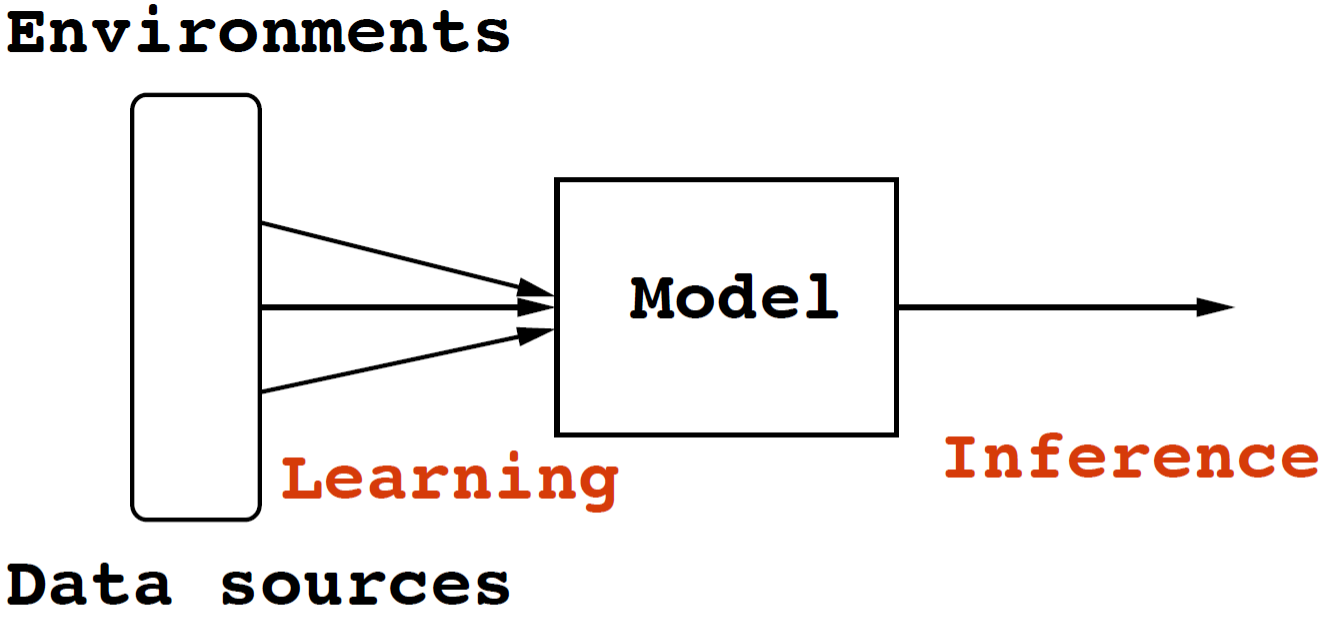


Semi-Supervised Learning: Generative Models

Pilsung Kang
School of Industrial Management Engineering
Korea University

Discriminative vs. Generative

Choi (2015)



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.

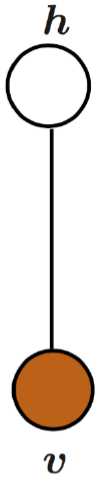
Discriminative vs. Generative

Choi (2015)

Generative model

Discriminative model

Undirected model



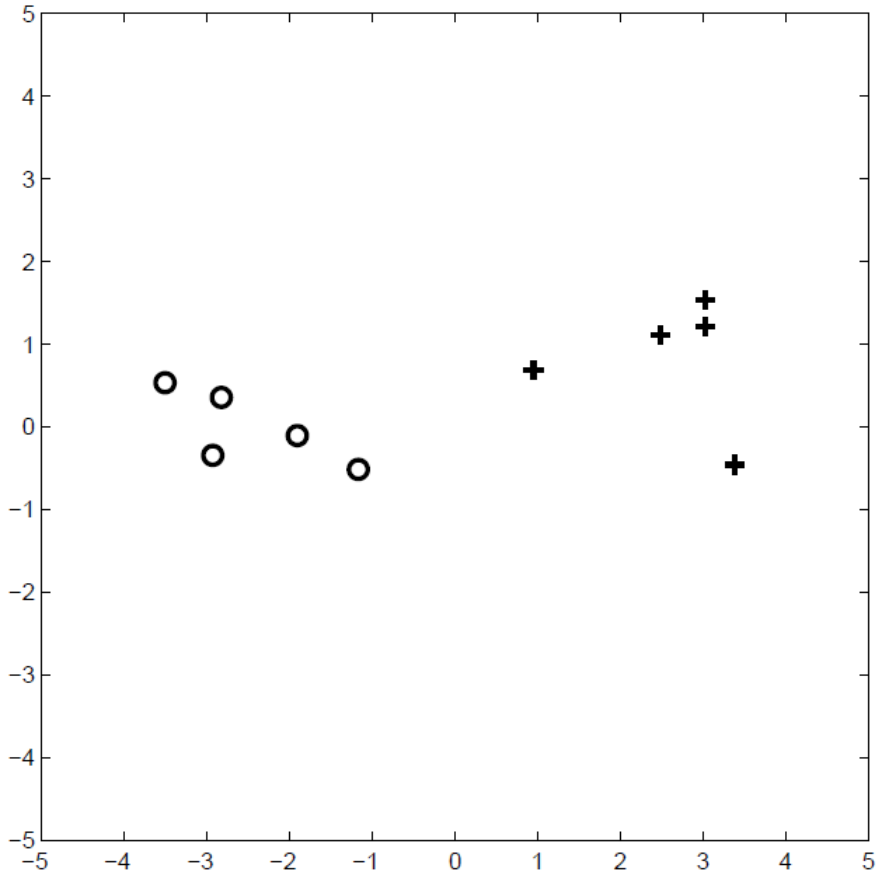
- Generative model: Joint distribution $p(\boldsymbol{v}, \boldsymbol{h}) = p(\boldsymbol{v}|\boldsymbol{h})p(\boldsymbol{h})$
- Discriminative model: Directly model $p(\boldsymbol{h}|\boldsymbol{v})$
- Undirected model: Energy-based model

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

Generative Models

Zhu (2007)

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



$$\text{Model parameters :}$$

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

$$p(x, y|\theta) = p(y|\theta)p(x|y, \theta)$$

$$= w_y \mathcal{N}(x; \mu_y, \Sigma_y)$$

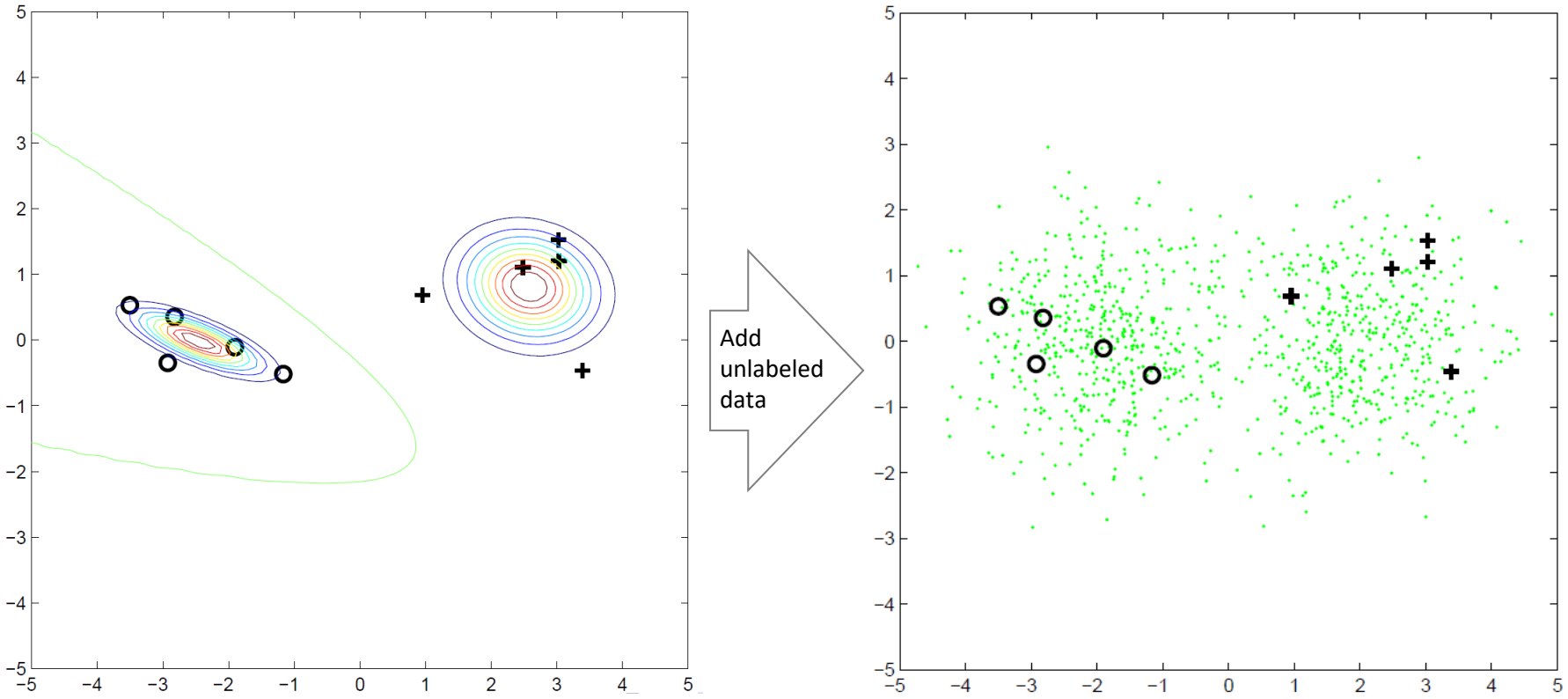
$$\text{Classification :}$$

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

Generative Models

Zhu (2007)

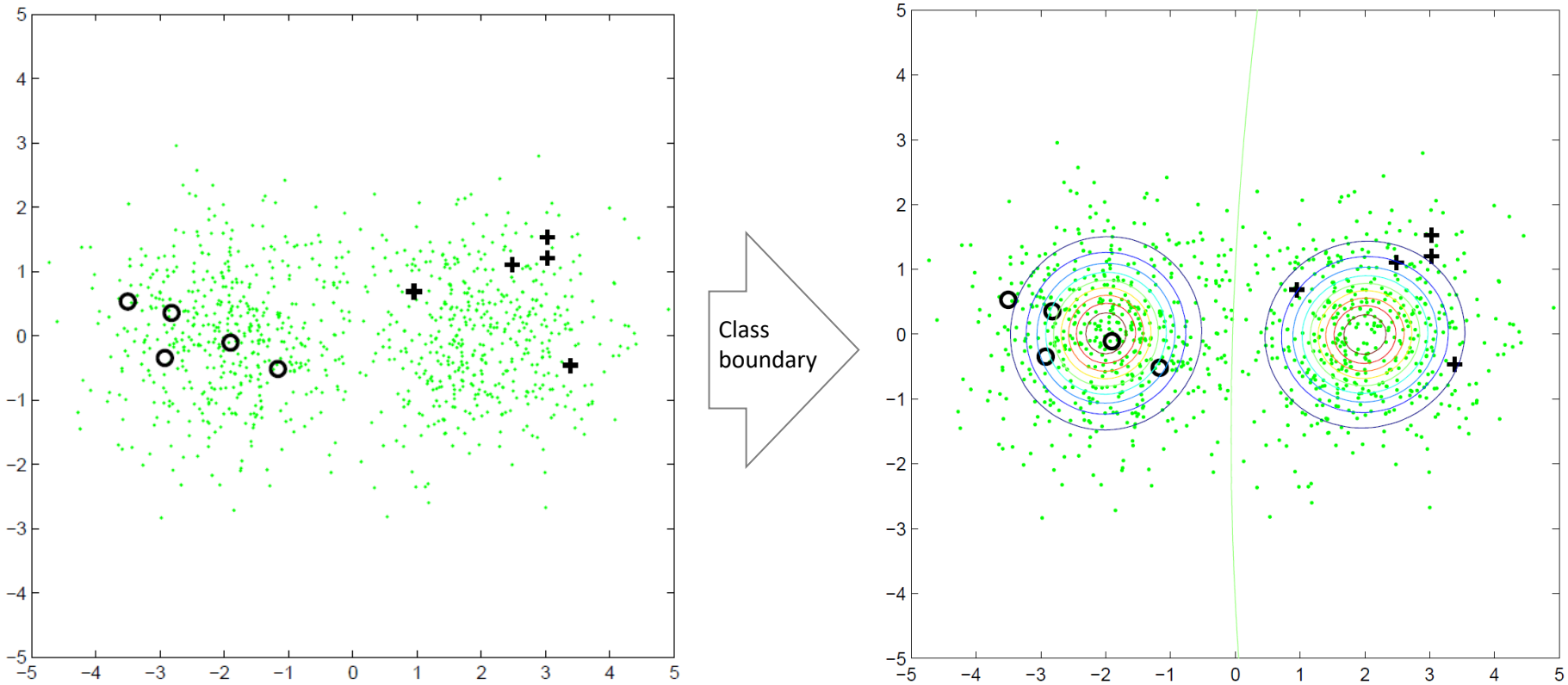
- Example
  - ✓ The most likely model, and its decision boundary:



Generative Models

Zhu (2007)

- Example
  - ✓ The most likely model, and its decision boundary:

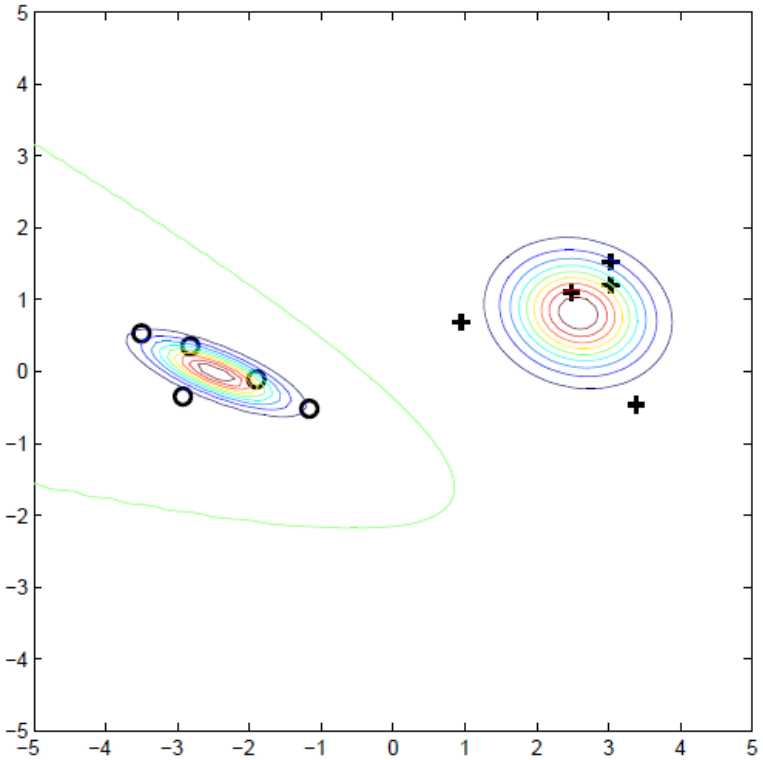


Generative Models

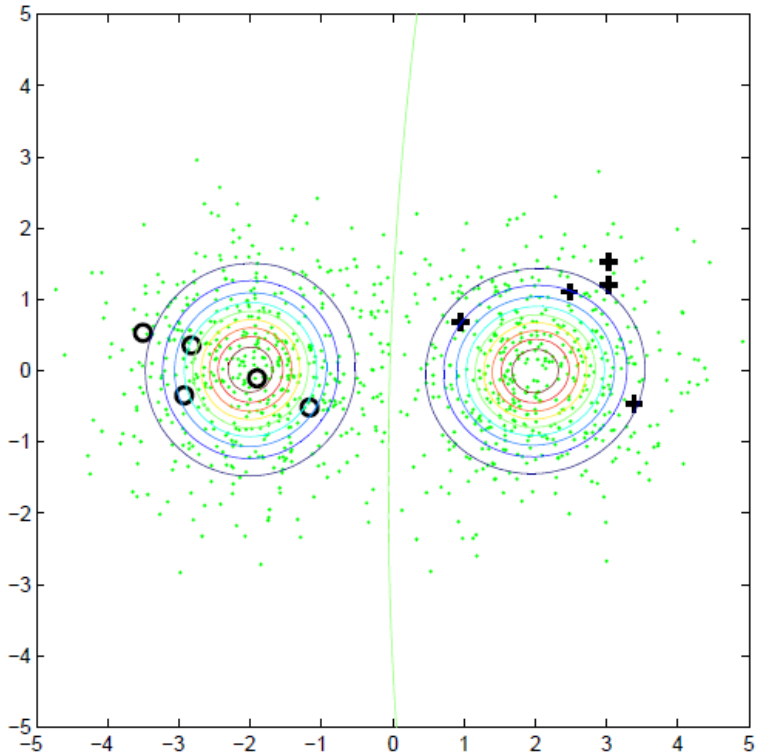
Zhu (2007)

- Example
  - ✓ They are different because they maximize different quantities

$p(X_l, Y_l|\theta)$



$p(X_l, Y_l, X_u|\theta)$



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 is θ 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 **x** with class 1
    - label $p(y = 2|\mathbf{x}, \theta)$-fraction of **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
    - $\sum_c$: 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)

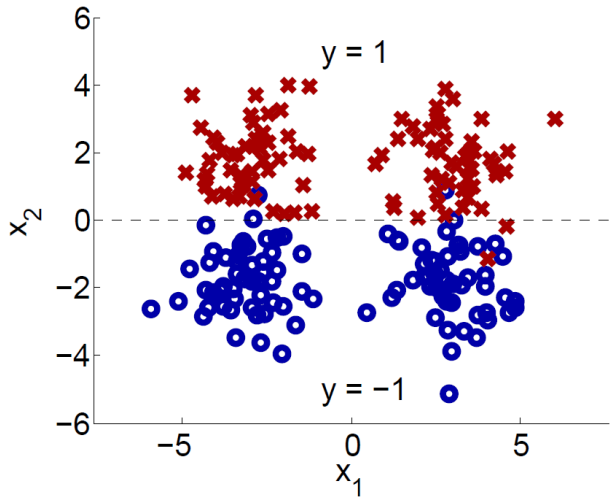
- The EM algorithm in general
  - ✓ Key is to maximize the posterior probability
  - ✓ EM is just one way to maximize it; other ways to find parameters are possible (variational approximation, direct optimization, etc.)

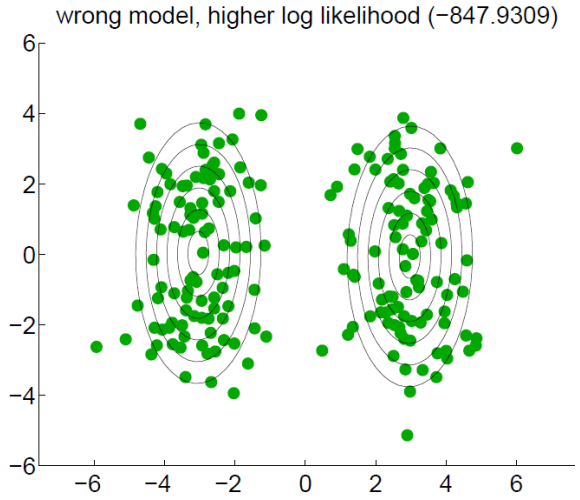
- Advantages
  - ✓ Clear, well-studied probabilistic framework
  - ✓ Can be extremely effective, if the model is close to correct

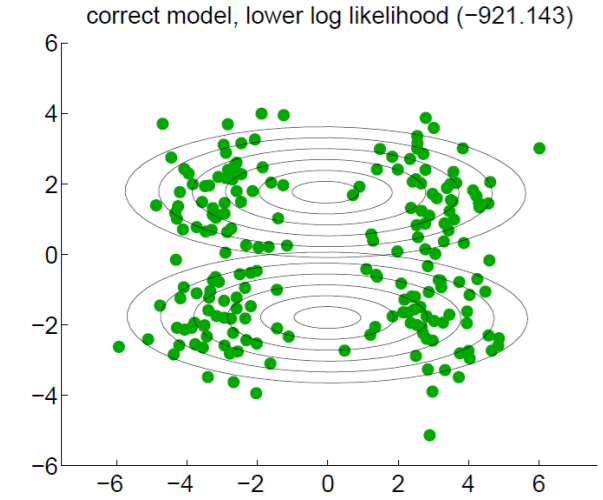
Generative Models: Gaussian Mixture Model

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

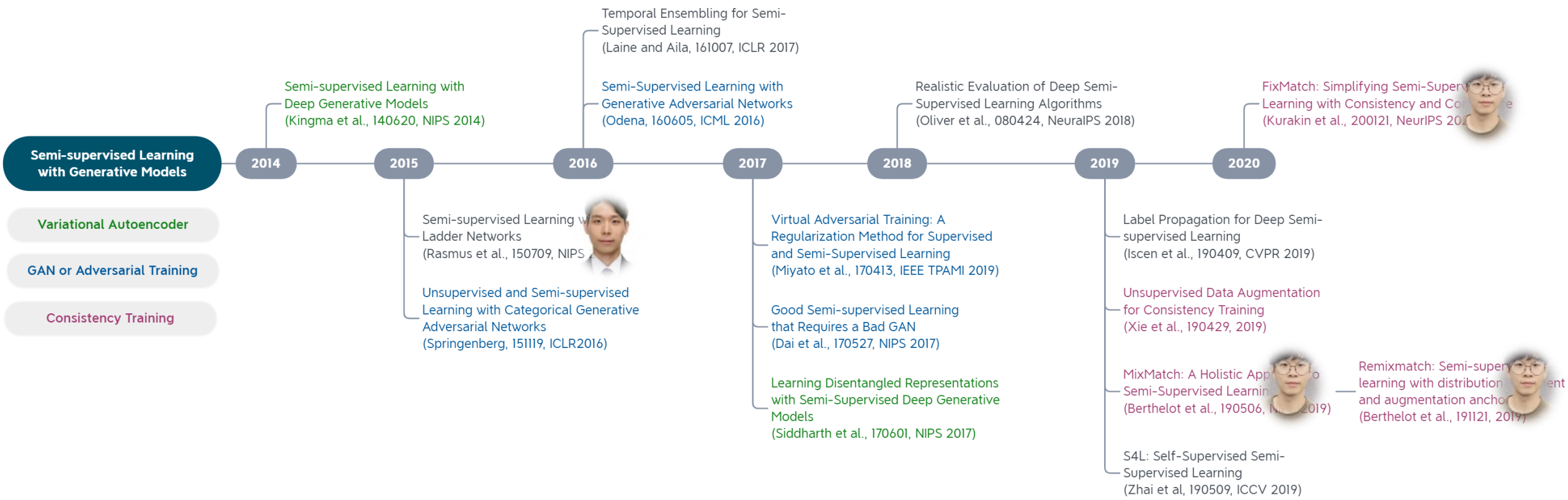






Semi-supervised Learning with Generative Models

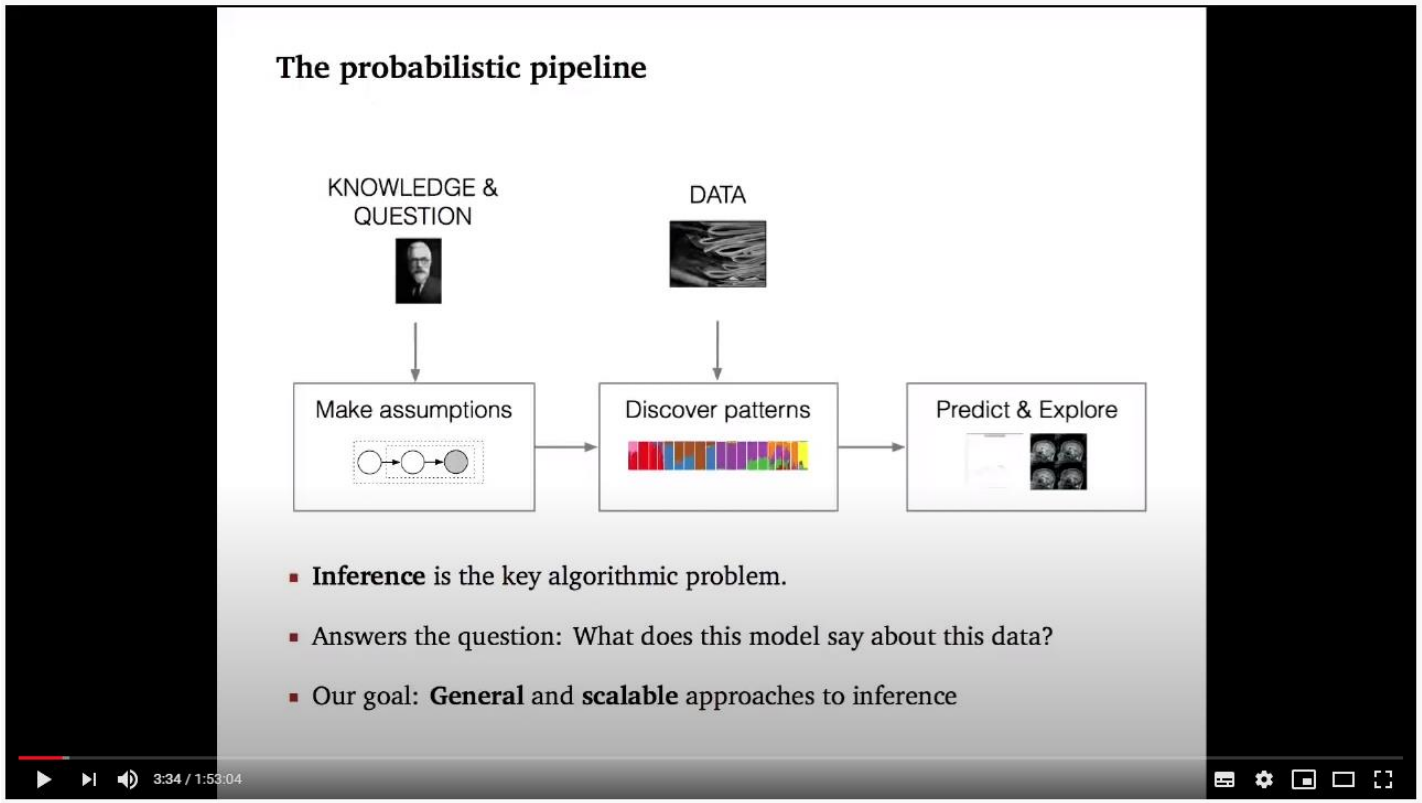
- Recent Advances



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



Deep Generative Models

Kingma et al. (2014)

- Variational Lower Bound
  - ✓ We have some data $\boldsymbol{X}$, a generative probability model $P(\boldsymbol{X}|\theta)$ that shows us how to randomly sample (e.g., generate) data points that follow distribution of $\boldsymbol{X}$, 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 $P(\theta|\boldsymbol{X})$, 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 $P(\boldsymbol{X}|\theta)$
  - ✓ The problem is intractable because of its denominator

Deep Generative Models

Kingma et al. (2014)

- The solution: Approximation
  - ✓ Approximate $P(\theta|\boldsymbol{X})$ by another function $Q(\theta|\boldsymbol{X})$
    - Solving for Q is relatively fast because we can assume a particular shape for $Q(\theta|\boldsymbol{X})$ and turn the inference problem (finding $P(\theta|\boldsymbol{X})$) into an optimization problem (finding Q)
    - $Q(\theta|\boldsymbol{X})$ should be as close as possible to $P(\theta|\boldsymbol{X})$
  - ✓ 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

$$\log p(\mathbf{X}) = -E_q\left[\log \frac{q(\theta|\mathbf{X})}{p(\theta,\mathbf{X})}\right] + D_{KL}(Q||P)$$

$$\log p(\mathbf{X}) \geq -E_q\left[\log \frac{q(\theta|\mathbf{X})}{p(\theta,\mathbf{X})}\right]$$

$$= E_q[\log p(\theta,\mathbf{X}) - \log q(\theta|\mathbf{X})]$$

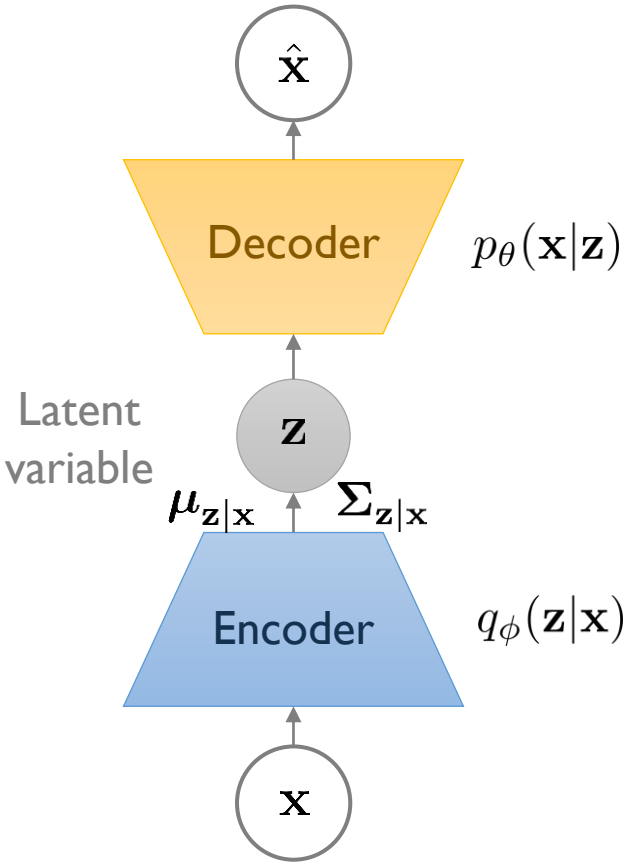
$$= E_q[\log p(\mathbf{X}|\theta) + \log p(\theta) - \log q(\theta|\mathbf{X})]$$

$$= E_q[\text{likelohood} + \text{prior} - \text{approx.posterior}]$$

Deep Generative Models

Kingma et al. (2014)

- A Vanilla VAE for Semi-supervised Learning (M1 Model)
  - ✓ Phase 1: train a variational auto-encoder (VAE) based on both labeled and unlabeled data



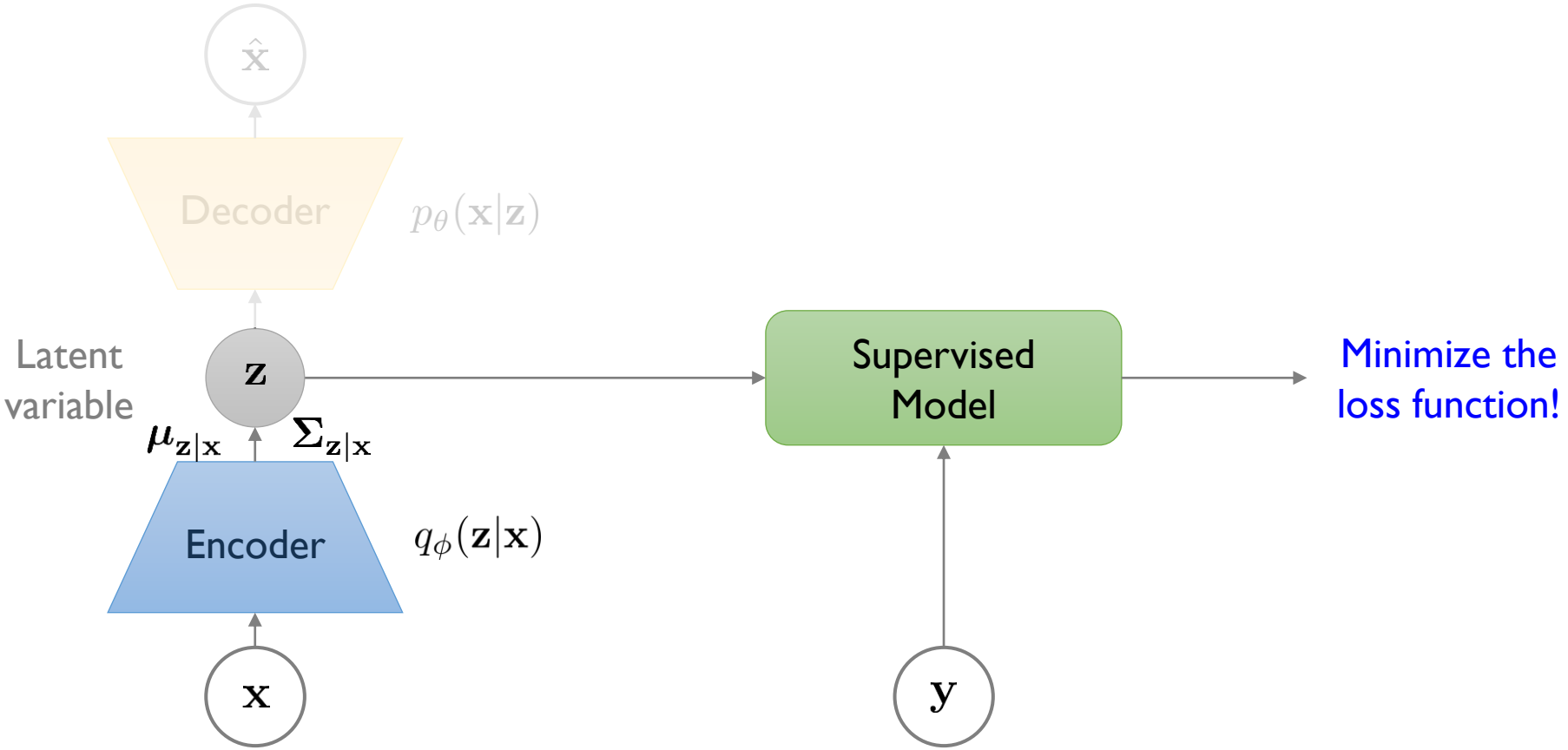
Variational Bound

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}|\mathbf{z})\right] - D_{KL}\left[q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})\right]$$

Deep Generative Models

Kingma et al. (2014)

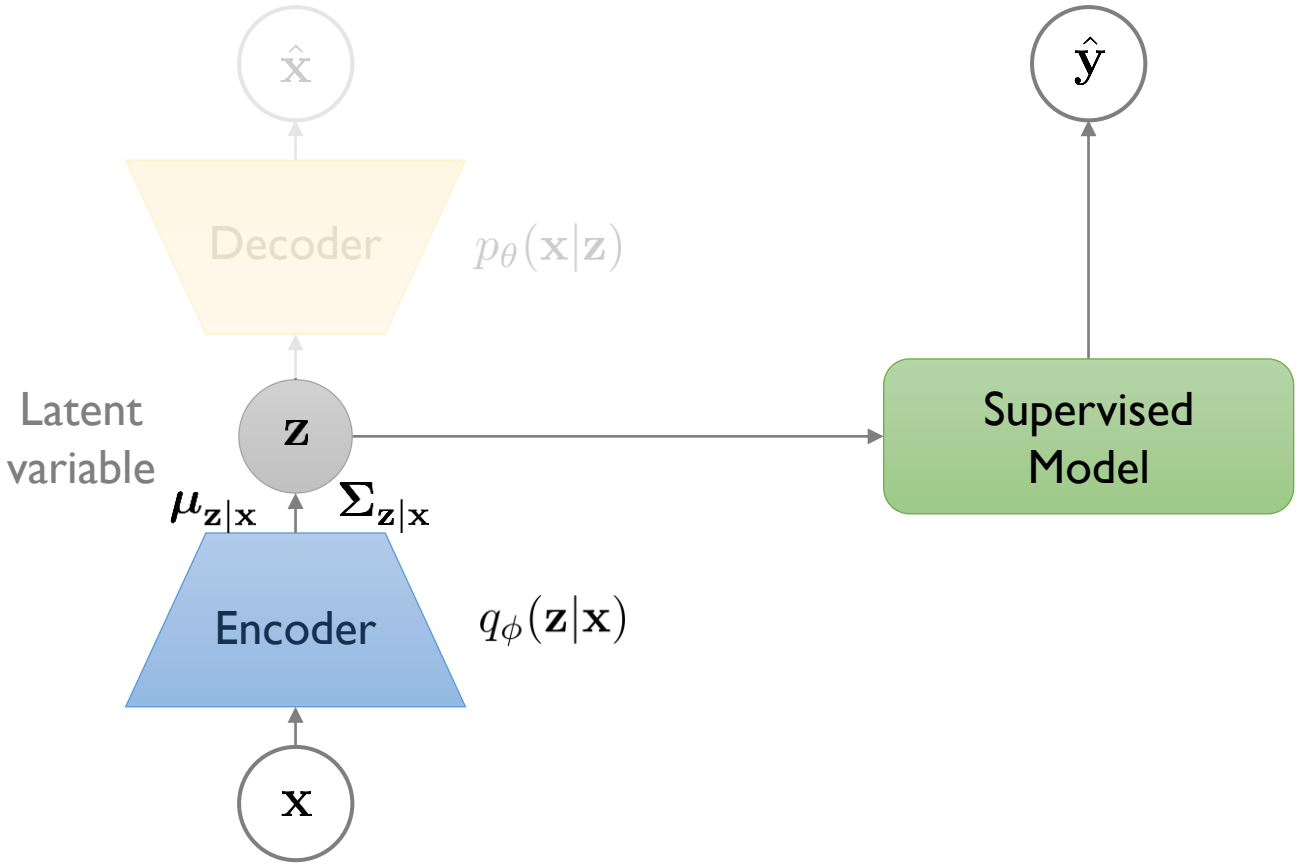
- A Vanilla VAE for Semi-supervised Learning (M1 Model)
  - ✓ Phase 2: Solve a standard supervised learning problem on the labeled data using $(\mathbf{Z}, \mathbf{y})$ pairs



Deep Generative Models

Kingma et al. (2014)

- A Vanilla VAE for Semi-supervised Learning (M1 Model)
  - ✓ Phase 3: Inference for unlabeled data or new test data

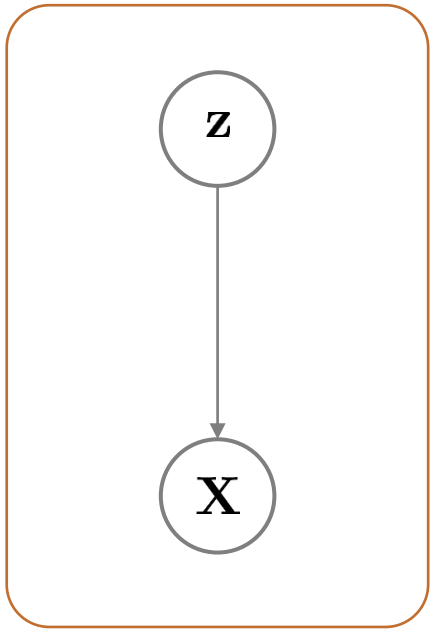


Deep Generative Models

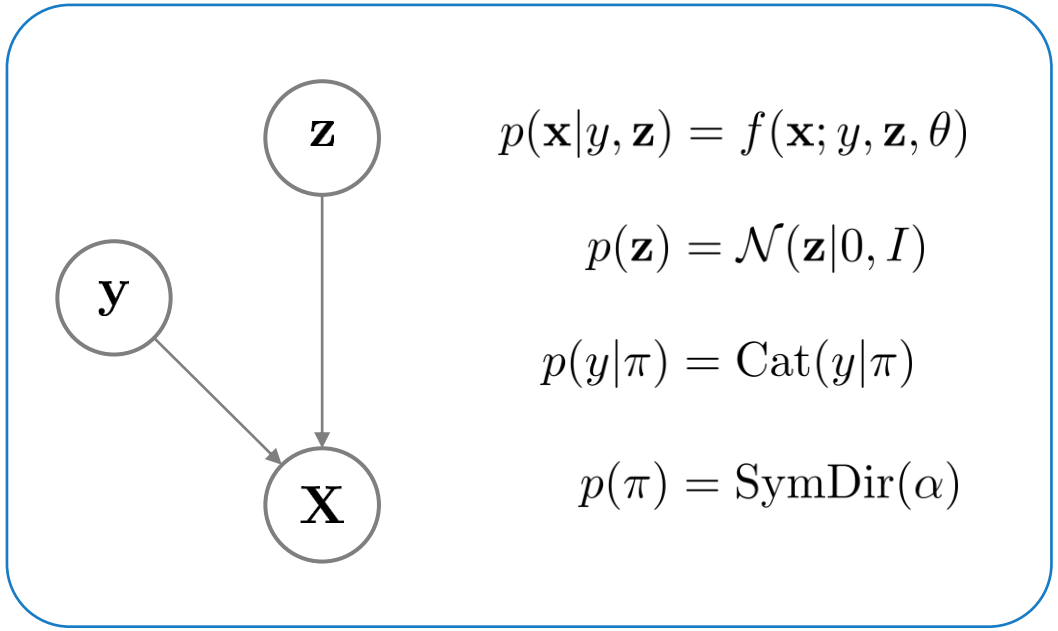
Kingma et al. (2014)

- 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



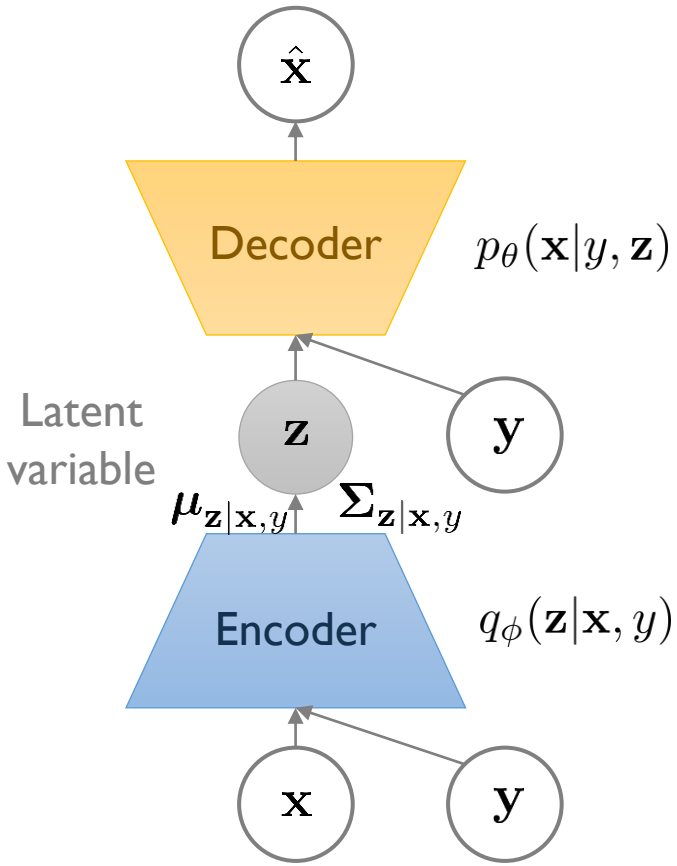
M2 Model



Deep Generative Models

Kingma et al. (2014)

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



Variational Bound for labeled data

$$\log p_\theta(\mathbf{x},y) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x},y)}\left[\log p_\theta(\mathbf{x}|y,\mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x},y)\right]$$

Variational Bound for unlabeled data

$$\log p_\theta(\mathbf{x},y) \geq \mathbb{E}_{q_\phi(y,\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}|y,\mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi(y,\mathbf{z}|\mathbf{x})\right]$$

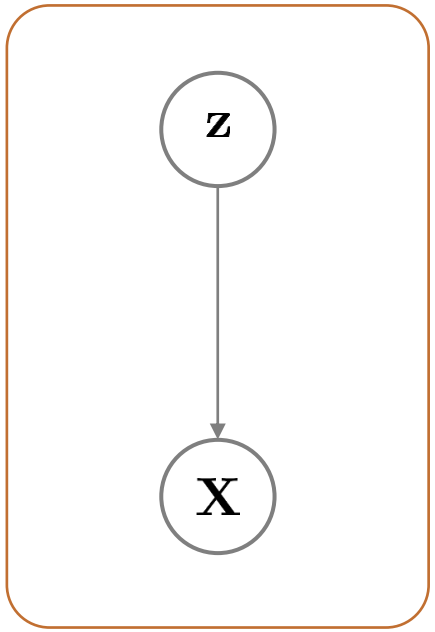
Deep Generative Models

Kingma et al. (2014)

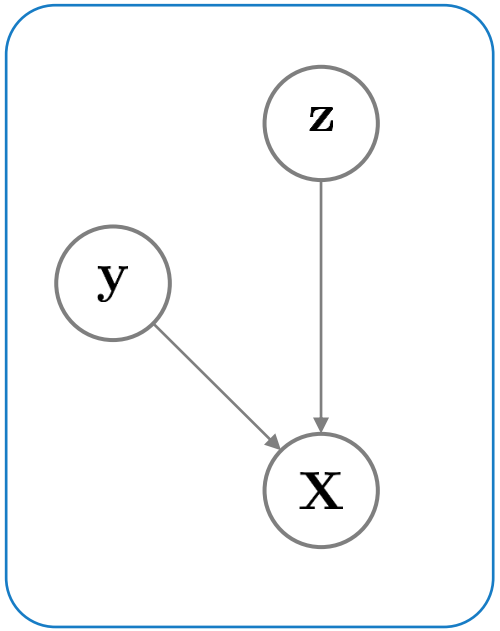
- Stack of M1 and M2
  - ✓ Train generative semi-supervised model (M2) on unsupervised features z_1 from latent feature model (M1)

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

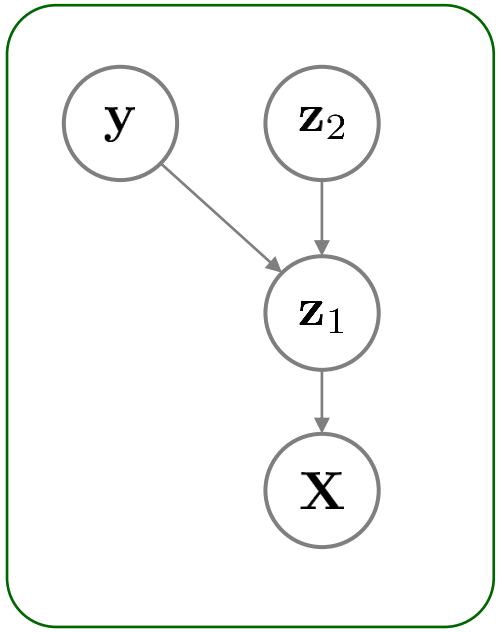
M1 Model



M2 Model



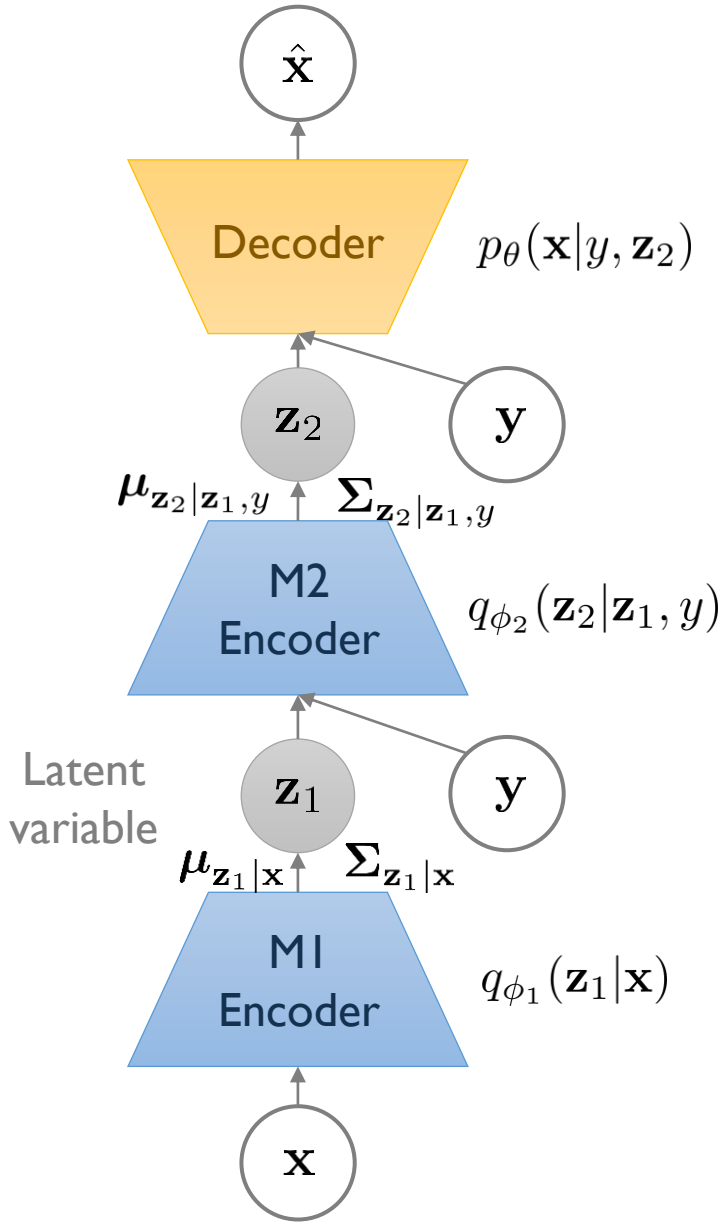
M1+M2 Model



Deep Generative Models

Kingma et al. (2014)

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



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
PCA + SVM	0.692	0.871	0.891	0.911	0.929
CNN	0.262	0.921	0.934	0.955	0.978
M1	0.628	0.885	0.905	0.921	0.933
M2	•	•	0.975	•	•

Table 1: MNIST Results

Model	N=1000	N=2000	N=5000	N=10000	N=25000
CNN	0.433	0.4844	0.610	0.673	0.767
Inception	0.661	0.684	0.728	0.751	0.773
PCA + SVM	0.356	0.384	0.420	0.446	0.482
M1	0.321	0.362	0.375	0.389	0.409
M2	0.420	•	•	•	•

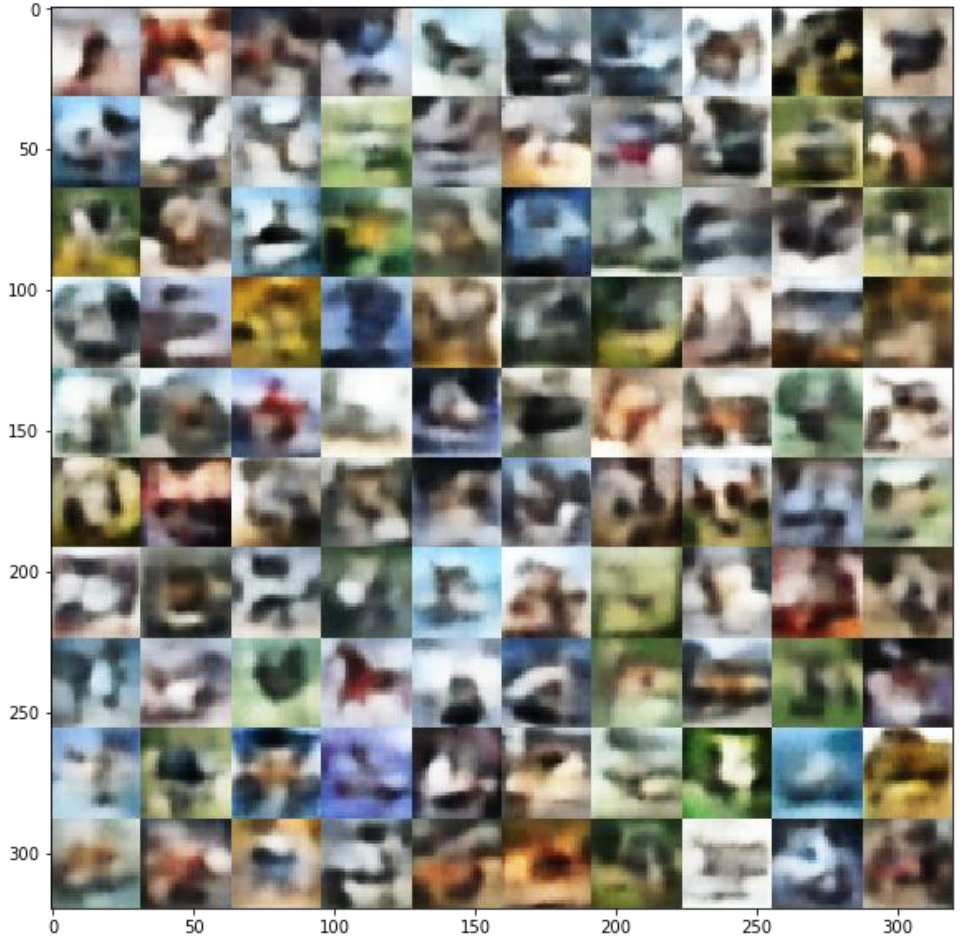
Table 2: CIFAR10 Results

Deep Generative Models

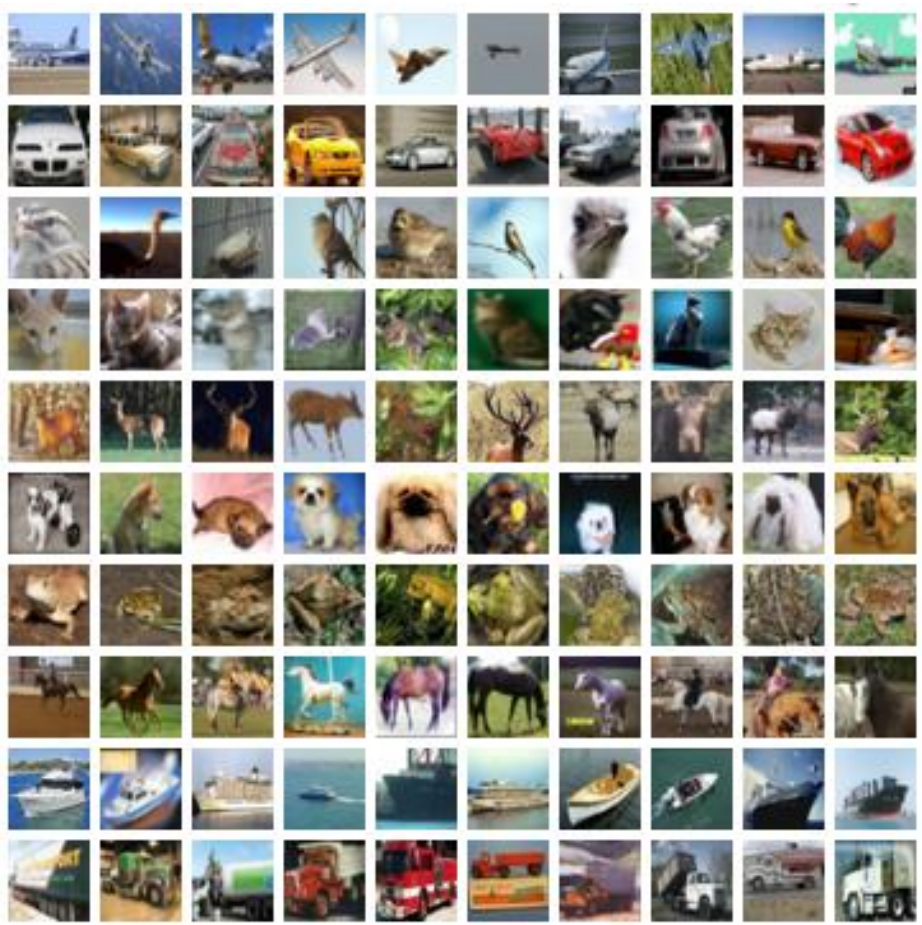
Kingma et al. (2014)

- Images generated from M2 VAE model trained on CIFAR data

Generated images



Original images



Unsupervised Data Augmentation for Consistency Training

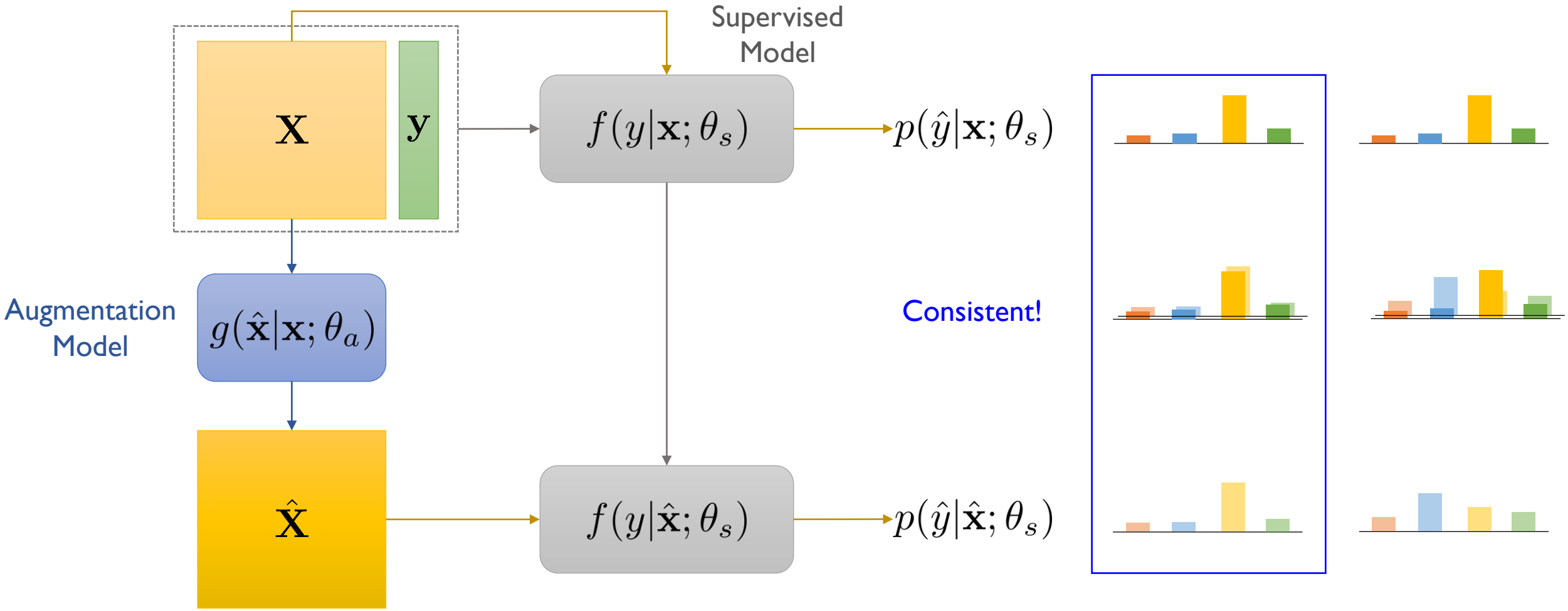
Xie et al. (2019)

- 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

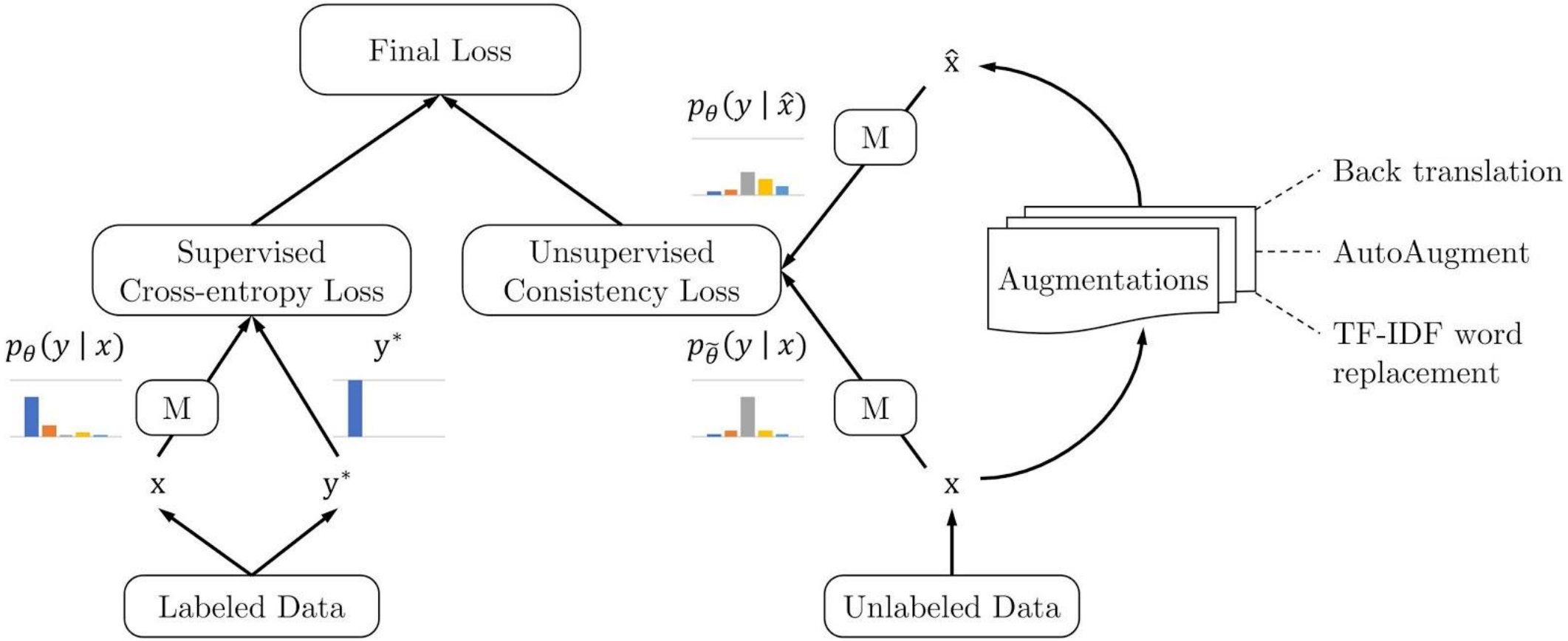
- Consistency Training



Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

- UDA at a glance

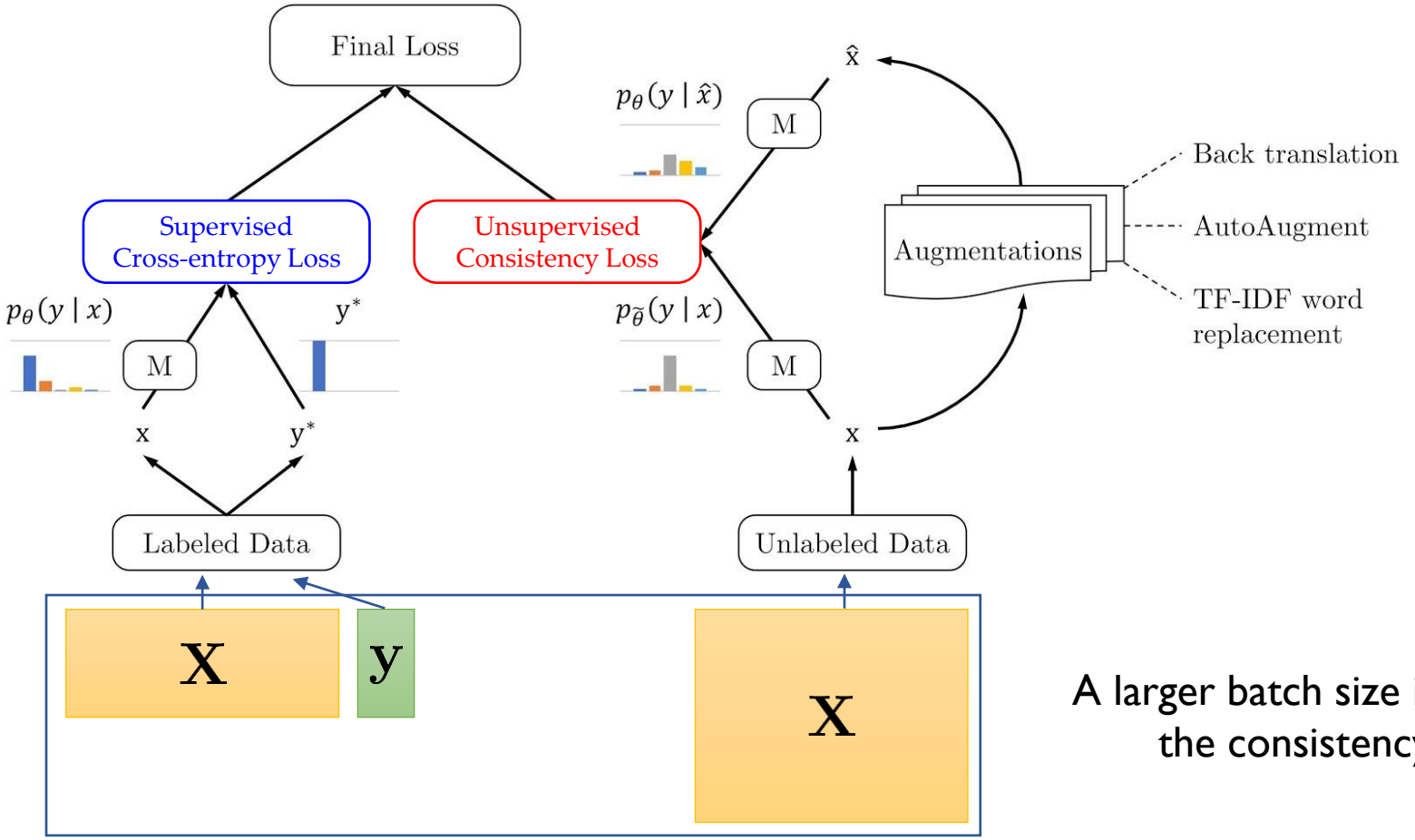


Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)

- Training Objective

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

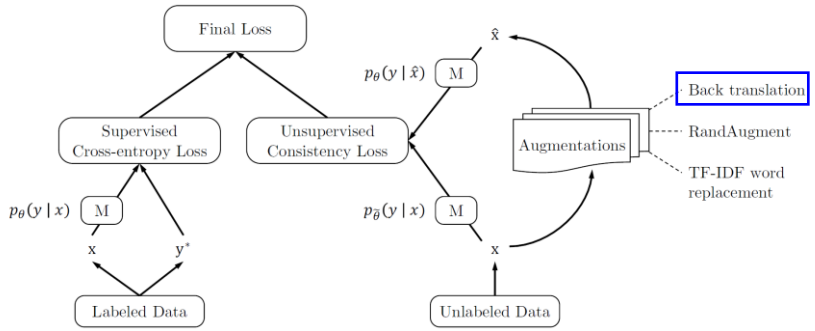


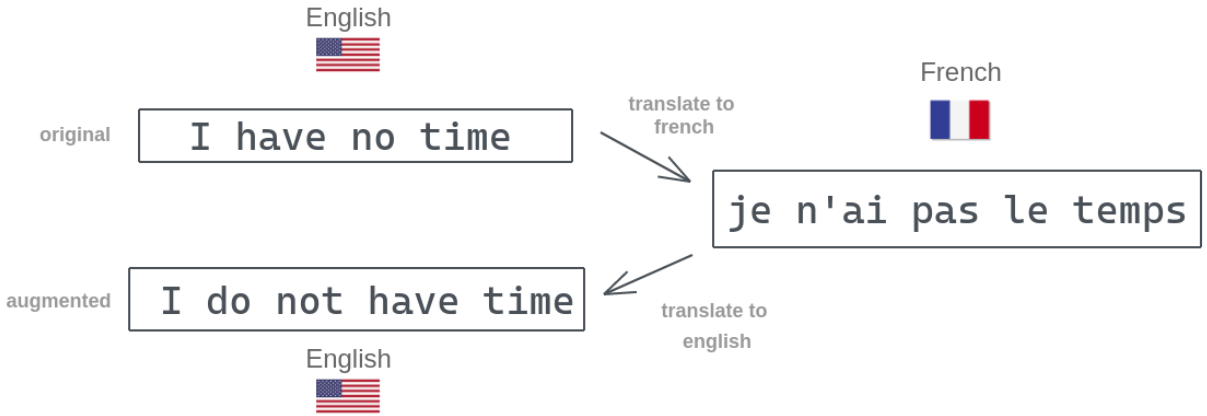
A larger batch size is used for the consistency loss

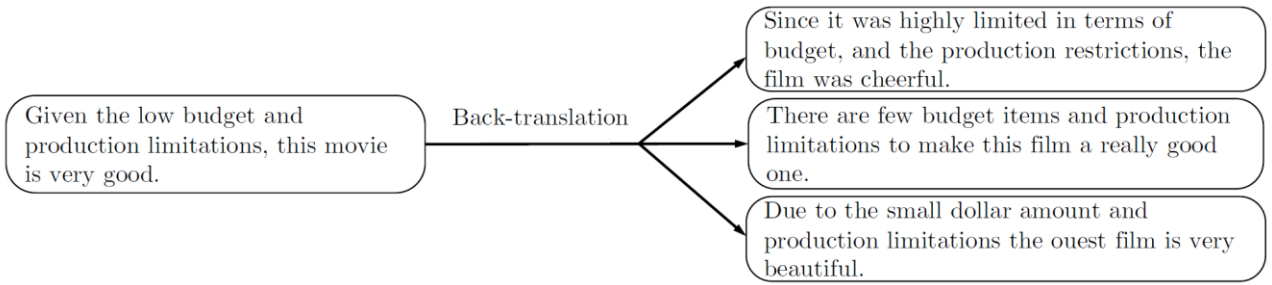
Unsupervised Data Augmentation for Consistency Training

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



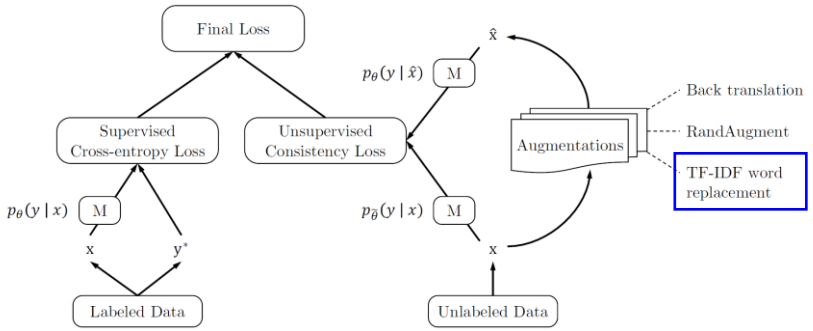




https://amitness.com/2020/02/back-translation-in-google-sheets/

Unsupervised Data Augmentation for Consistency Training

Xie et al. (2019)



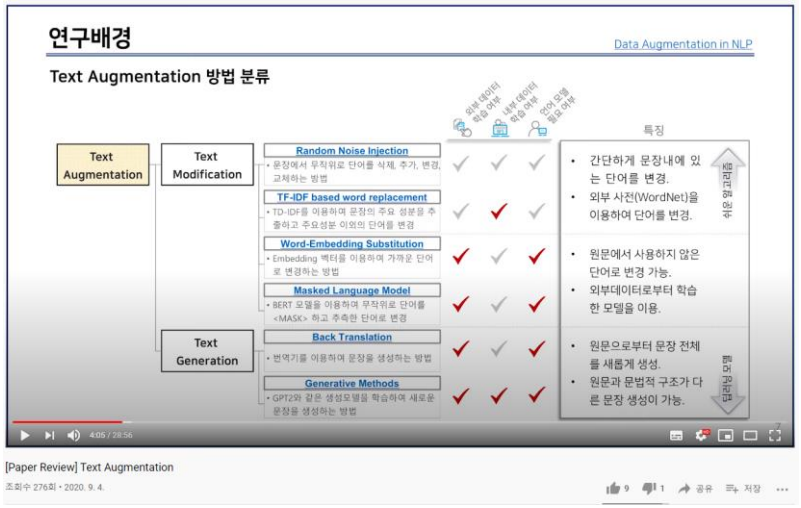
- Augmentation Methods
  - ✓ Word replacing with TF-IDF for Text Classification
    - Replaces uninformative words with low TF-IDF scores
    - While keeping those with high TF-IDF values

This virus has spread worldwide

↓

A virus has spread worldwide

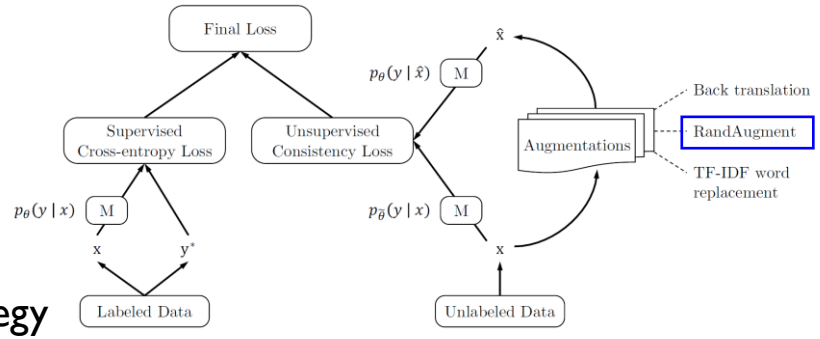
- For more text augmentation methods, refer to Junghee Kim's presentation at DSBA seminar



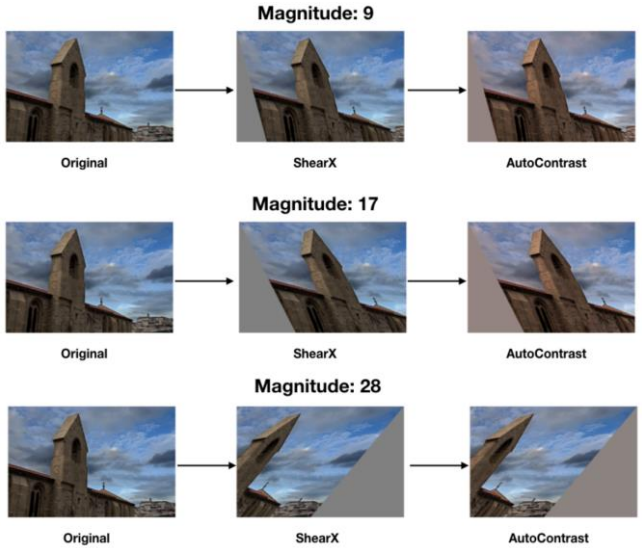
https://youtu.be/UVtMqh3agQY

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 nood 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)

- Performance

Image Classification

Method	Model	# Param	CIFAR-10 (4k)	SVHN (1k)
Π-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**	-

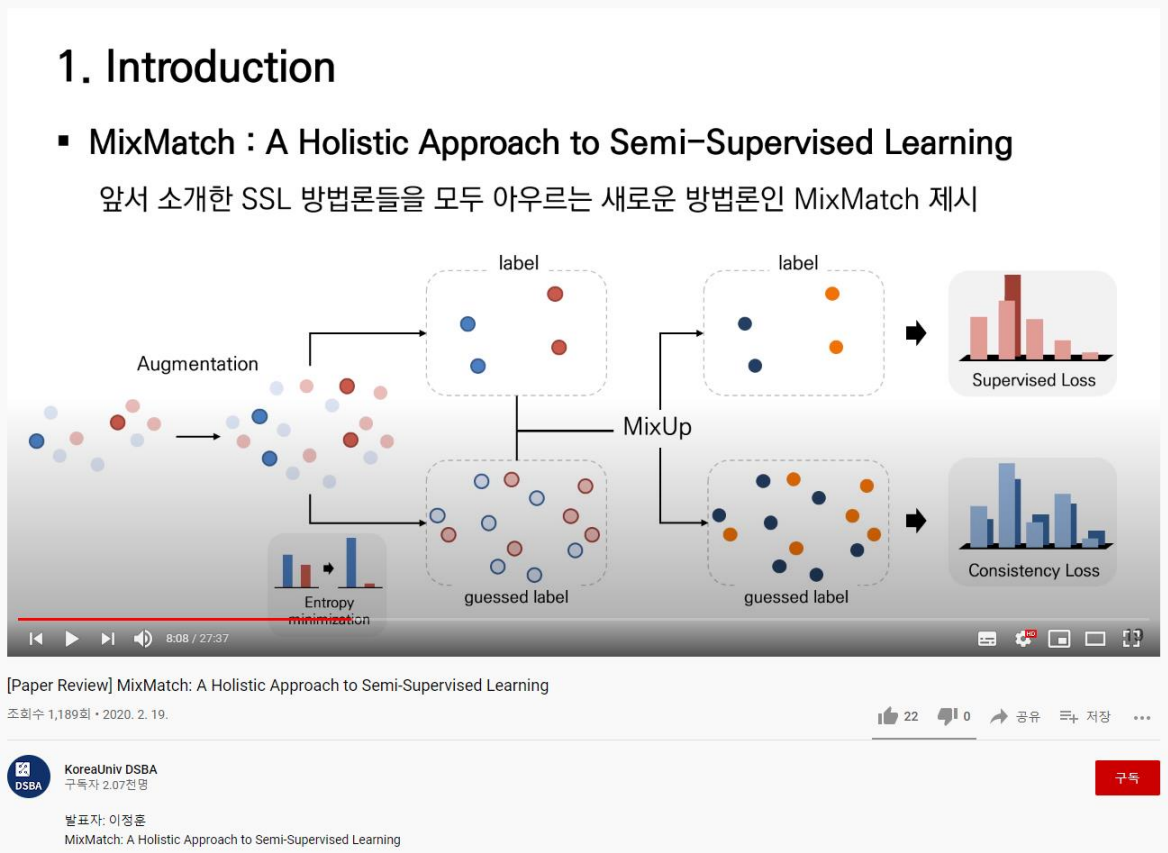
Text Classification

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
$\text{BERT}_{\text{LARGE}}$		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
$\text{BERT}_{\text{BASE}}$	✗	18.40	13.60	41.00	26.75	44.09	2.58
	✓	5.45	2.61	33.80	3.96	38.40	1.33
$\text{BERT}_{\text{LARGE}}$	✗	11.72	10.55	38.90	15.54	42.30	1.68
	✓	4.78	2.50	33.54	3.93	37.80	1.09
$\text{BERT}_{\text{FINETUNE}}$	✗	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



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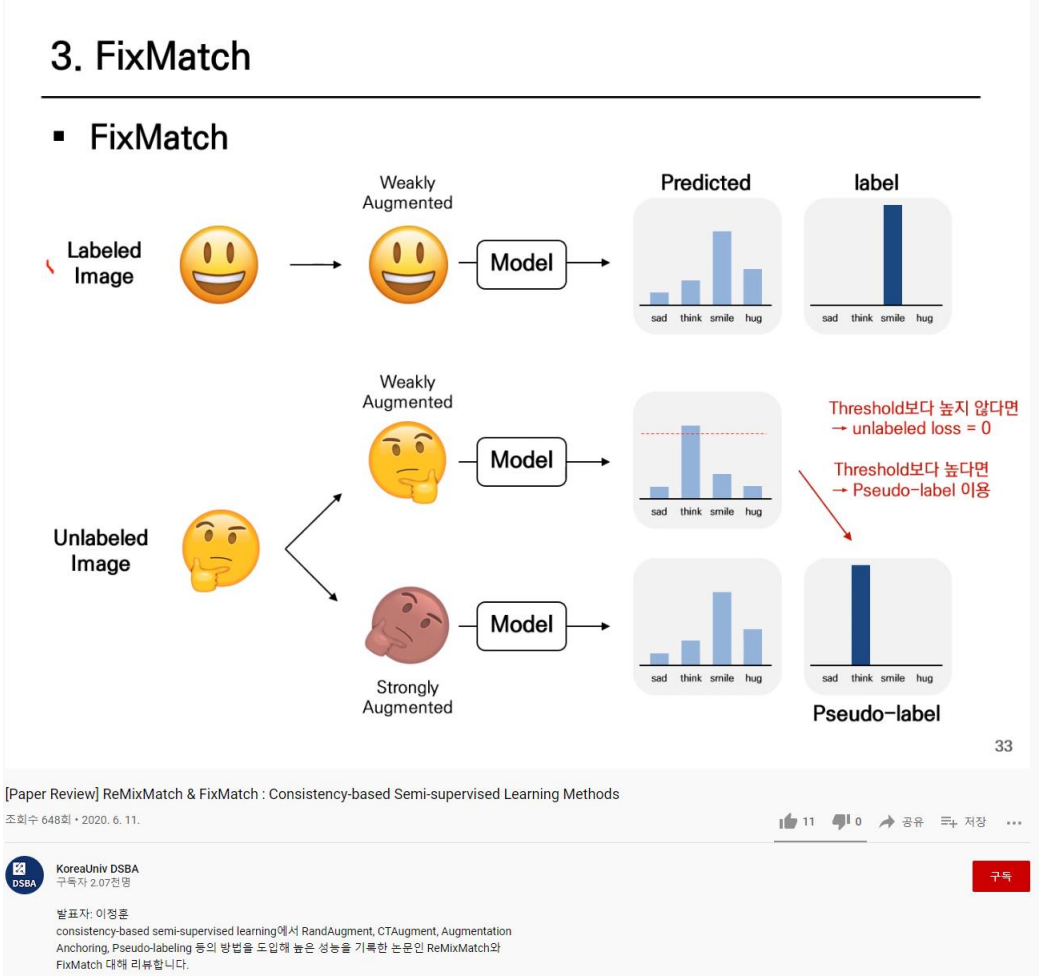

https://youtu.be/mXiPbkyGJ9g


Q & A

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References

Other materials

- Figures in the first page: 하상욱 단편시집 – 서울 시
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