

| Deep Bayesian Active Learning with Image Data |

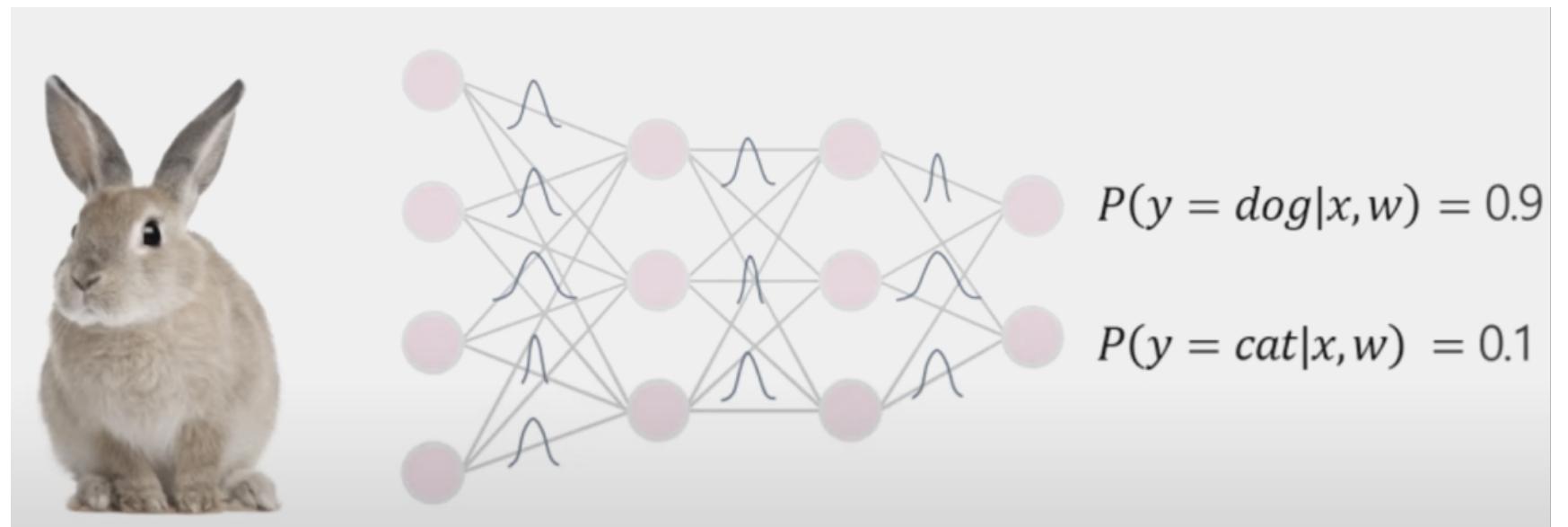
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2022.05.16

Uncertainty

- Over-confidence 문제
- Uncertainty 정량화 필요성
- Distribution의 variance



Bayesian Neural Network(BNN)

- 저자는 또 다른 논문에서 posterior를 추정을 MC dropout과 L2 regularization로 쉽게 구할 수 있음을 증명함.
- Prior distribution은 보통 Gaussian으로 둠(mean=0,variance=1).
- 최종적인 값은 여러 예측 값의 평균
- Uncertainty는 variance

$$p(W|X, Y) = \frac{p(Y|X, W)p(w)}{p(Y|X)}$$

Posterior Likelihood Prior
Evidence

$$p(Y|X) = \int p(Y|X, W)p(W)dW$$

Evidence

$$p(y = c|x, \omega) = \text{softmax}(\mathbf{f}^\omega(\mathbf{x}))$$

$$\text{ELBO} = \int q_\theta(\mathbf{w}) \log p(\mathbf{Y}|\mathbf{X}, \mathbf{w}) d\mathbf{w} - \text{KL}(q_\theta(\mathbf{w}) || p(\mathbf{w}))$$

$$\text{Minimize} -\frac{1}{M} \sum_{i \in S} \ln(p(y_i | f^{g(\theta, \hat{\epsilon})}(x_i))) + \lambda_1 \|M_1\|^2 + \lambda_2 \|M_2\|^2 + \lambda_3 \|b\|^2$$

$$\mathbb{E}[\mathbf{y}^*] \approx \frac{1}{T} \sum_{t=1}^T \hat{\mathbf{y}}_t^*(\mathbf{x}^*)$$

$$\text{Var}[\mathbf{y}^*] \approx \tau^{-1} \mathbf{I}_D + \frac{1}{T} \sum_{t=1}^T \hat{\mathbf{y}}_t^*(\mathbf{x}^*)^T \hat{\mathbf{y}}_t^*(\mathbf{x}^*) - \mathbb{E}[\mathbf{y}^*]^T \mathbb{E}[\mathbf{y}^*].$$

Bayesian Neural Network(BNN)

- Deterministic Neural Network vs. Bayesian Neural Network

Neural Network

Training:

$$\theta^* = \arg \max_{\theta} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}_{\text{tr}}} \log[p(y_i | \mathbf{x}_i, \theta)]$$

Likelihood

$$\theta^* = \arg \min_{\theta} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}_{\text{tr}}} \mathcal{L}(F_{\theta}(\mathbf{x}_i), y_i)$$

Prediction:

$$p(\hat{y} | \hat{\mathbf{x}}, \theta^*)$$

$$\hat{y} = F_{\theta^*}(\hat{\mathbf{x}})$$

Bayesian Neural Network

Training:

$$\mu^*, \Sigma^* = \arg \max_{\mu, \Sigma} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}_{\text{tr}}} \log[p(y_i | \mathbf{x}_i, \theta)] - \text{KL}[p(\theta), p(\theta_0)]$$

$$\theta \sim \mathcal{N}(\mu, \Sigma) \quad \theta_0 \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\mu^*, \Sigma^* = \arg \min_{\mu, \Sigma} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}_{\text{tr}}} \mathcal{L}(F_{\theta}(\mathbf{x}_i), y_i) + \text{KL}[p(\theta), p(\theta_0)]$$

Regularization

Prediction:

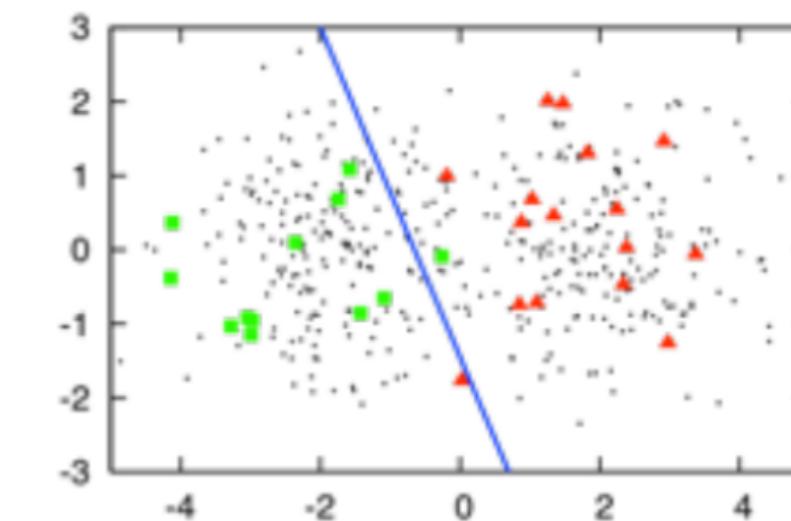
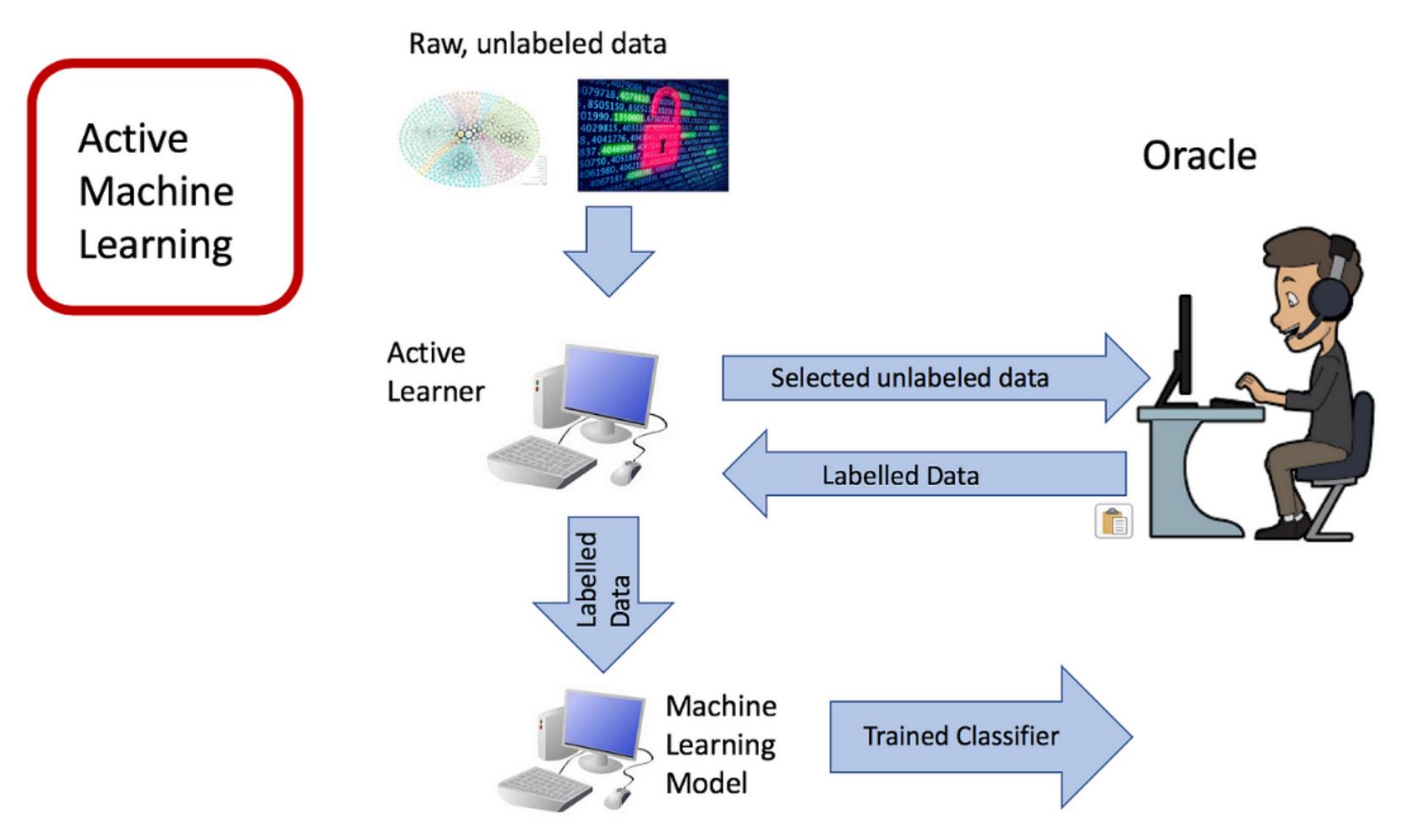
$$p(\hat{y} | \hat{\mathbf{x}}, \mathcal{D}_{\text{tr}}) = \int p(\hat{y} | \hat{\mathbf{x}}, \theta^*) p(\theta^* | \mathcal{D}_{\text{tr}}) d\theta^*$$

$$\theta^* \sim \mathcal{N}(\mu^*, \Sigma^*)$$

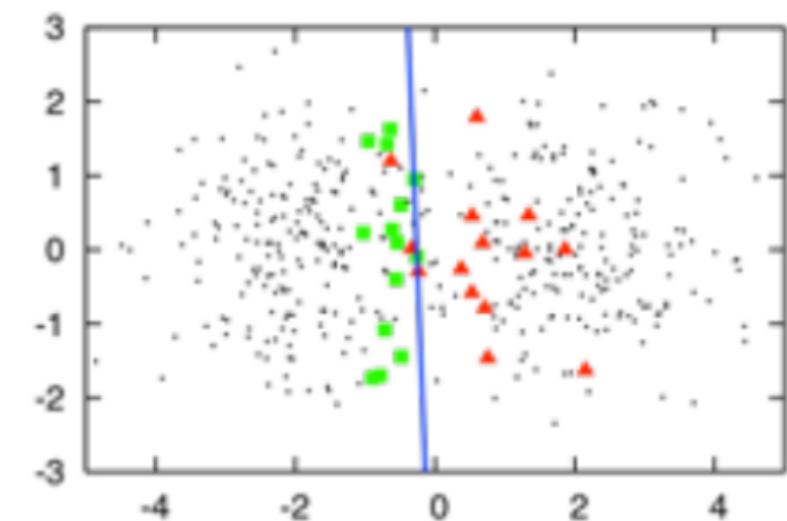
$$\hat{y} = \frac{1}{K} \sum_{k=1}^K F_{\theta_k^*}(\hat{\mathbf{x}}) \quad \theta_k^* \sim \mathcal{N}(\mu^*, \Sigma^*)$$

Active Learning

- 사람이 모두 라벨링하는 기존의 Passive Learning과 다름
- 모델은 Labeling할 데이터를 제시 (Enrich해줄 수 있는 데이터)
- 하지만, AutoLabeling과 달리 마지막엔 사람이 labeling



random sampling
30 labeled instances
(accuracy=0.7)



active learning
30 labeled instances
(accuracy=0.9)

Active Learning with BNN

- 선행 연구들은 저차원 데이터, kernel method만 대부분 사용하여 Active learning
- 그러나 이 경우엔 고차원 데이터를 다루지 못함.
- 본 논문에서는 BNN을 활용하여 이미지 데이터를 다룸.
- Acquisition Function
 - Variantion Ratios
 - Max Entropy
 - BALD
 - Mean STD

$$x^* = \operatorname{argmax}_{x \in \mathcal{D}_{\text{pool}}} a(x, \mathcal{M}).$$

$$\text{variation-ratio}[\mathbf{x}] := 1 - \max_y p(y|\mathbf{x}, \mathcal{D}_{\text{train}})$$

$$\mathbb{H}[y|\mathbf{x}, \mathcal{D}_{\text{train}}] :=$$

$$-\sum_c p(y=c|\mathbf{x}, \mathcal{D}_{\text{train}}) \log p(y=c|\mathbf{x}, \mathcal{D}_{\text{train}}).$$

$$\mathbb{I}[y, \boldsymbol{\omega}|\mathbf{x}, \mathcal{D}_{\text{train}}] = \mathbb{H}[y|\mathbf{x}, \mathcal{D}_{\text{train}}] - \mathbb{E}_{p(\boldsymbol{\omega}|\mathcal{D}_{\text{train}})} [\mathbb{H}[y|\mathbf{x}, \boldsymbol{\omega}]]$$

$$\sigma_c = \sqrt{\mathbb{E}_{q(\boldsymbol{\omega})}[p(y=c|\mathbf{x}, \boldsymbol{\omega})^2] - \mathbb{E}_{q(\boldsymbol{\omega})}[p(y=c|\mathbf{x}, \boldsymbol{\omega})]^2}$$

$$\sigma(\mathbf{x}) = \frac{1}{C} \sum_c \sigma_c$$

Experiments(MNIST)

- convolution-reluconvolution-relu-max pooling-dropout-dense-relu-dropoutdense-softmax
- 32 convolution kernels, 4x4 kernel size, 2x2 pooling, dense layer with 128 units, dropout probabilities 0.25 and 0.5
- acquisition until 1000
- Comparison to semi-supervised learning

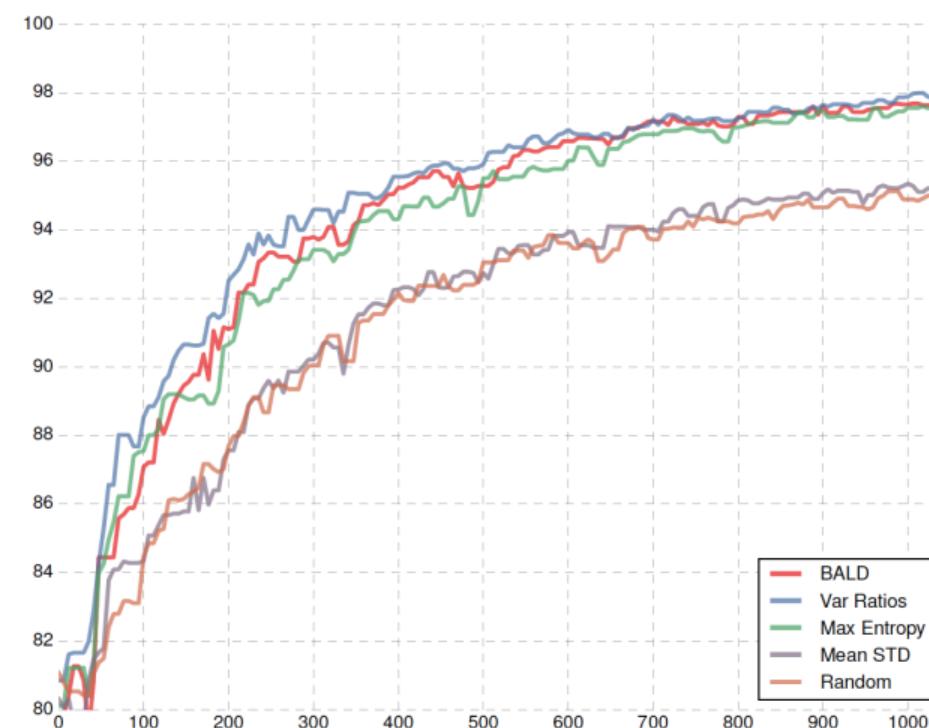
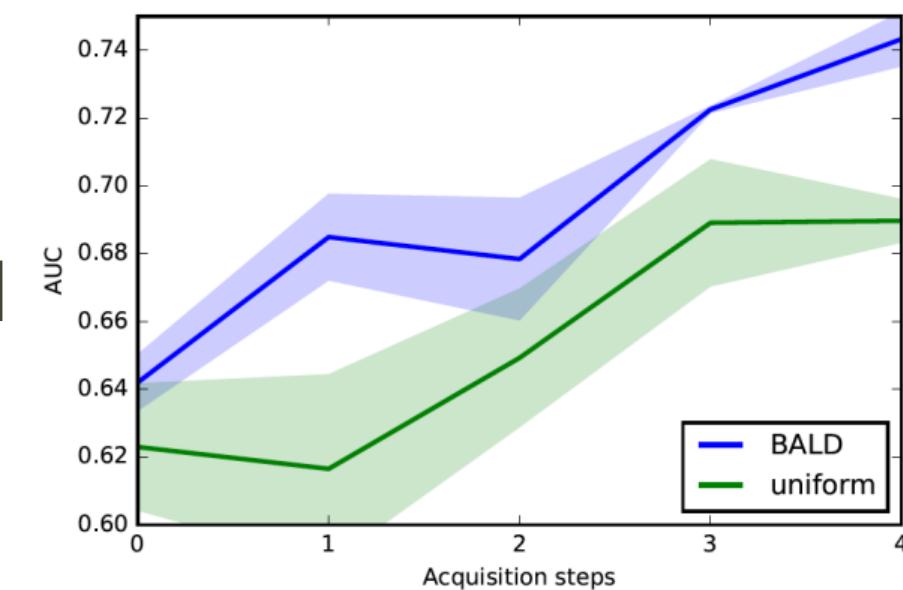
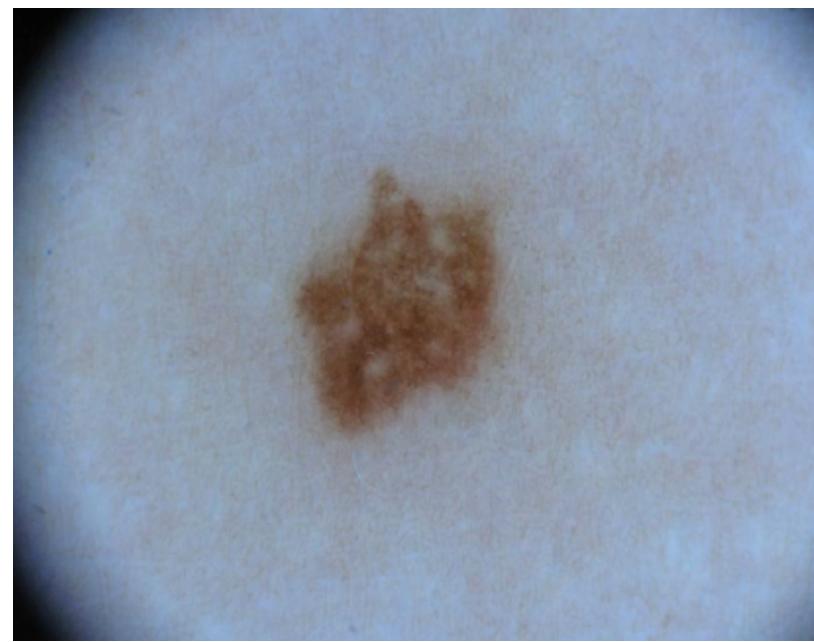


Figure 1. MNIST test accuracy as a function of number of acquired images from the pool set (up to 1000 images, using validation set size 100, and averaged over 3 repetitions). Four acquisition functions (*BALD*, *Variation Ratios*, *Max Entropy*, and *Mean STD*) are evaluated and compared to a *Random* acquisition function.

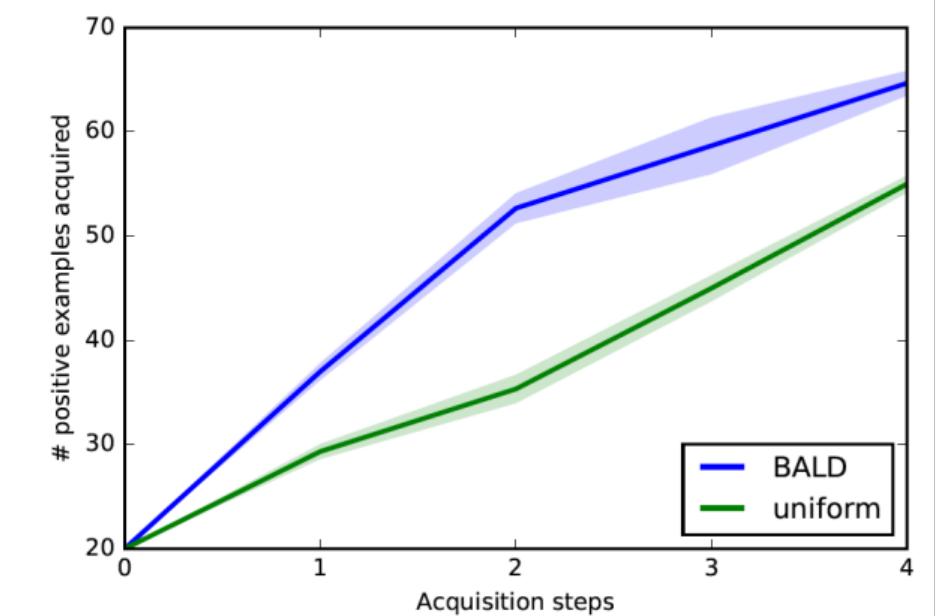
Technique	Test error
Semi-supervised:	
Semi-sup. Embedding (Weston et al., 2012)	5.73%
Transductive SVM (Weston et al., 2012)	5.38%
MTC (Rifai et al., 2011)	3.64%
Pseudo-label (Lee, 2013)	3.46%
AtlasRBF (Pitelis et al., 2014)	3.68%
DGN (Kingma et al., 2014)	2.40%
Virtual Adversarial (Miyato et al., 2015)	1.32%
Ladder Network (Γ -model) (Rasmus et al., 2015)	1.53%
Ladder Network (full) (Rasmus et al., 2015)	0.84%
Active learning with various acquisitions:	
Random	4.66%
BALD	1.80%
Max Entropy	1.74%
Var Ratios	1.64%

Experiments (ISIC 2016 melanoma diagnosis dataset)

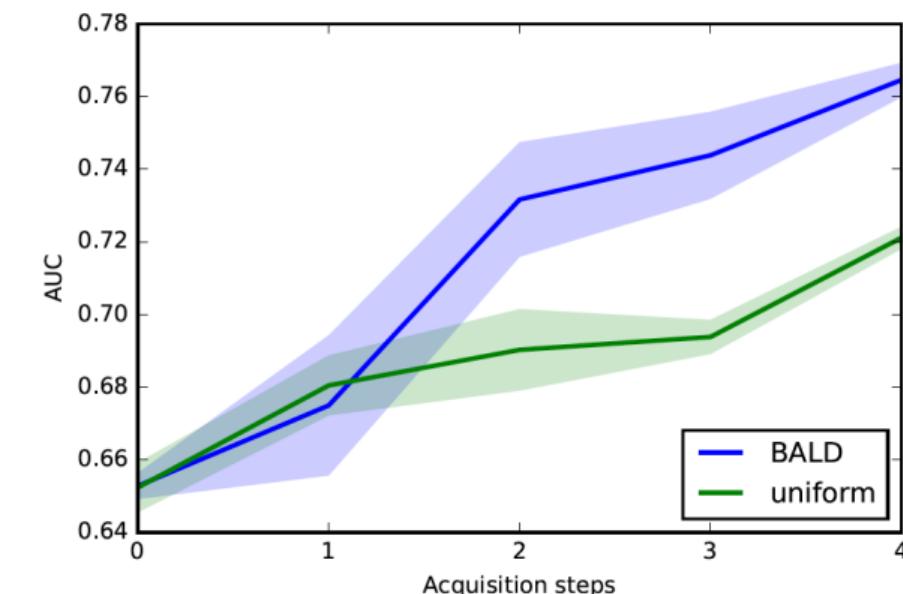
- Model : VGG16 (Simonyan & Zisserman, 2015) / 2 classification (malignant/benign)
- Small and imbalanced dataset
- initial dataset : 80 negative / 20 positive
- acquisition until all pool sets have been exhausted



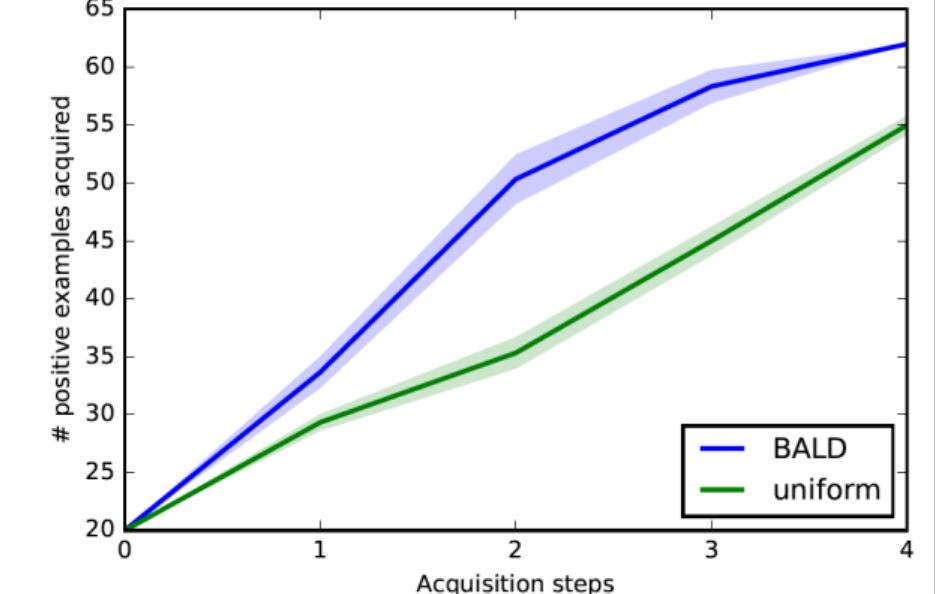
(a) AUC as a function of acquisition step, first test split



(b) # of positive examples acquired as a function of acquisition step, first test split



(c) AUC as a function of acquisition step, second test split



(d) # of positive examples acquired as a function of acquisition step, second test split

Discussion

- 두 번째 Real dataset에서 Acquisition function 간의 성능 차이를 보여주기보다는 Active learning을 통해서 학습했을 때와 전체 데이터셋을 사용해서 학습했을 때의 성능 차이를 보여주는 게 더 낫지 않았을까
- 성능 차이가 그렇게 크지 않다면 Semi-supervised learning보다 확실히 나은 점이 무엇일까

Reference...

- Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning
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- [Open DMQA Seminar] Uncertainty Quantification in Deep Learning
 - <https://www.youtube.com/watch?v=oCVEFv5P088&t=3421s>
- Bayesian Deep Learning Course
 - Seong-Jun Choi, <https://www.edwith.org/bayesandeeplearning>