# Semi-supervised Learning with Deep Generative Models

## Kingma et. al. (2014)

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CS 7180

# Motivating Question

How can we model data of increasing size when obtaining label information is difficult?

# High-level Answer

We can estimate missing label information by using a probabilistic model.

# Most Relevant Previous Work

Pitelis, N., Russell, C., and Agapito, L. (2014). Semi-supervised learning using an unsupervised atlas. *In Proceddings of the European Conference on Machine Learning (ECML)*, volume LNCS 8725, pages 565 – 580.

- Observing that high-dimensional datasets often lie on or near *manifolds* of locally low rank can help avoid the *curse of dimensionality*
- Experiments show how using unlabelled data to learn the underlying manifold improves classifier accuracy when trained on limited labelled data
  1. **Unsupervised learning of the underlying manifold:** Approximate the manifold of data on the original space by fitting an atlas of low-dimensional overlapping affine charts.
  2. **Supervised training of an SVM:** Proposed a new family of Mercer Kernels for SVM-based supervised learning which uses soft-assignment of datapoints to the underlying low-dimensional affine charts to generate the kernels

# Specifying the Probabilistic Model for Missing Labels

Kingma et. al. (2014)

- Data appears as pairs $(\mathbf{X}, \mathbf{Y}) = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_N, y_N)\}$ with the $i$-th observation $x_i \in \mathbb{R}^D$ and a corresponding class label $y_i \in \{1, ..., L\}$
    - Each pair of observations $(x_i, y_i)$ has a corresponding latent variable $z_i$
    - Empirical distribution over the labelled and unabelled subsets is referred to as $\tilde{p}_l(\mathbf{x}, y)$ and $\tilde{p}_u(\mathbf{x})$
- We can estimate $y_i$ for $x_i$ in distribution $\tilde{p}_u(\mathbf{x})$ by finding the maximum probability of $p(y_i)$ by using a set of features related to $z_i$ and a predictive model
    1. **Latent-feature discriminative model (M1)**
    2. **Generative semi-supervised model (M2)**
    3. **Stacked generative semi-supervised model (M1+M2)**

# Bayes Rule is used when specifying M1 & M2

$$\begin{aligned} p(x, y) &= p(x)p(y|x) \\ &= p(y)p(x|y) \\ p(x|y) &= \frac{p(x)p(y|x)}{p(y)} \end{aligned}$$

for models M1 [1], $p(z|x)$, and M2 [2]; $p(y|x)$

[1] Kingma et. al. (2014) equation (1)

[2] Kingma et. al. (2014) equation (2)

# (M1) Latent-feature discriminative model

$$y \Leftarrow p(z|x) = \frac{p(z)p(x|z)}{p(x)}$$

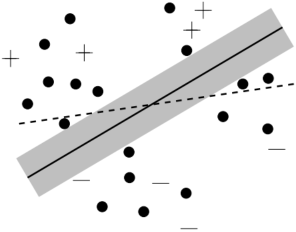
where

$$\begin{aligned} p(z) &= \mathcal{N}(z|0,I) && \text{Gaussian distribution of } z \text{ given a missing label } y \\ p(x|z) &= f(x; z, \theta) && \text{likelihood function, parameters } \theta \text{ of a set of } z \\ p(x) &= \tilde{p}_u(x) && \text{unlabelled subset of } x_i \in \mathbb{R}^D \end{aligned}$$

Kingma et. al. (2014) eq. (1)

# (M1) Predicting Class Labels $y$

Approximate samples from the posterior distribution over the latent variables $p(z|x)$ are used as features to train a classifier that predicts class labels $y$



(transductive) SVM[3]finds the largest margin w.r.t. the training **and** the test vectors

[3] See Figure 6.2 from Chapelle, O., B. Schölkopf, and A. Zien. "Semi-Supervised Learning." (2006).

# (M2) Generative semi-supervised model

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

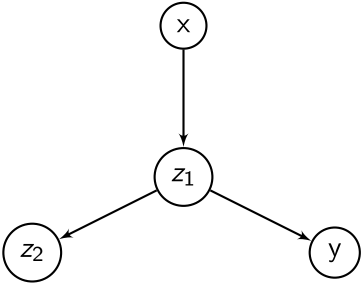
where

| | |
|---|---|
| $p(y) = Cat(y\|\pi)$ | multinomial distribution, $y$ can be latent |
| $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}\|\mathbf{0},\mathbf{I})$ | Gaussian distribution of $z$ when missing $y$ |
| $p_\theta(\mathbf{x}\|y,z) = f(\mathbf{x};y,\mathbf{z},\theta)$ | likelihood function, nonlinear parameters |
| $p(x)$ | all $x$ in dist. of real numbers; $x \in \mathbb{R}^D$ |

# Stacked generative semi-supervised model (M1 + M2)

Combine M1 and M2

1. Learn a new latent representation $z_1$ from M1
2. Use embeddings from $z_1$ instead of raw data $x$, to create a generative semi-supervised model M2



$$p_\theta(x, y, z_1, z_2) = p(y)p(z_2)p_\theta(z_1|y, z_2)p_\theta(x|z_1)$$

# Scaling Up: Lower Bound Objective

Lower Bound Objective[4]: computation of the exact posterior distribution is intractable for models M1 and M2

$$\text{M1: } q_\phi(z|x) = \mathcal{N}(z|u_\phi(x), \text{diag}(\sigma^2_\phi(\mathbf{x}))) \tag{3}$$

$$\begin{aligned} \text{M2: } q_\phi(\mathbf{z}|y, \mathbf{x}) &= \mathcal{N}(\mathbf{z}|\mu_\phi(y, \mathbf{x}), \text{diag}(\sigma^2_\phi(\mathbf{x}))); \\ q_\phi(y|\mathbf{z}) &= \text{Cat}(y|\pi_\phi(x)), \end{aligned} \tag{4}$$

where

| | |
|---|---|
| $\sigma_\phi(x)$ | vector of standard deviations |
| $\pi_\phi(x)$ | probability vector |
| $\mu_\phi(x), \sigma_\phi(x), \pi_\sigma(x)$ | Maximum likelihood Priors (MLPs) |

[4] Kingma et. al. (2014) equations (3), (4)

# Scaling Up: M1 Model Objective

Variational bound $\mathcal{J}(x)$ on the marginal likelihood of a single data point is[5]

$$\log p_\theta(x) \geq \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - KL[q_\phi(z|x)||p_\theta(z)] = -\mathcal{J}(x)$$

Approximate posterior is used as a feature extractor for the labelled data set, and the features used for training the classifier

[5] Kingma et. al. (2014) Equation 5

# Scaling Up: M2 Model Objective

When $y_i$ is observed for the $(x_i, y_i)$ data pair, extend from M1

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

In the case where $y_i$ is missing,

$$\begin{aligned}\log p_\theta(x) \geq \mathbb{E}_{q_\phi(y,z|x)}[&\log p_\theta(x|y,z) + \log p_\theta(y) \\ &+ \log p(z) - \log q_\phi(y,z|x)] \\ = \sum_y &q_\phi(y|x)(-\mathcal{L}(x,y)) + \mathcal{H}(q_\phi(y|x)) \\ = -&\mathcal{U}(x)\end{aligned}$$

The bound on the marginal likelihood for the entire dataset is now[6]

$$\mathcal{J} = \sum_{(x,y)\sim\tilde{p}_l} \mathcal{L}(x,y) + \sum_{x\sim\tilde{p}_u} \mathcal{U}(x)$$

[6] See Kingma et. al. (2014) equations 6-9

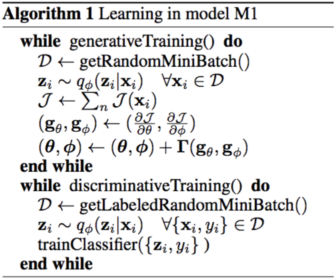
# Optimization Techniques

- Bounds from M1 and M2 objective function equations provides for optimization of both $\theta$ and $\phi$ parameters
  - Optimization can be done *jointly* without using the EM Algorithm
- Use deterministic reparameterizations of the expectations in the objective function and *Monte Carlo* approximation
- Previous work refers to this as *stochastic gradient variational Bayes*[7]and *stochastic backpropagation*[8]

[7] Kingma, D. P. and Welling, M. (2014). Auto-encoding variational Bayes. *In Proceedings of the International Conference on Learning Representations (ICLR)*.

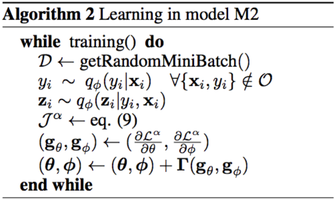
[8] Rezende, D. J., Mohamed, S., and Wierstra, D. (2014). Stochastic backpropagation and approximate inference in deep generative models. *In Proceedings of the International Conference on Machine Learning (ICML)*, volume 32 of JMLR WCP.

# Optimization Algorithms



**Algorithm 1** Learning in model M1

```
while generativeTraining() do
    $\mathcal{D} \leftarrow$ getRandomMiniBatch()
    $\mathbf{z}_i \sim q_\phi(\mathbf{z}_i|\mathbf{x}_i) \quad \forall \mathbf{x}_i \in \mathcal{D}$
    $\mathcal{J} \leftarrow \sum_n \mathcal{J}(\mathbf{x}_i)$
    $(\mathbf{g}_\theta, \mathbf{g}_\phi) \leftarrow (\frac{\partial \mathcal{J}}{\partial \theta}, \frac{\partial \mathcal{J}}{\partial \phi})$
    $(\boldsymbol{\theta}, \boldsymbol{\phi}) \leftarrow (\boldsymbol{\theta}, \boldsymbol{\phi}) + \boldsymbol{\Gamma}(\mathbf{g}_\theta, \mathbf{g}_\phi)$
end while
while discriminativeTraining() do
    $\mathcal{D} \leftarrow$ getLabeledRandomMiniBatch()
    $\mathbf{z}_i \sim q_\phi(\mathbf{z}_i|\mathbf{x}_i) \quad \forall \{\mathbf{x}_i, y_i\} \in \mathcal{D}$
    trainClassifier($\{\mathbf{z}_i, y_i\}$ )
end while
```



**Algorithm 2** Learning in model M2

```
while training() do
    $\mathcal{D} \leftarrow$ getRandomMiniBatch()
    $y_i \sim q_\phi(y_i|\mathbf{x}_i) \quad \forall \{\mathbf{x}_i, y_i\} \notin \mathcal{O}$
    $\mathbf{z}_i \sim q_\phi(\mathbf{z}_i|y_i, \mathbf{x}_i)$
    $\mathcal{J}^\alpha \leftarrow$ eq. (9)
    $(\mathbf{g}_\theta, \mathbf{g}_\phi) \leftarrow (\frac{\partial \mathcal{L}^\alpha}{\partial \theta}, \frac{\partial \mathcal{L}^\alpha}{\partial \phi})$
    $(\boldsymbol{\theta}, \boldsymbol{\phi}) \leftarrow (\boldsymbol{\theta}, \boldsymbol{\phi}) + \boldsymbol{\Gamma}(\mathbf{g}_\theta, \mathbf{g}_\phi)$
end while
```

Gradients w.r.t. generative parameters $\theta$ and variational parameters $\phi$ can be efficiently computed as expectations of simple gradients[9]

$$\nabla_{\{\theta,\phi\}}\mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] = \mathbb{E}_{\mathcal{N}(\epsilon|0,I)}[\nabla_{\{\theta,\phi\}}\log p_\theta(x|\mu_\theta(x)+\sigma_\phi(x)\odot\epsilon)].$$

[9] Kingma et. al. (2014) equation 11, regarding M1

# Results: Benchmark Classification

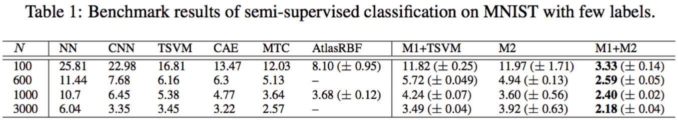
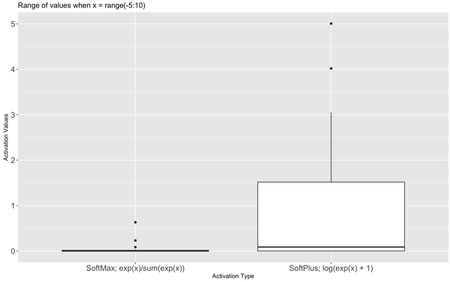


Table 1: Benchmark results of semi-supervised classification on MNIST with few labels.

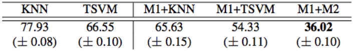
| *N* | NN | CNN | TSVM | CAE | MTC | AtlasRBF | M1+TSVM | M2 | M1+M2 |
|---|---|---|---|---|---|---|---|---|---|
| 100 | 25.81 | 22.98 | 16.81 | 13.47 | 12.03 | 8.10 (± 0.95) | 11.82 (± 0.25) | 11.97 (± 1.71) | **3.33** (± 0.14) |
| 600 | 11.44 | 7.68 | 6.16 | 6.3 | 5.13 | – | 5.72 (± 0.049) | 4.94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

- Varying the size of labelled data from 100 to 3000
- SoftPlus Activation function



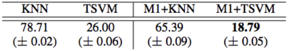
# Results: Image Classification

Table 2: Semi-supervised classification on the SVHN dataset with 1000 labels.



| KNN | TSVM | M1+KNN | M1+TSVM | M1+M2 |
|---|---|---|---|---|
| 77.93<br>(± 0.08) | 66.55<br>(± 0.10) | 65.63<br>(± 0.15) | 54.33<br>(± 0.11) | **36.02**<br>(± 0.10) |

Table 3: Semi-supervised classification on the NORB dataset with 1000 labels.



| KNN | TSVM | M1+KNN | M1+TSVM |
|---|---|---|---|
| 78.71<br>(± 0.02) | 26.00<br>(± 0.06) | 65.39<br>(± 0.09) | **18.79**<br>(± 0.05) |

- No comparative results in semi-supervised setting exists for SVHN and NORB image data sets
- Performed nearest-neighbor and TSVM classification with RBF kernels
- Compared performance on features generated by their latent-feature discriminative model to the original features

# Discussion

- Approximate inference methods can be extended to learn the model's parameters; helps with model selection
- Image classification tasks, can combine the approach presented with a CNN
- Limitation of the model is linear scaling with the number of classes in the datasets
  - Re-evaluating the generative likelihood for each class during training is an expensive operation

**Any questions? Thanks!**