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

$p(z) = \mathcal{N}(z|0, I)$ Gaussian distribution of z given a missing label y

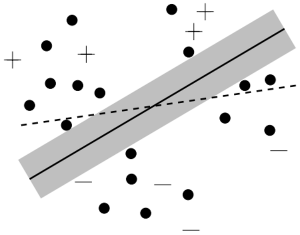
$p(x|z) = f(x; z, \theta)$ likelihood function, parameters θ of a set of z

$p(x) = \tilde{p_u}(x)$ unlabelled subset of $x_i \in \mathbb{R}^D$

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

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

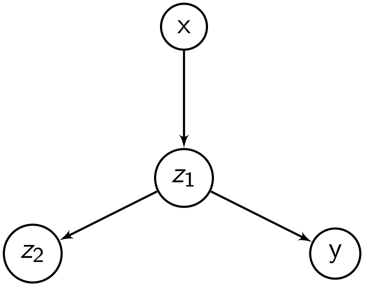
where

$p(y) = Cat(y\|\pi)$	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

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

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

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 θ and ϕ 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]

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[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 θ and variational parameters ϕ 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 ($\pm$ 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)

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 (± 0.08)	66.55 (± 0.10)	65.63 (± 0.15)	54.33 (± 0.11)	**36.02** (± 0.10)

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

KNN	TSVM	M1+KNN	M1+TSVM
78.71 (± 0.02)	26.00 (± 0.06)	65.39 (± 0.09)	**18.79** (± 0.05)

Discussion

You can use this model for a few things
TODO: just summarize their discussion

Any questions? Thanks!