An Unsupervised Learning Method Exploiting Sequential Output Statistics

Yu Liu* 1  Jianshu Chen* 1  Li Deng* 1

Abstract

We address a class of unsupervised learning problems where the same goal of supervised learning is aimed except with no output labels provided for training classifiers. This type of unsupervised learning is highly valuable in machine learning practice since obtaining labels in training data is often costly. Instead of pairing input-output samples, we exploit sequential statistics of output labels, in the form of N-gram language models, which can be obtained independently of input data and thus with low or no cost. We introduce a novel cost function in this unsupervised learning setting, whose profiles are analyzed and shown to be highly non-convex with large barriers near the global optimum. A new stochastic primal-dual gradient method is developed to optimize this very difficult type of cost function via the use of dual variables to reduce the barriers. We demonstrate in experimental evaluation, with both synthetic and real-world data sets, that the new method for unsupervised learning gives drastically lower errors and higher learning efficiency than the standard stochastic gradient descent, reaching classification errors about twice of those obtained by fully supervised learning. We also show the crucial role of labels’ sequential statistics exploited for label-free training with the new method, reflected by the significantly lower classification errors when higher-order language models are used in unsupervised learning than low-order ones.

1. Introduction

Unsupervised learning is one of the most challenging problems in machine learning, and has often been formulated as one that performs internal modeling of how the world works without requiring a huge amount of effort by humans to train such unsupervised learning systems; e.g. (Chintala & LeCun, 2016). To reach this grand goal, which currently suffers from lacking commonly agreeable evaluation measures, it is necessary to first solve a sub-goal of unsupervised learning that nevertheless has high practical value — learning to predict output labels from input data without requiring costly labeled data. Toward this end, we report in this paper our recent success of a practical approach to grounding unsupervised learning using the same evaluation measure as that for supervised learning in classification tasks.

During the past two years or so, various solutions have been proposed to address the input-to-output prediction problem without using labeled output data in the training phase, all without demonstrated successes (Deng, 2015; Sutskever et al., 2015; Chen et al., 2016). For example, the work reported in (Chen et al., 2016) proposes the use of a quantity related to expected cross-entropy as the cost function to train a classifier, where the need for explicitly labeled data in training is eliminated by averaging out the role of labeled data while retaining part of the discriminative power of cross-entropy that proves highly successful in recent supervised deep learning and neural network applications (Hinton et al., 2012; Krizhevsky et al., 2012; Mesnil et al., 2015; Fang et al., 2015). It was shown that the highly non-convex profile of the cost function constructed without labeled data has very high barriers near the global optimum, making parameter estimation difficult although adding a regularization term into the cost function mitigated the problem somewhat.

The solution provided in this paper fundamentally improves the cost function proposed in (Chen et al., 2016) in three important aspects. First, the cost function for unsupervised learning is revised to take into account more information, including non-uniform class probabilities, contained in the sequential statistics. Second, given the form of the new cost function with log sum of the batch of data, which makes the standard gradient computation and mini-batch training inefficient and intrinsically biased, a stochastic primal-dual gradient (SPDG) algorithm is developed to overcome these difficulties. Our analysis of SPDG reported in this paper also demonstrates how it is able to naturally reduce the high barriers in the cost function expressed in the primal domain via joint optimization of primal and dual variables. Most importantly, we demonstrate the new cost function and the associated SPDG optimization algorithm work well in two
classification tasks for evaluating unsupervised learning.

The organization of this paper is as follows. In Section 2, we survey the previous work on unsupervised learning related to our approach. The problem formulation of learning predictive functions using no explicit and costly output labels is presented in Section 3, together with a proposal of a novel cost function. Section 4 describes the SPDG method devised to minimize the cost function taking into account its special log-sum and non-convex properties. An analysis of the highly non-convex nature of the unsupervised cost function including visualization of its profile with respect to the parameters is detailed in Section 5. Experimental evaluation using both synthetic and real-world data sets described in Section 6 shows the effectiveness of our unsupervised learning paradigm presented in this paper.

2. Related Work

In machine learning literature, most studies on unsupervised learning concern automatic discovery of inherent regularities in the data without labels (Goodfellow et al., 2016). This also amounts to learning density functions for or feature representations from the data without labels. An important line of research has been to focus on exploiting the structure of input data by learning the data distribution using maximum likelihood rule. The most successful examples in this category include the restricted Boltzmann machine (RBM) (Smolensky, 1986; Hinton & Salakhutdinov, 2006), the deep belief network (Hinton et al., 2006), topic models (Blei et al., 2003), etc. Various approximate methods have been developed, such as variational inference (Jordan et al., 1999) and Monte Carlo methods (Hastings, 1970) to address computational difficulties. Further methods in this category include autoencoders (Bengio, 2009), denoising autoencoders (Vincent et al., 2010), variational autoencoders (Kingma & Welling, 2013), and generative adversarial networks (GAN) (Goodfellow et al., 2014; Goodfellow, 2016).

The above unsupervised learning methods have been developed to learn the input data distribution instead of the input-to-output prediction from unpaired input-output data. For applications of unsupervised learning to prediction tasks, a number of approaches have also been taken in the past, the majority of which has been to exploit the learned representations of the input data as feature vectors that are subsequently fed to a separate classifier; e.g., (Le et al., 2012). This approach, albeit widely used, is usually less effective than end-to-end learning with labeled data (Chen et al., 2015). Another important line of work on using unsupervised learning to help prediction is pre-training, where an unsupervised model trained using unlabeled data is used to initialize a separate supervised learning algorithm (Dahl et al., 2012; Hinton & Salakhutdinov, 2006; Bengio et al., 2007; Mikolov et al., 2013; Dai & Le, 2015). Pre-training is shown to be effective only when there is a small amount of labeled data available (Hinton et al., 2012). In prediction tasks with large amounts of paired training data, all the above unsupervised methods have played only an auxiliary role in helping supervised learning.

Several recent studies on unsupervised learning more closely related to and motivated the current work are (Deng, 2015; Sutskever et al., 2015; Chen et al., 2016). Deng (2015) proposed the use of the similarities between distributions of the language model prior and of the predicted word sequence as an alternative unsupervised learning objective to the likelihood function of the input data. Sutskever et al. (2015) used the more general concept of the output distribution matching (ODM). The ODM cost function measures how well the distribution of predicted outputs (integrated over the input space, which is computational infeasible) matches the distribution of target output samples. Dual autoencoders and GANs were used to implement the learning algorithm approximately without success. Further, ODM does not exploit any structure of the output samples, which may be one reason why ODM method failed based on the results we will present in Section 6 of this paper showing the importance of exploiting the sequential structure of the output labels.

As discussed in Section 1, the more recent work reported in (Chen et al., 2016), like the work presented in this paper, explicitly exploited the sequence prior, a type of structure commonly found in natural language data, of the output samples. The sequence prior is a very strong one when the order is high, and in many possible applications such as speech recognition, machine translation, and image/video captioning, this sequence prior can be obtained from language models trained using a very large amount of text data freely available and without labeling cost. The power of such a strong prior of language models in unsupervised learning was also demonstrated in earlier studies reported in (Knight et al., 2006; Berg-Kirkpatrick et al., 2013). However, due possibly to inappropriately formulated cost functions and to inappropriate choices of optimization methods, these earlier methods did not perform well in practical prediction tasks with real-world data without using additional strong generative models.

Finally, the most recent work on unsupervised learning for prediction closely related to our paper appeared in (Stewart & Ermon, 2017). It shares the same motivations as (Deng, 2015; Sutskever et al., 2015; Chen et al., 2016; Berg-Kirkpatrick et al., 2013) and our current work in recognizing the high cost of obtaining labeled data in prediction tasks. Different from our current approach based on exploiting sequential statistics in the output labels in the applications with natural language as the output, they exploit prior domain knowledge derived from laws of physics in computer vision applications.
3. Formulation of Unsupervised Learning for Label-Free Prediction

3.1. Problem setup

In this paper, we consider the unsupervised learning of a classifier without using paired training samples. Before we formally state our problem, we first briefly review the supervised learning problem. Let \( x_t \) denote a \( d \)-dimensional input vector and \( y_t \) be the associated \( C \)-dimensional output vector, where the subscript \( t \) denotes the \( t \)-th sample. The supervised learning problem could be formulated as using a set of paired training samples \( \{(x_t, y_t)\}_{t=1}^T \) to train a posterior probability \( p_\theta(y_t|x_t) \) so that it can be used to predict (unseen) test samples. \( \theta \) denotes the model parameters that could be estimated via solving the following problem

\[
\max_{\theta} \sum_{t=1}^T \ln p_\theta(y_t|x_t) \tag{1}
\]

In our unsupervised learning setup, we consider the learning of the posterior probability \( p_\theta(y_t|x_t) \) without using paired examples \( \{(x_t, y_t)\}_{t=1}^T \). Instead, the learner is only presented with a sequence of input data \( \mathcal{X} = (x_1, ..., x_T) \) and a separate output sequence \( \mathcal{Y} = (y_1, ..., y_T) \) that are not aligned with the input data samples, where \( T \) and \( T' \) are the number of their samples, respectively. Furthermore, we assume that the output \( (y_1, y_2, ..., y_T) \) admits sequential structure, which, for example, can be characterized by the following \( N \)-gram joint probability distribution

\[
p_{\text{LM}}(y_{t-N+1} = i_1, ..., y_t = i_t) = p_{\text{LM}}(i_1, ..., i_N) \tag{2}
\]

where the subscript “LM” stands for language model. In practice, the dataset \( \mathcal{Y} \) is used to estimate \( p_{\text{LM}}(i_1, ..., i_N) \). Then we learn \( p_\theta(y_t|x_t) \) from \( \mathcal{X} \) by exploiting this estimated \( p_{\text{LM}}(i_1, ..., i_N) \). Therefore, instead of pairing input-output samples, we exploit sequential statistics of output labels, \( (N\text{-gram language models here}) \), which can be obtained independently of input data and thus with low or even no cost. This scenario is useful in many practical problems where the output has strong sequence structure. For example, in optimal character recognition (OCR) tasks, \( y_t \) could be an English character and \( x_t \) is the input image containing a certain character. We can estimate an \( N \)-gram character-level language model from a separate text corpus, and then we can train the classifier by using the input images and the estimated \( N \)-gram language model, without any aligned input-output pairs. In our experiment section, we will demonstrate the effectiveness of our method on such a real OCR task.

3.2. The cost function in (Chen et al., 2016)

We now formally formulate the problem as an optimization problem. The key step is to derive a cost function that can effectively exploit the structure in \( p_{\text{LM}}(i_1, ..., i_N) \). Chen et al. (2016) proposed to use the expected negative log-likelihood function as the cost function to exploit the output sequential statistics, where the expectation is with respect to the posterior distribution defined by the model:

\[
E[-\ln p_{\text{LM}}(y_1, ..., y_T)|x_1, ..., x_T] \approx \sum_{(y_1, ..., y_T)} p_\theta(y_t|x_t) \ln p_{\text{LM}}(y_1, ..., y_T) \tag{2}
\]

where the sum above is over all possible values of \((y_1, ..., y_T)\). This cost function has the following interpretation. For a given input sequence \((x_1, ..., x_T)\), let \((y_1, ..., y_T)\) be a sequence sampled from the distribution \(\prod_{t=1}^T p_\theta(y_t|x_t)\), which is the parametric posterior model to be learned. Then the estimated language model can measure the quality of the sampled output sequence \((y_1, ..., y_T)\) by assigning it with a negative log-likelihood:

\[-\ln p_{\text{LM}}(y_1, ..., y_T)\]. The cost function in (2) is then the expected score of the output sequences generated from the predictor \(\prod_{t=1}^T p_\theta(y_t|x_t)\). Chen et al. (2016) showed that minimizing this cost function alone would lead to trivial solutions and proposed to combine it with an additional generative regularization term. We now give an in-depth analysis of this cost function (2) and develop a better form of cost function that can overcome these problems.

First, it can be shown that, under \( N \)-gram model, the cost function (2) is equivalent to the following cross entropy form (see the derivation in supplementary material):

\[-T \sum_{i_1, ..., i_N \in \{1, ..., C\}} p_\theta(i_1, ..., i_N) \ln p_{\text{LM}}(i_N|i_{N-1}, ..., i_1) \tag{3}\]

where \( p_{\text{LM}}(i_N|i_{N-1}, ..., i_1) \) denotes the probability of \( y_t = i_t \) given \( y_{t-1} = i_{t-1}, ..., y_{t-N+1} = i_1 \), and

\[
p_\theta(i_1, ..., i_N) \triangleq \frac{1}{T} \sum_{t=1}^T \prod_{k=0}^{N-1} p_\theta(y_{t-k} = i_{N-k}|x_{t-k}) \tag{4}\]

\( p_\theta(i_1, ..., i_N) \) can be interpreted as the expected frequency of the \( N \)-gram \((i_1, ..., i_N)\) in the output sequence \((y_1, ..., y_T)\) when applying \(\prod_{t=1}^T p_\theta(y_t|x_t)\) to the training input sequence \((x_1, ..., x_T)\) (see supplementary material).

3.3. The proposed cost function

Note that the cost function (3) is the negative cross entropy between \( p_\theta(i_1, ..., i_N) \) and \( p_{\text{LM}}(i_N|i_{N-1}, ..., i_1) \). We argue that it is more preferable to use an alternative form of cross entropy by swapping \( p_\theta(i_1, ..., i_N) \) and \( p_{\text{LM}}(i_N|i_{N-1}, ..., i_1) \). To see this, we first note that

- \( p_{\text{LM}}(i_N|i_{N-1}, ..., i_1) \to 0 \) and \( p_\theta(i_1, ..., i_N) > 0 \):

\[- p_\theta(i_1, ..., i_N) \ln p_{\text{LM}}(i_N|i_{N-1}, ..., i_1) \to +\infty\]
We have verified that this new form of cost function is less
which is already available in

\[ p_{LM}(i_N | i_{N-1}, \ldots, i_1) > 0 \text{ and } p_{\theta}(i_1, \ldots, i_N) \rightarrow 0: \]
\[ -p_{LM}(i_N | i_{N-1}, \ldots, i_1) \ln p_{\theta}(i_1, \ldots, i_N) \rightarrow 0 \]

\( \cdot \) \[ p_{LM}(i_N | i_{N-1}, \ldots, i_1) > 0 \text{ and } p_{\theta}(i_1, \ldots, i_N) \rightarrow 0: \]
\[ -p_{\theta}(i_1, \ldots, i_N) \ln p_{LM}(i_N | i_{N-1}, \ldots, i_1) \rightarrow 0 \]
\[ -p_{LM}(i_N | i_{N-1}, \ldots, i_1) \ln p_{\theta}(i_1, \ldots, i_N) \rightarrow +\infty \]

Therefore, the cost function (3) will heavily penalize the
classifier if it predicts an output that is believed to be less
probable by the prior language model. On the other hand,
the cost function (3) will not penalize the classifier when it
does not predict an output that the language model believes
to be probable. In other words, the classifier is encouraged
to be "conservative"; it tends to predict outputs with high
probability from the language model. This probably
explains the behavior observed in (Chen et al., 2016): the
training process could be easily converge to trivial local
optimal solutions of predicting the same output if the addi-
tional generative regularization is not added. On the other
hand, if we consider the cost function

\[ - \sum_{i_1, \ldots, i_{N-1}} \sum_{i_N} p_{LM}(i_N | i_{N-1}, \ldots, i_1) \ln p_{\theta}(i_1, \ldots, i_N) \quad (5) \]

it will heavily penalize the classifier if it does not predict
the output that the language model believes to be probable,
and will penalize less if the classifier predicts outputs that
the language model believes to be not probable. That is,
this cost will encourage the classifier to (i) trust the prior
language model more if \( p_{LM}(i_N | i_{N-1}, \ldots, i_1) \) is large and
(ii) trust it less otherwise. Ideally, if the language model is
precise, the situation (ii) is also less favorable. However,
in practice, the small values in \( p_{LM}(i_N | i_{N-1}, \ldots, i_1) \) are
usually less reliable as it is estimated from fewer examples.
We have verified that this new form of cost function is less
inclined to learn trivial solutions and is more robust.

In this paper, we consider a further improved version of (5)
as a cost function:

\[ - \sum_{i_1, \ldots, i_{N-1}} \sum_{i_N} p_{LM}(i_1, \ldots, i_{N-1}) \times \sum_{i_N} p_{LM}(i_N | i_{N-1}, \ldots, i_1) \ln p_{\theta}(i_1, \ldots, i_N) \quad (6) \]

which replaces the uniform sum in (5) by a weighted sum
with weights being \( p_{LM}(i_1, \ldots, i_{N-1}) \). This effectively
takes the non-uniform distribution of \( (i_1, \ldots, i_{N-1}) \) into ac-
count by exploiting the information in \( p_{LM}(i_1, \ldots, i_{N-1}) \),
which is already available in \( p_{LM}(i_1, \ldots, i_N) \). This non-
uniform class prior information was missing in the cost
proposed in (Chen et al., 2016).

Based on the above argument, we will learn \( p_{\theta}(y_t | x_t) \) by
minimizing the cost function (6), which can be rewritten in
the following form after substituting (4):

\[ \min_{\theta} \left\{ J(\theta) \triangleq - \sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \times \ln \left( \frac{1}{T} \sum_{t=1}^{T} \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \right) \right\} \quad (7) \]

The main challenge with (7) is that the sample average is in-
side the logarithmic loss, which is different from traditional
empirical risk minimization problems where the sum is out-
side the loss. This special form prevents us from applying
stochastic gradient descent (SGD) to minimize the cost. To
see this, we can express the (full batch) gradient of \( J(\theta) \) as

\[ \nabla_{\theta} J(\theta) = - \sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \times \frac{1}{T} \sum_{t=1}^{T} \nabla_{\theta} \left( \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \right) \times \frac{1}{T} \sum_{t=1}^{T} \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \quad (8) \]

Note that the gradient expression has sample averages in
both the numerator and denominator. Therefore, full batch
gradient method is less scalable as it needs to go over the
entire training set to compute \( \nabla_{\theta} J(\theta) \) at each update. To
apply SGD, we may obtain an unbiased estimate of it by
sampling the numerator with a single component while keep-
ing the denominator the same:

\[ -\sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \nabla_{\theta} \left( \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \right) \quad \frac{1}{T} \sum_{t=1}^{T} \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \]

However, this implementation is still not scalable as it needs
to average over the entire training set at each update to
compute the denominator. On the other hand, if we sample
both the numerator and the denominator, i.e.,

\[ -\sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \nabla_{\theta} \left( \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \right) \quad \frac{1}{T} \sum_{t=1}^{T} \prod_{k=0}^{N-1} p_{\theta}(y_{t-k} = i_{N-k} | x_{t-k}) \]

then it will be a biased estimate of the gradient (8). Our
experiments in Section 6 show that this biased SGD does not
perform well on the unsupervised learning problem. In the
next section, we will transform the cost function (7) into an
equivalent min-max problem, which allows us to efficiently
obtain unbiased stochastic gradient.

The posterior probability \( p_{\theta}(y_t | x_t) \) used to describe the clas-
sifier could admit different parametric forms, such as neural
networks, where \( \theta \) denotes all network weights. However,
in this paper, we focus on log-linear model, where \( p_{\theta}(y_t | x_t) \)
could be expressed as a softmax function:

\[ p_{\theta}(y_t = i | x_t) = \frac{e^{\gamma w^T y t}}{\sum_{j=1}^{C} e^{\gamma w^T j x t}} \quad (9) \]
where $\theta \triangleq \{ w_i \in \mathbb{R}^d, i = 1, \ldots, C \}$ denotes the collection of the model parameters.

4. SPDG: Learn to Predict without Labels

4.1. Equivalent primal-dual formulation

In order to correctly apply stochastic gradient descent to solve (7), we need to transform it so that the sum over $t$ is brought out of the logarithmic loss. To this end, we first introduce the concept of convex conjugate functions. For a given convex function $f(u)$, its convex conjugate function $f^*(\nu)$ is defined as $f^*(\nu) \triangleq \sup_{u} (\nu^T u - f(u))$ (Boyd & Vandenberghe, 2004, pp. 90-95). Furthermore, it holds that

$$f(u) = \sup_{\nu} (u^T \nu - f^*(\nu))$$  \hfill (10)

Consider a function $f(u) = -\ln u$ where $u > 0$ is a scalar, then its conjugate function is $f^*(\nu) = -1 - \ln(-\nu)$ with $\nu < 0$. Therefore, by (10), we have the following relation

$$-\ln u = \max_{\nu} (u \nu + 1 + \ln(-\nu))$$  \hfill (11)

where the $\sup$ is replaced by $\max$ because the supremum is attainable. Substituting (11) into (7), the original minimization problem (7) can be shown to be equivalent to solving the following min-max problem:

$$\min_{\theta} \max_{\nu_1, \ldots, \nu_N < 0} \left\{ \mathcal{L}(\theta, V) \triangleq \frac{1}{T} \sum_{t=1}^{T} L_t(\theta, V) + \sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \ln(-\nu_{i_1, \ldots, i_N}) \right\}$$  \hfill (12)

where $V \triangleq \{ \nu_{i_1, \ldots, i_N} \}$ is a collection of all the dual variables $\nu_{i_1, \ldots, i_N}$, and $L_t(\theta, V)$ is the $t$-th component function:

$$L_t(\theta, V) \triangleq \sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \nu_{i_1, \ldots, i_N} \times \prod_{k=0}^{N-1} p_{h}(y_{t-k} = i_{N-k} | x_{t-k})$$

The optimal solution $(\theta^*, V^*)$ to (12) is called the saddle point of $\mathcal{L}(\theta, V)$ (Boyd & Vandenberghe, 2004). Once $(\theta^*, V^*)$ is obtained, we only keep the primal variable $\theta^*$ as the learned model parameters.

4.2. Stochastic primal-dual gradient method (SPDG)

In the equivalent min-max problem (12), we find the optimal solution $(\theta^*, V^*)$ by minimizing $\mathcal{L}(\theta, V)$ with respect to $\theta$ and maximizing $\mathcal{L}(\theta, V)$ with respect to $V$. The obtained $\theta^*$ will also be the optimal solution to (7). We further note that the equivalent min-max problem (12) now becomes a sum over $T$ component functions $L_t(\theta, V), t = 1, \ldots, T$.

**Algorithm 1 Stochastic Primal-Dual Gradient Method**

1: Input data: $X = (x_1, \ldots, x_T)$ and $p_{LM}(i_1, \ldots, i_N)$.
2: Initialize $\theta$ and $V$ where the elements of $V$ are negative
3: repeat
4: Randomly sample a mini-batch of $B$ subsequences of length $N$, i.e., $B = \{(x_{t_n-N+1}, \ldots, x_{t_m})\}_{m=1}^{B}$, from $X$.
5: Compute the stochastic gradients for each subsequence in the mini-batch and average them
$$\Delta \theta = \frac{1}{B} \sum_{m=1}^{B} \frac{\partial L_m}{\partial \theta}$$
$$\Delta V = \frac{1}{B} \sum_{m=1}^{B} \frac{\partial L_m}{\partial V} + \frac{\partial}{\partial \nu_{i_1, \ldots, i_N}} \sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \ln(-\nu_{i_1, \ldots, i_N})$$
6: Update $\theta$ and $V$ according to
$$\theta \leftarrow \theta - \mu_\theta \Delta \theta, \quad V \leftarrow V + \mu_v \Delta V$$
7: until convergence or a certain stopping condition is met

Therefore, the minimization with respect to $\theta$ and the maximization with respect to $V$ could be solved by stochastic gradient descent of $\mathcal{L}(\theta, V)$ with respect to the primal variable $\theta$ and by stochastic gradient ascent of $\mathcal{L}(\theta, V)$ with respect to the dual variable $V$, respectively, and we name this algorithm stochastic primal-dual gradient (SPDG) method. To compute the stochastic gradients, we express the full batch gradients of $\mathcal{L}(\theta, V)$ as

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{1}{T} \sum_{t=1}^{T} \frac{\partial L_t}{\partial \theta}$$
$$\frac{\partial \mathcal{L}}{\partial V} = \frac{1}{T} \sum_{t=1}^{T} \frac{\partial L_t}{\partial V} + \frac{\partial}{\partial \nu_{i_1, \ldots, i_N}} \sum_{i_1, \ldots, i_N} p_{LM}(i_1, \ldots, i_N) \ln(-\nu_{i_1, \ldots, i_N})$$

To compute the stochastic gradients, we replace each sample average of $\partial L_t / \partial \theta$ and $\partial L_t / \partial V$ by their respective randomly sampled component $\partial L_m / \partial \theta$ and $\partial L_m / \partial V$ (or their mini-batch averages), respectively, where $t_m$ is a uniform random variable over $\{1, \ldots, T\}$. In Algorithm 1, we summarize the SPDG method with mini-batch gradient, where the gradients are computed automatically in Tensor-Flow implementation. Furthermore, the negative constraint on dual variables $\nu_{i_1, \ldots, i_N}$ can be automatically enforced due to the inherent log-barrier $\ln(-\nu_{i_1, \ldots, i_N})$ appearing in (12) (Boyd & Vandenberghe, 2004). Therefore, we do not need a separate method to enforce the constraint.

5. Analyzing the Profiles of the Cost Function

In this section, we analyze the profiles of the proposed cost functions $\mathcal{J}(\theta)$ in (7) and the function $\mathcal{L}(\theta, V)$ in (12). We will show below the difficulty of optimizing the original
cost function $J(\theta)$ and how the primal-dual reformulation makes the problem much easier.

### 5.1. Profiles in the primal domain

We first examine the profile of the cost function $J(\theta)$. However, since $J(\theta)$ is a high-dimensional function, it is hard to visualize its full profile. To address this difficult, we use the following procedure to partially visualize $J(\theta)$ to analyze its properties. First, since with linear classifiers the supervised learning problem (1) is a convex optimization problem with a global optimal solution, we find $\theta^*$ by solving the supervised learning problem (1)\(^1\). Afterwards, we randomly generate two parameter vectors $\theta_1$ and $\theta_2$ and plot the two-dimensional function $J(\theta^* + \lambda_1(\theta_1 - \theta^*) + \lambda_2(\theta_2 - \theta^*))$ with respect to $\lambda_1, \lambda_2 \in \mathbb{R}$, which is the slice of the cost function on the two-dimensional affine space spanned by $\theta_1 - \theta^*$ and $\theta_2 - \theta^*$ and translated by vector $\theta^*$. In Figure 1, we show one slice of $J(\theta)$ on the OCR dataset that we will use in our experiment, viewed from different angles. (More slices and a video of the profiles from many angles can be found in the supplementary material.) From the figures, we find that the cost function $J(\theta)$ is highly non-convex even with linear classifiers. There are local optimal solutions and there are high barriers between the local optimal solution and the global optimal solution (the supervised solution). Therefore, besides the difficulty of having the sample average inside the logarithmic loss (see the discussion in Section 4), minimizing this cost function directly is also extremely difficult; it would be hard to cross the high barriers to reach the global optimal solution if not properly initialized.

### 5.2. Profiles in the primal-dual domain

Next, we proceed to examine the profile of $\mathcal{L}(\theta, V)$ in the min-max problem (12). Similar to the case of $J(\theta)$, in order to visualize $\mathcal{L}(\theta, V)$, we first solve the supervised learning problem to get $\theta^*$, and then by (12), the optimal dual variable $V^* = [v_{1, \ldots, i_N}]$ obtained by maximizing $\nu_{1, \ldots, i_N}$ with $\theta = \theta^*$, which is given by

$$
\nu_{1, \ldots, i_N} = -\frac{1}{\mathcal{L}} \sum_{i=1}^{\mathcal{L}} \prod_{k=0}^{N-1} p_{\theta^*}(y_{i-k} = i_{N-k} | x_{i-k})
$$

Afterwards, we randomly generate $\theta_1$ and $V_1$ (with the elements of $V_1$ being negative) and plot the values of $\mathcal{L}(\theta^* + \lambda_p(\theta_1 - \theta^*), V^* + \lambda_d(V_1 - V^*))$ for different values of $\lambda_p, \lambda_d \in \mathbb{R}$ in Figure 2a. It is clear that the optimal solution (red dot) is at the saddle point of the profile. Furthermore, comparing Figure 2a to Figure 1, we observe that the profile of $\mathcal{L}(\theta, V)$ is much smoother than that of $J(\theta)$ and the barrier is much lower. To further compare $J(\theta)$ and $\mathcal{L}(\theta, V)$, we plot the values of $J(\theta)$ and $\mathcal{L}(\theta, V)$ along the same line of $\theta^* + \lambda_p(\theta_1 - \theta^*)$ for $\lambda_p \in \mathbb{R}$ in Figure 2b. It also shows that the barrier $\mathcal{L}(\theta, V)$ along the primal direction is also lower than that of $J(\theta)$. Roughly speaking, these observations imply that, with the introduction of auxiliary dual variables, the cost function becomes much better conditioned to work with, and that the equivalent min-max problem (12) becomes nicer than the original minimization problem (7). This further justifies the use of SPDG method for solving the unsupervised learning problem (7).

### 6. Experimental Evaluation

#### 6.1. Experimental setup

We evaluate our unsupervised learning scheme described in earlier sections using two prediction tasks, unsupervised character-level OCR and unsupervised English Spelling Correction (Spell-Corr).

For the OCR task, we generate our dataset from a public database UWIII English Document Image Database (Phillips et al.), which contains images of lines and corresponding groundtruth. We first segment the image of lines into characters tiles and assign each tile with one character. We employ a heuristic method using Tesseract (Kay, 2007) for segmentation. We verify the segmentation by training a simple neural network classifier on the segmented results and achieve 0.9% error rate on the test set. Then, we select sentence segments that are longer than 100 and contain only lower case English characters and common punctuations (space, comma, and period). As a result, we have a vocabulary of size 29 and we obtain 1175 sentence segments and 153221 characters for our OCR task. Specifically, to represent images, we extract VGG19 features with $\text{dim} = 4096$, and them project into $\text{dim} = 200$ using Principal Component Analysis.

In training out-of-domain language models (LM) for use in providing sequence statistics in the OCR task, we select sentences from another public database English Gigaword (Parker, 2009), from which we select three different language partitions (CNA, NYT, XIN) in our experiments reported later in this section.

In Spell-Corr task, we learn to correct the spelling from a mis-spelling text. From the AFP partition of the Gigaword database, we select 500 sentence segments into our Spell-Corr dataset. Each sentence is selected to be longer than 100 and contains English characters and common punctuation only, resulting in a total of 83567 characters. To create mis-spelling, we use substitution simulations to generate noisy text. The noisy text is treated as our input, and the goal of prediction is to recover the original text. There is no original text (“labels”) available in our training of the

---

\(^1\)Note that, we solve the supervised learning only for the purpose of understanding our proposed unsupervised learning cost $J(\theta)$. In our implementation of the unsupervised learning algorithm, we do not use any of the training label information nor supervised learning algorithms.
An Unsupervised Learning Method Exploiting Sequential Output Statistics

Figure 1. The profiles of $J(\theta)$ for the OCR dataset on a two-dimensional affine space that passes through the supervised solution. The three figures show the same profile from different angles, where the red dot is the supervised solution. The contours of the profiles are also shown at the bottom.

Figure 2. The profiles of $L(\theta, V)$ for the OCR dataset. (a) The profile on a two-dimensional affine space that passes through the optimal solution, where the red dot is the optimal solution (saddle point). (b) The profile along the line of $\theta^* + \lambda_p(\theta_1 - \theta^*)$ with $\lambda_p \in \mathbb{R}$, where the circles are the optimal solutions.

prediction model, hence an unsupervised learning task. 2

6.2. Results: Comparing optimization algorithms

In the first set of experiments, we aim to evaluate the effectiveness of the SPDG method as described in Section 4 that is designed for optimizing the unsupervised cost function described in Section 3. The analysis provided in Section 5 sheds insight to why SPDG is superior to the standard stochastic gradient descent (SGD) method — the barriers in the highly non-convex profile of the cost function can be naturally reduced via simultaneously optimizing dual variables.

Table 1 provides strong experimental evidence demonstrating the substantially greater effectiveness of the primal-dual method over the SGD one using the OCR data set (the second column) and the Spelling Correction data set (the third column). Let’s examine the results on the OCR in detail. First, the SPGD on the unsupervised cost function achieves 9.21% error rate, much lower than error rates of any of mini-batch SGD runs, where the size of the mini-batches ranges from 10 to 10000. All these results are obtained where the training runs for the same large number of parameter updates. Note that, in sharp contrast to supervised learning with SGD, larger mini-batch sizes produce lower errors here.

This leads to the second observation from Table 1. That is, when the mini-batch size is as small as 10, the high error rate of 83.09% is close to a guess by majority rule — predicting the character (space) that has a largest proportion in the train set; i.e. $\frac{25}{153.221} = 83.37\%$.

Third, perhaps most interestingly, with no labels provided

---

2 We gratefully acknowledge the discussions with Prof. Hermann Ney for private discussions on this task and his work on using likelihood as the objective function for unsupervised training.
in the training, the classification errors produced by our method are only about twice compared with supervised learning (4.63% shown in Table 1). This clearly demonstrates that the unsupervised learning scheme proposed in this paper is an effective one.

For the Spelling Correction data set with the results shown in the third column in Table 1, we observe rather consistent results with the OCR data set.

Table 1. Test error rates on two data sets: OCR and Spelling Corrections. Comparing SPDG with plain SGD. The 2-gram character language model is trained using in-domain data

| Data-sets       | OCR    | Spell-Corr |
|-----------------|--------|------------|
| SPDG (this paper) | **9.59%** | **1.94%**  |
| SGD (miniBatch,10) | 83.09% | 82.91%      |
| SGD (miniBatch,100) | 78.05% | 72.93%      |
| SGD (miniBatch,1000) | 67.14% | 65.69%      |
| SGD (miniBatch,10000) | 56.48% | 45.24%      |
| Supervised learning | 4.63% | 0.00%       |
| Guess by majority rule | 83.37% | 82.91%      |

6.3. Results: Comparing orders of language modeling

In the second set of experiments, we aim to examine to what extent the use of higher order sequential statistics (e.g. 2- and 3-gram LMs) can do better than low-order uni-gram LM in unsupervised learning. As the use of 3-gram LM requires more characters to carry out the LM estimation independently of the input data, we use out-of-domain data sets which have no corresponding input data.

The unsupervised prediction results are shown in Table 2, using various kinds of data sources to estimate N-gram LM parameters. Consistent across all four ways of estimating reliable N-gram LMs, we observe significantly lower error rates when the unsupervised learning exploits 2-gram and 3-gram LM as sequential statistics compared with exploiting the prior with no sequential statistics (i.e. 1-gram). In three of four cases, exploiting a 3-gram LM gives better results than a 2-gram LM.

Further, the comparable error rate rate associated with 3-gram using out-of-domain output character data (10.17% in Table 2) to that using in-domain output character data (9.59% in Table 2) indicates that the effectiveness of the unsupervised learning paradigm presented in this paper is robust to the quality of the LM acting as the sequential prior.

Table 2. Test error rates on the OCR dataset. Character language models (LMs), with the order ranging from one to three, are trained using three out-of-domain data sets as well as fused in-domain and out-of-domain data

|          | NYT-LM | XIN-LM | CNA-LM | Fused-LM |
|----------|--------|--------|--------|----------|
| No. Sents| 1206903| 155647 | 12234  | 15409    |
| No. Chars| 86005542| 18626451| 1911124| 2064345  |
| 1-gram   | 71.83%| 72.14%| 71.51%| 71.25%   |
| 2-gram   | 10.93%| 12.55%| 10.56%| 10.33%   |
| 3-gram   | 10.17%| 12.89%| 10.29%| 9.21%    |

7. Conclusions and future work

The main contributions of this paper are as follows. First, we are moving towards solving unsupervised learning in a cleanly measurable and practically valuable manners — using the same measure of prediction accuracy as for supervised learning but eliminating the requirement for labeled outputs each being paired with input samples in the training set. The practical benefit of such unsupervised learning is tremendous. For example, in large scale commercial speech recognition systems, the currently dominant supervised learning methods typically require a few thousand hours of training material where each utterance in the acoustic form needs to be explicitly labeled with the corresponding word sequence by humans. Although there are millions of hours of natural speech data available for training, labeling all of such acoustic data followed by supervised learning is simply not feasible. To make effective use of such huge amounts of acoustic data in speech recognition, the practical unsupervised learning approach discussed in this paper would be called for. Similar applications such as machine translation, automatic image and video captioning and so on can all be benefiting from our unsupervised learning paradigm here, since their outputs have the common structure of natural language, the kind of sequential statistics demonstrated in Section 6 to be essential as the structured prior for unsupervised learning to work well. Second, the cost function for unsupervised learning presented in (Chen et al., 2016) is significantly improved so that it becomes much better able to exploit the structured prior of n-gram LM. Third, a novel SPDG algorithm is developed to optimize the new cost function, taking into account its special property. An analysis of the algorithm, together with examinations of the profiles of the cost function, sheds insight to why SPDG works well and why previous methods failed. Finally, we demonstrate in two data sets that our label-free unsupervised learning is highly effective, producing only about twice errors as fully supervised learning, which no previous unsupervised learning could produce without additional step of supervised learning.

While the current work is limited to unsupervised linear models for prediction, it is straightforward to generalize the current cost function and SPDG algorithm to nonlinear models such as deep neural nets (Hinton et al., 2012). We also plan to extend our current method from exploiting N-gram LM to exploiting state-of-art current neural network...
An Unsupervised Learning Method Exploiting Sequential Output Statistics

LM so that the full unsupervised learning and prediction can be formulated as an end-to-end system.

References

Bengio, Yoshua. Learning deep architectures for AI. *Foundations and Trends in Machine Learning*, 2(1):1–127, January 2009. ISSN 1935-8237.

Bengio, Yoshua, Lamblin, Pascal, Popovici, Dan, and Larochelle, Hugo. Greedy layer-wise training of deep networks. In *Proceedings of the Advances in Neural Information Processing Systems (NIPS)*, pp. 153–160, 2007.

Berg-Kirkpatrick, Taylor, Durrett, Greg, and Klein, Dan. Unsupervised transcription of historical documents. In *Proceedings of the 51st Annual Meeting of the Association for Computational Linguistics*, pp. 207–217, 2013.

Blei, David M., Ng, Andrew Y., and Jordan, Michael I. Latent dirichlet allocation. *The Journal of Machine Learning Research*, 3:993–1022, March 2003. ISSN 1532-4435.

Boyd, Stephen and Vandenberghe, Lieven. *Convex optimization*. Cambridge university press, 2004.

Chen, Jianshu, He, Ji, Shen, Yelong, Xiao, Lin, He, Xiaodong, Gao, Jianfeng, Song, Xinying, and Deng, Li. End-to-end learning of lda by mirror-descent back propagation over a deep architecture. In *Proceedings of the Advances in Neural Information Processing Systems (NIPS)*, pp. 1765–1773, 2015.

Chen, Jianshu, Huang, Po-Sen, He, Xiaodong, Gao, Jianfeng, and Deng, Li. Unsupervised learning of predictors from unpaired input-output samples. *arXiv:1606.04646*, 2016.

Chintala, Soumith and LeCun, Yann. A path to unsupervised learning through adversarial networks. In *https://code.facebook.com/posts/1587249151575490/a-path-to-unsupervised-learning-through-adversarial-networks/*, 2016.

Dahl, George E, Yu, Dong, Deng, Li, and Acero, Alex. Context-dependent pre-trained deep neural networks for large-vocabulary speech recognition. *Audio, Speech, and Language Processing, IEEE Transactions on*, 20(1):30–42, 2012.

Dai, Andrew M and Le, Quoc V. Semi-supervised sequence learning. In *Proceedings of the Advances in Neural Information Processing Systems (NIPS)*, pp. 3079–3087, 2015.

Deng, Li. Deep learning for speech and language processing. In *Tutorial at Interspeech Conf, Dresden, Germany, https://www.microsoft.com/en-us/research/wp-content/uploads/2016/07/interspeech-tutorial-2015-lideng-sep16a.pdf*, Aug-Sept, 2015.

Fang, Hao, Gupta, Saurabh, Iandola, Forrest, Srivastava, Rupesh, Deng, Li, Dollar, Piotr, Gao, Jianfeng, He, Xiaodong, Mitchell, Margaret, Platt, John, Zitnick, Lawrence, and Zweig, Geoffrey. From captions to visual concepts and back. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2015.

Goodfellow, Ian. Generative adversarial nets. In *Tutorial at NIPS, http://www.cs.toronto.edu/~dtkarlo/pos14/talks/goodfellow.pdf*, 2016.

Goodfellow, Ian, Pouget-Abadie, Jean, Mirza, Mehdi, Xu, Bing, Warde-Farley, David, Ozair, Sherjil, Courville, Aaron, and Bengio, Yoshua. Generative adversarial nets. In *Proceedings of the Advances in Neural Information Processing Systems (NIPS)*, pp. 2672–2680, 2014.

Goodfellow, Ian, Bengio, Yoshua, and Courville, Aaron. *Deep Learning*, by MIT Press. 2016.

Hastings, W Keith. Monte carlo sampling methods using markov chains and their applications. *Biometrika*, 57(1):97–109, 1970.

Hinton, Geoffrey, Deng, Li, Yu, Dong, Dahl, George E, Mohamed, Abdel-Rahman, Jaitly, Navdeep, Senior, Andrew, Vanhoucke, Vincent, Nguyen, Patrick, Sainath, Tara N., and Kingsbury, B. Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups. *IEEE Signal Processing Magazine*, 29 (6):82–97, November 2012.

Hinton, Geoffrey E and Salakhutdinov, Ruslan R. Reducing the dimensionality of data with neural networks. *Science*, 313(5786):504–507, 2006.

Hinton, Geoffrey E, Osindero, Simon, and Teh, Yee-Whye. A fast learning algorithm for deep belief nets. *Neural computation*, 18(7):1527–1554, 2006.

Jordan, Michael I, Ghahramani, Zoubin, Jaakkola, Tommi S, and Saul, Lawrence K. An introduction to variational methods for graphical models. *Machine learning*, 37(2):183–233, 1999.

Kay, Anthony. Tesseract: An open-source optical character recognition engine. *Linux Journal*, 2007.

Kingma, Diederik P and Welling, Max. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*, 2013.

Knight, Kevin, Nair, Anish, Radhod, Nishit, and Yamada, Kenji. Unsupervised analysis for decipherment problems. In *Proceedings of the COLING/ACL*, pp. 499–506, 2006.
Krizhevsky, Alex, Sutskever, Ilya, and Hinton, Geoffrey E. ImageNet classification with deep convolutional neural networks. In *Proceedings of the Advances in Neural Information Processing Systems (NIPS)*, pp. 1097–1105, 2012.

Le, Quoc, Ranzato, Marc’Aurelio, Monga, Rajat, Devin, Matthieu, Chen, Kai, Corrado, Greg, Dean, Jeff, and Ng, Andrew. Building high-level features using large scale unsupervised learning. In *International Conference in Machine Learning*, 2012.

Mesnil, Grégoire, Dauphin, Yann, Yao, Kaisheng, Bengio, Yoshua, Deng, Li, Hakkani-Tur, Dilek, He, Xiaodong, Heck, Larry, Tur, Gokhan, Yu, Dong, et al. Using recurrent neural networks for slot filling in spoken language understanding. *Audio, Speech, and Language Processing, IEEE/ACM Transactions on*, 23(3):530–539, 2015.

Mikolov, Tomas, Chen, Kai, Corrado, Greg, and Dean, Jeffrey. Efficient estimation of word representations in vector space. *arXiv preprint arXiv:1301.3781*, 2013.

Parker, Robert et al. English gigaword fourth edition ldc2009t13. *Philadelphia: Linguistic Data Consortium*, 2009.

Phillips, Ihsin, Chanda, Bhabatosh, and Haralick, Robert. http://isis-data.science.uva.nl/events/dlia/datasets/uwash3.html.

Smolensky, P. Parallel distributed processing: Explorations in the microstructure of cognition, vol. 1. chapter Information Processing in Dynamical Systems: Foundations of Harmony Theory, pp. 194–281. 1986.

Stewart, Russell and Ermon, Stefano. Label-free supervision of neural networks with physics and domain knowledge. In *Proceedings of AAAI*, 2017.

Sutskever, Ilya, Jozefowicz, Rafal, Gregor, Karol, Rezende, Danilo, Lillicrap, Tim, and Vinyals, Oriol. Towards principled unsupervised learning. *arXiv preprint arXiv:1511.06440*, 2015.

Vincent, Pascal, Larochelle, Hugo, Lajoie, Isabelle, Bengio, Yoshua, and Manzagol, Pierre-Antoine. Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion. *The Journal of Machine Learning Research*, 11:3371–3408, 2010.
A. Derivation of the equivalent form of the cost in (Chen et al., 2016)

In N-gram case, the language model can be written as

\[ \text{PLM}(y_1, \ldots, y_T) = \prod_{t=1}^{T} \text{PLM}(y_t | y_{t-1}, \ldots, y_{t-N+1}) \]

Substituting the above expression into the cost (2), we obtain

\[
\mathbb{E}[-\ln \text{PLM}(y_1, \ldots, y_T)| x_1, \ldots, x_T]
= - \sum_{(y_1, \ldots, y_T)} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \ln \text{PLM}(y_1, \ldots, y_T)
\]
\[
= - \sum_{(y_1, \ldots, y_T)} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1}|x_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_1, \ldots, y_{t-1}, \ldots, y_{t-N+1})
\]
\[
= - \sum_{(y_1, \ldots, y_{t-N+1})} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1}|x_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_1, \ldots, y_{t-1}, \ldots, y_{t-N+1})
\]
\[
= - \sum_{(y_1, \ldots, y_{t-N+1})} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1}|x_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_1, \ldots, y_{t-1}, \ldots, y_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_{t-N+1}, \ldots, y_{t-N})
\]
\[
= - \sum_{(y_1, \ldots, y_{t-N+1})} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1}|x_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_1, \ldots, y_{t-1}, \ldots, y_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_{t-N+1}, \ldots, y_{t-N})
\]
\[
= - \sum_{(y_1, \ldots, y_{t-N+1})} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1}|x_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_1, \ldots, y_{t-1}, \ldots, y_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_{t-N+1}, \ldots, y_{t-N})
\]
\[
= - \sum_{(y_1, \ldots, y_{t-N+1})} \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1}|x_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_1, \ldots, y_{t-1}, \ldots, y_{t-N+1})
\]
\[
\times \ln \text{PLM}(y_{t-N+1}, \ldots, y_{t-N})
\]
\[
= - T \sum_{i_1, \ldots, i_T} \ln p_{\theta}(y_t = i_T|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1} = i_{t-N+1}|x_{t-N+1})
\]
\[
\times \sum_{i_T} \sum_{i_{T-1}} \ldots \sum_{i_1} \prod_{t=1}^{T} p_{\theta}(y_t = i_T|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1} = i_{t-N+1}|x_{t-N+1})
\]
\[
= \frac{1}{T} \sum_{t=1}^{T} \sum_{i_T} \sum_{i_{T-1}} \ldots \sum_{i_1} \prod_{t=1}^{T} p_{\theta}(y_t = i_T|x_t) \cdot \prod_{t=1}^{T} p_{\theta}(y_{t-N+1} = i_{t-N+1}|x_{t-N+1})
\]

B. Interpretation of \( \mathbb{P}_\theta(i_1, \ldots, i_N) \)

In this section, we formally derive the following relation, which interprets \( \mathbb{P}_\theta(i_1, \ldots, i_N) \) as the expected frequency of \( (i_1, \ldots, i_N) \) in the output sequence:

\[ \mathbb{P}_\theta(i_1, \ldots, i_N) = \mathbb{E}_{\prod_{t=1}^{T} p_{\theta}(y_t|x_t)} \left[ \frac{n(i_1, \ldots, i_N)}{T} \right] \]

Let \( (x_1, \ldots, x_T) \) be a given input training sequence, and let \( (y_1, \ldots, y_T) \) be a sequence generated according to the posterior \( \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \) (which is the classifier). Furthermore, let \( \mathbb{I}_t(i_1, \ldots, i_N) \) denote the indicator function of the event \( \{y_{t-N+1} = i_1, \ldots, y_t = i_N\} \), and let \( n(i_1, \ldots, i_N) \) denote the number of the N-gram \( (i_1, \ldots, i_N) \) appearing in the output sequence \( (y_1, \ldots, y_T) \). Then, we have the following relation:

\[ n(i_1, \ldots, i_N) = \sum_{t=1}^{T} \mathbb{I}_t(i_1, \ldots, i_N) \]

(13)

Obviously, \( n(i_1, \ldots, i_N) \) is a function of \( (y_1, \ldots, y_T) \) and is thus a random variable. Taking the conditional expectation of the above expression with respect to \( \prod_{t=1}^{T} p_{\theta}(y_t|x_t) \), we obtain

\[ \mathbb{E}_{\prod_{t=1}^{T} p_{\theta}(y_t|x_t)} [n(i_1, \ldots, i_N)] \]
\[ = \sum_{t=1}^{T} \mathbb{E}_{\prod_{t=1}^{T} p_{\theta}(y_t|x_t)} [\mathbb{I}_t(i_1, \ldots, i_N)] \]
\[ = \sum_{t=1}^{T} \prod_{k=0}^{T-1} p_{\theta}(y_{t-k} = i_N-k|x_{t-k}) \]

where step (a) uses the fact that the expectation of an indicator function of an event equals the probability of the event. Divide both sides by \( T \), the right hand side of the above expression becomes \( \mathbb{P}_\theta(i_1, \ldots, i_N) \), and we conclude our proof of

\[ \mathbb{P}_\theta(i_N, \ldots, i_1) = \mathbb{E}_{\prod_{t=1}^{T} p_{\theta}(y_t|x_t)} \left[ \frac{n(i_1, \ldots, i_N)}{T} \right] \]

C. Additional visualization of \( J(\theta) \)

In Figures 3, 4 and 5, we show three visualization examples of \( J(\theta) \) for the OCR dataset on three different affine spaces, part of the first example was included in Figure 1. The six sub-figures in each example show the same profile from six different angles, spinning clock-wise from (a)-(f). The red dots indicate the global minimum.
In Figure 6, we show the same type of profiles as above except using synthetic data for a binary classification problem. First, we sequentially generated a sequence of states from 0, 1 by a hidden Markov model. Then we sample the corresponding data points from two separate 2-dimensional Gaussian models accordingly.

**D. Additional visualization of $\mathcal{L}(\theta, V)$**

Figure 7 shows the profile of $\mathcal{L}(\theta, V)$ for the OCR data set on a two-dimensional affine space viewed from nine different angles. The red dots show the saddle points of the profile, one for each angle.

**E. Experiment Details**

In the experiment, we implement the model with Python 2.7 and Tensorflow 0.12.

In training of models both on OCR and Spell-Corr task, we initialize the primal parameters in Formula (9) with $w_{\text{init}} = 1/dim(x)$ and $\gamma = 10$, where $dim(x)$ is the dimension of input. And we initialize the dual parameters $V_{\text{init}}$ with uniformly distributed random variables $v \sim U(-1, 0)$. We set the learning rate for primal parameter $\mu_\theta = 10^{-6}$ and learning rate for dual parameter $\mu_v = 10^{-4}$. We use Adam optimization to train our model.

The test set of OCR is generated also from UWIII database, but avoiding overlap with training set. The size of test set of OCR is 15000. Furthermore, the size of the test set of Spell-Corr is also 15000 without overlapping with the training set.
An Unsupervised Learning Method Exploiting Sequential Output Statistics

Figure 3. Profile Example I: $\mathcal{J}(\theta)$ for the OCR dataset on a two-dimensional affine space

Figure 4. Profile Example II: $\mathcal{J}(\theta)$ for the OCR dataset on a two-dimensional affine space
Figure 5. Profile Example III: \(J(\theta)\) for the OCR dataset on a two-dimensional affine space

Figure 6. Complete \(J(\theta)\) profile created from 2-dim synthetic data with two parameters
Figure 7. Profile of $\mathcal{L}(\theta, V)$ for the OCR dataset on a two-dimensional affine space. Red dots show the saddle points (the optimal solution) of the profile from nine different angles.