Learning Generative ConvNet with Continuous Latent Factors by Alternating Back-Propagation

Tian Han, Yang Lu, Song-Chun Zhu, and Ying Nian Wu
Department of Statistics
University of California, Los Angeles

Abstract

The supervised learning of the discriminative convolutional neural network (ConvNet or CNN) is powered by back-propagation on the parameters. In this paper, we show that the unsupervised learning of a popular top-down generative ConvNet model with latent continuous factors can be accomplished by a learning algorithm that consists of alternatively performing back-propagation on both the latent factors and the parameters. The model is a non-linear generalization of factor analysis, where the high-dimensional observed data vector, such as an image, is assumed to be the noisy version of a vector generated by a non-linear transformation of a low-dimensional vector of continuous latent factors. Furthermore, it is assumed that these latent factors follow known independent distributions, such as standard normal distributions, and the non-linear transformation is assumed to be parametrized by a top-down ConvNet, which is capable of approximating the highly non-linear mapping from the latent factors to the image. We explore a simple and natural learning algorithm for this model that alternates between the following two steps: (1) inferring the latent factors by Langevin dynamics or gradient descent, and (2) updating the parameters of the ConvNet by gradient descent. Step (1) is based on the gradient of the reconstruction error with respect to the latent factors, which is readily available by back-propagation. We call this step inferential back-propagation. Step (2) is based on the gradient of the reconstruction error with respect to the parameters, and is also obtained by back-propagation. We refer to this step as learning back-propagation. The code for inferential back-propagation in (1) is actually part of the code for learning back-propagation in (2), and thus the inferential back-propagation in (1) is actually a by-product of the learning back-propagation in (2). We show that such an alternating back-propagation algorithm can learn realistic generative models of natural images and sounds.

1 Introduction

1.1 Top down generative ConvNet

The convolutional neural network (ConvNet or CNN) (LeCun et al., 1998) has proven to be a powerful tool for approximating highly non-linear continuous mappings. Recent successes in image classification and supervised learning (Krizhevsky et al., 2012) have underscored the utility of the ConvNet in a wide range of learning tasks. The expressive power of the ConvNet has also been exploited for image generation (Dosovitskiy et al., 2015; Gatys et al., 2015): in this generative context, the ConvNet is often referred to as the inverse ConvNet (Dosovitskiy et al., 2015), the deconvolution network (Zeiler et al., 2011; Zeiler & Fergus, 2014), the generator network (in the context of a generator-discriminator adversarial pair) (Goodfellow et al., 2014; Radford et al., 2015), or the generative ConvNet (Dai et al., 2015; Lu et al., 2016).

In this paper, we consider a model that has become increasingly popular in the recent literature on deep generative models (Goodfellow et al., 2014; Kingma & Welling, 2014; Rezende et al., 2014; Mnih & Gregor, 2014; Denton et al., 2015; Kulkarni et al., 2015; Gregor et al., 2015; Radford et al., 2015).

*Equal contributions.
For want of a name that is both concrete and informative, we temporarily refer to it as the top-down generative ConvNet model with continuous latent factors. The model assumes that the high-dimensional observed data vector, e.g., an image, is generated by a low-dimensional vector of latent continuous factors. Furthermore, the latent factors are assumed to be independent and follow known distributions such as standard normal distributions. The transformation that maps the vector of latent factors to the observed data vector is assumed to be parametrized by a feedforward network such as a ConvNet. Since the transformation is from the latent factors to the image, we refer to it as the top-down network or the top-down ConvNet. Because of its power of representing complex non-linear continuous transformations, the top-down ConvNet is able to transform the simple distribution of the latent factors into the highly complex distribution of the observed data vector.

Such a latent factor model has the following advantages. (1) Analysis: the model disentangles the variations in the observed data vectors into independent variations of latent factors, which trace out the non-linear variations in the observed data. (2) Synthesis: the model can easily synthesize new images by sampling the factors from the known distribution and transforming the factors into the image. This feature of the model is highly advantageous when compared to other models that require Markov chain Monte Carlo (MCMC) for sampling. (3) Embedding: the model embeds the high-dimensional non-Euclidean manifold formed by the observed data vectors into the low-dimensional Euclidean space of latent factors, so that linear interpolation or extrapolation in the low-dimensional factor space results in meaningful and continuous non-linear interpolation or extrapolation in the data space.

1.2 Modeling spatial and temporal processes

To model spatial processes and time series that exhibit stochastic repetitiveness or stationarity in the spatial or temporal domains (or both), we may assume that the independent and identically distributed latent factors form an image or a sequence, and use the top-down ConvNet to transform the latent factors into the signals. Because of the translation invariant nature of the convolutions in the ConvNet, the generated signals will naturally be stationary.

1.3 Alternating back-propagation

In our treatment of the above latent factor model, we assume that the observed data vector is a noisy version of the vector obtained by the ConvNet transformation of the latent factors. We also assume that the noise is Gaussian white noise - in other words, the latent factors only approximately reconstruct the observed data vector. Under the above assumption, we explore a simple and natural learning algorithm that alternates between the following two steps:

(1) Inferential back-propagation: Inferring the latent factors by gradient descent or Langevin dynamics based on the posterior distribution of the latent factors. This step is based on the gradient of the reconstruction error with respect to the latent factors, which is readily available via back-propagation.

(2) Learning back-propagation: Updating the parameters of the ConvNet given the inferred latent factors. This step is based on the gradient of the reconstruction error with respect to the parameters, and is also obtained by back-propagation.

The inferential back-propagation phase seeks to solve an inverse problem: invert the top-down ConvNet mapping from the latent factors to the image, in order to obtain the latent factors from the observed image. An appealing feature of the learning algorithm is that the code used for inferential back-propagation is part of the code used for learning back-propagation, so that inferential back-propagation is actually a by-product of learning back-propagation. We show that this alternating back-propagation algorithm can learn realistic generative models of natural images and sounds.

2 Related work and contribution

2.1 Assisting networks

The generative network with latent factors belongs to the broader family of direct generative models. Such generative models have been closely studied in recent years; see, for example, the recent work of Goodfellow et al. (2014), Denton et al. (2015), Radford et al. (2015) on the generative adversarial network, and the work of Kingma & Welling (2014), Rezende et al. (2014), Mnih & Gregor (2014) on
the variational Bayes auto-encoder. The paper of Goodfellow et al. (2014) also contains a summary and comparison of other types of generative models, but these are beyond the scope of this paper.

Learning direct generative models with latent variables is as interesting as it is difficult. For such models, the marginal distribution of the observed data vector often does not have a closed form because it involves integrating out the latent variables. As a result, the posterior distribution of the latent variables given the observed data vector, which is the basis for inferring the latent variables, does not have a closed form expression either. Learning such latent variable models often involves iterating between inferring the latent variables given the parameters, and updating the parameters given the hidden variables. This iterative learning scheme is typified by the EM algorithm (Dempster et al., 1977) and the data augmentation algorithm (Tanner & Wong, 1987), but the fact that the posterior distribution of the latent variables is not in closed form usually renders EM or data augmentation inapplicable.

Two ingenious schemes have recently been devised in order to address this problem, both of which involve an assisting network with a separate set of parameters in addition to the original network that generates the data vector. In the first scheme (Kingma & Welling, 2014; Rezende et al., 2014; Mnih & Gregor, 2014), the assisting network is an inferential network that seeks to approximate the posterior distribution of the latent factors given the observed data vector. This method can be traced back to the wake-sleep algorithm (Hinton et al., 1995) and is the product of the long tradition of the variational Bayes approach (Wainwright & Jordan, 2008) for learning latent variable models. The second approach (Goodfellow et al., 2014) is based on highly original game theoretical reasoning, where the assisting network is a discriminator network that plays an adversarial role against the generator network. Specifically, the discriminator seeks to separate the data generated by the generator and the observed data, while the generator seeks to generate data in order to fool the discriminator. Both classes of methods have been implemented using ConvNet, producing interesting and sometimes stunning results in image synthesis (Denton et al., 2015; Kulkarni et al., 2015; Gregor et al., 2015; Radford et al., 2015). Equally impressive are the work of Dinh et al. (2016) based on Dinh et al. (2014), and the work of Oord et al. (2016). These models assume auto-regressive structures on the latent variables or image pixels. They are beyond the scope of this paper.

The premise of the variational Bayes approach and adversarial training is that posterior inference of the latent variables is too expensive to be practical. Although this may be the case in general, for the generative ConvNet with a relatively small number of continuous latent factors at the top layer, posterior inference of the latent factors may not be prohibitively difficult since the gradient of the reconstruction error with respect to the latent factors can be efficiently obtained by back-propagation. Hence, in this paper we choose to explore the traditional and principled approach of unsupervised learning based on posterior inference of the latent factors. The alternating back-propagation scheme studied in this paper is both simple and natural. Compared to adversarial training, inferential back-propagation infers the latent factors explicitly, producing an explicit embedding of the high-dimensional data manifold into the low-dimensional Euclidean factor space. Compared to the variational Bayes approach, inferential back-propagation is derived as an inverse of the generative network, without relying on an approximate inferential network defined by a separate set of parameters.

Nonetheless, alternating back-propagation training is complementary to variational Bayes and adversarial training: the alternating back-propagation training may help initialize the adversarial or variational Bayes training, while the variational Bayes inferential network may help initialize inferential back-propagation. After alternating back-propagation training, the learned model can be used to generate data and to train an inferential network or a discriminative network for the purpose of learning bottom-up features for other tasks. Inferential back-propagation may also help assess the trained adversarial network to see if the learned generator network can reconstruct the observed images and if the inferred factors follow the prescribed prior distribution.

Our paper appears to be related to the recent paper of Bengio (2015), which explores Langevin inference in the general context of an energy based model and establishes its relationship with back-propagation. It appears that our work is a concrete instantiation of the general musing in Bengio (2015).

The main contribution of this paper is to draw attention to a simple and natural learning algorithm based on alternating gradient computations powered by back-propagation. The learning algorithm is more direct and basic than some of the recent inventions and may serve as a complement to the latter.
2.2 Factor analysis and generalizations

The latent factor model studied in this paper is a non-linear generalization of factor analysis (Rubin & Thayer, 1982), which can be considered the prototypical template for much of the subsequent development in unsupervised learning, such as independent component analysis (Hyvärinen et al., 2004), sparse coding (Olshausen & Field, 1997), non-negative matrix factorization (Lee & Seung, 2001; Paatero & Tapper, 1994), matrix factorization for recommender systems (Koren et al., 2009), local linear embedding (Roweis & Saul, 2000), the restricted Boltzmann machine (Hinton et al., 2006), and the auto-encoder (Bengio & Courville, 2016).

The alternating back-propagation algorithm follows the tradition of alternating sweep operators as in the EM learning of factor analysis (Rubin & Thayer, 1982; Liu et al., 1998), alternating least squares for matrix factorization (Koren et al., 2009; Kim & Park, 2008), and alternating gradient descent for sparse coding (Olshausen & Field, 1997).

2.3 Generative ConvNet with no explicit latent factors

Xie et al. (2016) recently proposed a generative ConvNet model that did not involve explicit latent factors. Their energy based model (LeCun et al., 2006; Ngiam et al., 2011; Zhu et al., 1997; Roth & Black, 2005), which can be derived from the commonly used discriminative ConvNet (Krizhevsky et al., 2012), is built on bottom-up filters but has a unique internal top-down representational structure where the filters play the role of basis functions whose coefficients are binary activation variables detected by the bottom-up filters. The binary activation variables are not explicit random variables as in Hinton et al. (2006); Salakhutdinov & Hinton (2009); Lee et al. (2009), but they emerge naturally as the binary switches of the rectified linear units (ReLU) in the modern ConvNet (Krizhevsky et al., 2012). The model of Xie et al. (2016) has a very interpretable “detect and reconstruct” auto-encoding logic in its ConvNet, whereas the ConvNet mapping in the model considered in this paper is still a bit alchemical. However, the latent factor model studied in this paper has the advantage that it can be sampled directly without MCMC, and the factors can still be interpreted by examining how they influence the generated data. In terms of the learning algorithm, the model of Xie et al. (2016) is also trained by an alternating back-propagation algorithm. However, in contrast to the latent factors used in this paper, their work relies on Langevin dynamics powered by back-propagation to sample the images.

Adopting the language of Zhu (2003), the latent factor model considered in this paper can be called a generative model based on explicit latent variables in a top-down structure; an example of such models is given in Olshausen & Field (1997). In contrast, the model of Xie et al. (2016) can be considered a descriptive model based on features in a bottom-up structure, a typical example of which is given by Zhu et al. (1997), though Xie et al. (2016) discovered an unusual top-down structure in terms of an auto-encoder hidden in the local energy minima.

3 Factor analysis with top-down ConvNet loading

3.1 Factor analysis and beyond

Let Y be a D-dimensional observed data vector, such as an image. Let Z be the d-dimensional vector of latent factors, Z = (z_k, k = 1, ..., d). The traditional factor analysis model is Y = WZ + ε, where W is a D × d matrix, and ε is a D-dimensional error vector or the observational noise. We can write W = (W_1, ..., W_d), where each W_k is a D-dimensional column vector. Then Y = ∑_{k=1}^{d} z_k W_k + ε, i.e., W_k are the basis vectors and z_k are the coefficients. We can also write W = (w_1, ..., w_d)^T, where w_j^T is the j-th row of W. Then y_j = (w_j, Z) + ε_j, where y_j and ε_j are the j-th components of Y and ε respectively. Each y_j is a loading of the d factors where w_j is a vector of loading weights, indicating which factors are important for determining y_j. W is called the loading matrix. The factor analysis model can be learned by the EM algorithm, which involves alternating regressions of Z on Y in the E-step and of Y on Z in the M-step, with both steps powered by the sweep operator (Rubin & Thayer, 1982; Liu et al., 1998).
The factor analysis model is the prototype of many subsequent models that generalize the prior model of $Z$. In independent component analysis (Hyvärinen et al. 2004), $d = D$, $\epsilon = 0$, and $z_k$ are assumed to follow independent heavy tailed distributions. In sparse coding (Olshausen & Field 1997), $d > D$, and $Z$ is assumed to be a redundant but sparse vector, i.e., only a small number of $z_k$ are nonzero or significantly different from zero. In non-negative matrix factorization (Lee & Seung 2001, Paatero & Tapper 1994), it is assumed that $z_k \geq 0$. In customer rating and recommender system (Koren et al. 2009), $Z$ is a vector of a customer’s desires in different aspects and $w_i$ is a vector of a product’s desirabilities in these aspects. The $\ell_2$ penalty term in matrix factorization corresponds to a Gaussian prior model of $Z$.

The factor analysis model is a special example where both the observed data model $p(Y|W)$ and the posterior distribution $p(Z|Y, W)$ are available in closed form. Any of the above mentioned generalizations of the model may result in implicit or intractable $p(Y|W)$, $p(Z|Y, W)$, or both.

3.2 Recursive and piecewise factor analysis with ReLU ConvNet

In addition to generalizing the prior distribution of the latent factors $Z$, we can also generalize the mapping from $Z$ to $Y$. In this paper, we consider the model that retains the assumptions that $d < D$, $Z \sim N(0, I_d)$, and $\epsilon \sim N(0, \sigma^2 I_D)$ as in traditional factor analysis, but generalizes the linear loading $WZ$ to a non-linear loading $f(Z; W)$, where $f$ is a ConvNet, and $W$ collects all the connection weights and bias terms of the ConvNet. Then the model becomes

$$Y = f(Z; W) + \epsilon,$$

$$Z \sim N(0, I_d), \quad \epsilon \sim N(0, \sigma^2 I_D), \quad d < D. \tag{1}$$

The reconstruction error is $||Y - f(Z; W)||^2$. We may also assume $\epsilon$ to be colored noise and weight the frequency bands of the residual image $Y - f(Z; W)$ differently, i.e., the frequency components of $\epsilon$ are assumed to have unequal variances. Although $f(Z; W)$ can be any non-linear mapping, the ConvNet parameterization of $f(Z; W)$ makes it particularly close to the original factor analysis. Specifically, we can write the top-down ConvNet as follows

$$f(Z; W) = f_1(W_1 f_2(W_2 ... f_L(W_L Z + b_L) + ... + b_2) + b_1), \tag{2}$$

where $f_1$ is element-wise non-linearity at layer $l$, $W_l$ is the matrix of connection weights, $b_l$ is the vector of bias terms at layer $l$, and $W = (W_l, b_l, l = 1, ..., L)$. We may write equation (2) recursively as

$$Z^{(l-1)} = f_l(W_l Z^{(l)} + b_l), \tag{3}$$

with $Z^{(0)} = f(Z; W)$, and $Z^{(L)} = Z$. The top-down ConvNet (3) can be considered a recursion of the original factor analysis model, where the factors at the layer $l-1$ are obtained by the linear superposition of the basis vectors or basis functions that are column vectors of $W_l$, with the factors at the layer $l$ being the coefficients of the linear superposition. In the case of ConvNet, the basis functions are shift-invariant versions of one another, like wavelets. The element-wise non-linearity $f_l$ in modern ConvNet is usually the two-piece linearity, such as ReLU (Krizhevsky et al. 2012) or the leaky ReLU (Maas et al. 2013, Xu et al. 2015). Each ReLU unit corresponds to a binary switch. For the case of non-leaky ReLU, following the analysis of Pascanu et al. (2013), we can write

$$Z^{(l-1)} = \delta_l(W_l Z^{(l)} + b_l), \tag{4}$$

where $\delta_l = \text{diag}(1(W_l Z^{(l)} + b_l > 0))$ is a diagonal matrix, 1() is an element-wise indicator function, and diag(vector) returns a diagonal matrix whose diagonal elements form the vector. For the case of leaky ReLU, the 0 values on the diagonal are replaced by a leaking factor (e.g., 0.2), $\delta = (\delta_l, l = 1, ..., L)$ forms a classification of $Z$ according to the network $W$. Specifically, the factor space of $Z$ is divided into a large number of pieces by the hyper-planes $W_l Z^{(l)} + b_l = 0$, and each piece is indexed by an instantiation of $\delta$. We can write $\delta = \delta(Z; W)$ to make explicit its dependence on $Z$ and $W$. On the piece indexed by $\delta$, $f(Z; W) = W_l Z + b_l$. Assuming $b_l = 0, \forall l$, for simplicity, we have $W_\delta = \delta_1 W_1 ... \delta_L W_L$. Thus each piece defined by $\delta = \delta(Z; W)$ corresponds to an original factor analysis $Y = W_\delta Z + \epsilon$, whose basis $W_\delta$ is a multiplicative recomposition of the basis functions at multiple layers $(W_l, l = 1, ..., L)$, and the recomposition is controlled by the
binary switches at multiple layers $\delta = (\delta_i, l = 1, \ldots, L)$. Hence the top-down ConvNet amounts to a reconﬁgurable basis $W_\delta$ for representing $Y$, and the model is a piecewise linear factor analysis.

Model (1) can be considered an explicit implementation of the local linear embedding (Roweis & Saul, 2000), where $Z$ is the embedding of $Y$. In local linear embedding, the mapping between $Z$ and $Y$ is implicit. In model (1), the mapping from $Z$ to $Y$ is explicit. With ReLU ConvNet, the mapping is piecewise linear, which is consistent with local linear embedding, except that the partition of the linear pieces by $\delta(Z; W)$ in model (1) is learned automatically without resorting to a pre-deﬁned neighborhood system in the high dimensional space of $Y$ as in local linear embedding. Model (1) is also related to the auto-encoder, where $Z$ is the encoding of $Y$, and $Y$ is the decoding of $Z$. The inference step seeks to encode $Y$ by $Z$.

4 Alternating back-propagation

4.1 Inference by gradient descent

If we observe a training set of data vectors $\{Y_i, i = 1, \ldots, n\}$, then each $Y_i$ has a corresponding $Z_i$, but all the $Y_i$ share the same ConvNet $W$. Intuitively, we should infer $\{Z_i\}$ and learn $W$ to minimize the reconstruction error $\sum_i ||Y_i - f(Z_i; W)||^2$ plus a regularization term that corresponds to the prior on $Z$.

More formally, the model can be written as $Z \sim p(Z)$ and $[Y|Z, W] \sim p(Y|Z, W)$. Adopting the language of the EM algorithm, the complete-data model is $p(Y, Z; W) = p(Z)p(Y|Z, W)$, and the observed-data model is $p(Y; W) = \int p(Z)p(Y|Z, W)dZ$. The posterior distribution of $Z$ is given by $p(Z|Y, W) = p(Y, Z; W)/p(Y; W) \propto p(Z)p(Y|Z, W)$ as a function of $Z$.

For the training data $\{Y_i\}$, the complete-data log-likelihood is

$$L(W, \{Z_i\}) = \sum_{i=1}^{n} \log p(Y_i, Z_i; W)$$

$$= - \sum_{i=1}^{n} \left[ \frac{||Y_i - f(Z_i; W)||^2}{2\sigma^2} + \frac{||Z_i||^2}{2} \right] + \text{constant},$$ (5)

where we assume $\sigma^2$ is given.

We can estimate $W$ and infer $Z_i$ by jointly maximizing $L(W, \{Z_i\})$. The gradients with respect to $Z_i$ and $W$ are respectively

$$\frac{\partial L}{\partial Z_i} = \frac{1}{\sigma^2}(Y_i - f(Z_i; W)) \frac{\partial f(Z_i; W)}{\partial Z_i} - Z_i,$$ (6)

$$\frac{\partial L}{\partial W} = \sum_{i=1}^{n} \frac{1}{\sigma^2}(Y_i - f(Z_i; W)) \frac{\partial f(Z_i; W)}{\partial W}.$$ (7)

Maximum likelihood estimation can be accomplished by the alternating gradient descent algorithm that iterates the following two steps: (1) Inference step: update $Z_i$ by running $L$ steps of gradient descent. (2) Learning step: update $W$ by one step of gradient descent.

Algorithm [1] describes the details of the alternating back-propagation learning algorithm.

Both the inferential back-propagation and the learning back-propagation stages are guided by the residual $Y_i - f(Z_i; W)$. Inferential back-propagation is based on $\partial f(Z; W)/\partial Z$ in (6), whereas learning back-propagation is based on $\partial f(Z; W)/\partial W$ in (7). Both gradients are readily available by back-propagation computations, which share most of their operations. Specifically, for the top-down ConvNet defined by (2) and (3), $\partial f(Z; W)/\partial W$ and $\partial f(Z; W)/\partial Z$ share the same code for the chain rule computation of $\partial Z(l_i)/\partial Z(l_j)$ for $l = 1, \ldots, L$. Thus, the code for $\partial f(Z; W)/\partial Z$ is part of the code for $\partial f(Z; W)/\partial W$. In fact, with $f(Z; W) = W_\delta Z$, $\partial f(Z; W)/\partial Z = W_\delta$. If $Z$ belongs to the piece defined by $\delta$, then the inferential back-propagation seeks to approximate $Y$ by the basis $W_\delta$ by ridge regression. Because $\delta(Z; W)$ keeps changing, the algorithm searches for the optimal reconﬁgurable basis $W_\delta$ to approximate $Y$. At the local stationary point, $Z$ satisfies an auto-encoder $Z = W_\delta^2 (Y - W_\delta Z)/\sigma^2$, with $\delta = \delta(Z; W)$. Assuming $\delta$ is ﬁxed, we can solve
Algorithm 1: Alternating back-propagation with gradient descent inference

Input:
1. (1) training images \{Y_i, i = 1, ..., n\}
2. number of gradient descent steps \(L\) in inference
3. number of learning iterations \(T\)

Output:
1. (1) estimated parameters \(W\)
2. inferred latent factors \(\{Z_i, i = 1, ..., n\}\)

1: Let \(t \leftarrow 0\), initialize \(W \leftarrow 0\).
2: Initialize \(Z_i \leftarrow 0\), for \(i = 1, ..., n\).
3: repeat
4:  **Inferential back-propagation:** For each \(i\), run \(L\) steps of gradient descent to update \(Z_i\), i.e., starting from the current value of \(Z_i\), each step is driven by the gradient given in (6).
5:  **Learning back-propagation:** Update \(W \leftarrow W + \eta \frac{\partial L(W, \{Z_i\})}{\partial W}\), where the gradient is given in (7), with step size \(\eta\).
6:  Let \(t \leftarrow t + 1\)
7: until \(t = T\)

\(Z = (W_\delta^\top W_\delta + \sigma^2 I_d)^{-1} W_\delta^\top Y\) by ridge regression. In general, we may solve \(Z\) by iterated ridge regression, \(Z_{\tau + 1} = (W_\delta^\top W_\delta + \sigma^2 I_d)^{-1} W_\delta^\top Y\), where \(\tau\) indexes the time steps, and \(\delta = \delta(Z_{\tau}; W)\), which can change over time \(\tau\). The iterated ridge regression is actually Newton-Raphson, where the Hessian matrix is \(W_\delta^\top W_\delta/\sigma^2 + I_d\). If we do not assume \(b_l = 0, \forall l\), then we should replace \(Y\) in the above iterated ridge regression by \(Y - b_\delta = Y - f(Z_{\tau}; W) + W_\delta Z_{\tau}\). The iterated ridge regression is computationally more expensive than the simple gradient descent.

We may also modify Algorithm 1 by a joint gradient descent on both \(W\) and \(\{Z_i\}\) simultaneously. In this joint back-propagation algorithm, both gradients are based on the same \(Y_i - f(Z_i; W)\), and \(\frac{\partial f(Z; W)}{\partial Z}\) is actually a by-product of \(\frac{\partial f(Z; W)}{\partial W}\) not only in coding, but also in actual computational results.

4.2 Inference by Langevin dynamics

A more rigorous approach to maximum likelihood learning involves maximizing the observed-data log-likelihood \(L(W) = \sum_{i=1}^n \log p(Y_i; W) = \sum_{i=1}^n \sum_{i=1}^{n} \log \int p(Y_i, Z_i; W)dZ_i\), where the latent factors have been integrated out. For convenience, we continue to use \(L()\) to denote the observed-data log-likelihood.

The gradient of \(L(W)\) can be calculated according to the following well-known fact

\[
\frac{\partial}{\partial W} \log p(Y; W) = \frac{1}{P(Y; W)} \frac{\partial}{\partial W} \int p(Y, Z; W)dZ = \frac{1}{P(Y; W)} \int \left[ \frac{\partial}{\partial W} \log p(Y, Z; W) \right] p(Y, Z; W)dZ = \frac{1}{P(Y; W)} \int \left[ \frac{\partial}{\partial W} \log p(Y, Z; W) \right] \frac{p(Y, Z; W)}{p(Y; W)}dZ = E_{p(Z|Y, W)} \left[ \frac{\partial}{\partial W} \log p(Y, Z; W) \right].
\]

(8)

The expectation with respect to \(p(Z|Y, W)\) can be approximated by drawing samples from \(p(Z|Y, W)\) and then computing the Monte Carlo average.

The above fact has a geometric interpretation that encodes the properties of the EM algorithm for maximizing \(L(W)\). Consider the curve \(l(W) = \log p(Y; W)\) and the curve \(q(W|W') = E_{p(Z|Y, W')} | \log p(Y, Z; W) + \text{entropy}, \text{ with } W' \text{ fixed}\). The entropy term is the entropy of \(p(Z|Y, W')\), which is constant relative to \(W\). These two curves touch at \(W'\) and they are co-tangent at \(W'\), i.e., both curves share the same tangent at \(W'\), according to (6). Moreover, \(l(W)\) majorizes \(q(W|W')\), i.e., \(l(W) \geq q(W|W')\) for all \(W\), justifying the monotonicity of EM.
To derive a loss function appropriate for learning, we first note that
\[ -\log p(Z|Y, W) = \frac{1}{2\sigma^2} \|Y - f(Z; W)\|^2 + \frac{1}{2} Z^2 + \text{constant}. \] (9)

Therefore, the Langevin dynamics for sampling Z is
\[ Z_{t+1} = Z_t + \Delta \frac{1}{\sigma^2} (Y - f(Z_t; W)) \frac{\partial}{\partial Z} f(Z_t; W) - Z_t + \Delta E, \] (10)

where \( \Delta \) denotes a random noise vector that follows \( N(0, \mathbb{I}) \). Although Langevin dynamics can be formally justified by stochastic differential equations, it can be more easily understood by analyzing the expectation and variance of the one-step displacement of a Metropolis algorithm whose base chain is a symmetric random walk with a step size \( \Delta \).

The stochastic gradient algorithm of [Younes, 1999] can be used for learning, where for each \( Z_i \), only a single copy of \( Z_i \) is sampled from \( p(Z_i|Y_i, W) \) by running a finite number of steps of Langevin dynamics starting from the current value of \( Z_i \). With \( \{Z_i\} \) sampled in this manner, we can update the parameter \( W \) based on the gradient \( \hat{L}'(W) \) which is an approximation to \( L'(W) \):
\[
\hat{L}'(W) = \sum_{i=1}^{n} \frac{\partial}{\partial W} \log p(Y_i, Z_i; W) = -\sum_{i=1}^{n} \frac{\partial}{\partial W} \frac{1}{2\sigma^2} ||Y_i - f(Z_i; W)||^2 \\
= \sum_{i=1}^{n} \frac{1}{\sigma^2} (Y_i - f(Z_i; W)) \frac{\partial}{\partial W} f(Z_i; W).
\] (11)

Algorithm 2 describes the details of the learning and sampling algorithm.

Algorithm 2: Alternating back-propagation with Langevin inference

**Input:**
1. Training images \( \{Y_i, i = 1, \ldots, n\} \)
2. Number of Langevin steps \( L \)
3. Number of learning iterations \( T \)

**Output:**
1. Estimated parameters \( W \)
2. Inferred latent factors \( \{Z_i, i = 1, \ldots, n\} \)

1. Let \( t \leftarrow 0 \), initialize \( W \leftarrow 0 \).
2. Initialize \( Z_i \leftarrow 0 \), for \( i = 1, \ldots, n \).
3. repeat
   4. **Inferential back-propagation:** For each \( i \), run \( L \) steps of Langevin dynamics to sample \( Z_i \sim p(Z_i|Y_i, W) \), i.e., starting from the current \( Z_i \), each step follows equation (10).
   5. **Learning back-propagation:** Update \( W \leftarrow W + \eta \hat{L}'(W) \), where \( \hat{L}'(W) \) is computed according to equation (11), with step size \( \eta \).
4. Let \( t \leftarrow t + 1 \)
5. until \( t = T \)

In Algorithm 2, the Langevin dynamics samples from a gradually changing posterior distribution \( p(Z_i|Y_i, W) \) because \( W \) keeps changing. The updatings of both \( Z_i \) and \( W \) collaborate to reduce the reconstruction error \( ||Y_i - f(Z_i; W)||^2 \). The parameter \( \sigma^2 \) plays the role of annealing or tempering in Langevin sampling. If \( \sigma^2 \) is very large, then the posterior is close to the prior \( N(0, \mathbb{I}) \). If \( \sigma^2 \) is very small, then the posterior may be multi-modal, but the changing energy landscape of \( p(Z_i|Y_i, W) \) may help alleviate the trapping of local modes. In practice, we tune the value of \( \sigma^2 \) instead of estimating it. The Langevin dynamics can be extended to Hamiltonian Monte Carlo [Neal, 2011] or more sophisticated versions [Girolami & Calderhead, 2011].

If the Gaussian noise in the Langevin inference is removed, then the above procedure becomes the alternating gradient descent given in Algorithm 1. Alternatively, if Gaussian noise is added to the learning step yielding Langevin dynamics in a full Bayesian treatment [Welling & Teh, 2011], then the algorithm will become an alternating Langevin dynamics that samples the joint posterior distribution of both \( \{Z_i\} \) and \( W \).
5 Experiments

The code in our experiments is based on the MatConvNet package of Vedaldi & Lenc (2015). The data, code and more results are available from the project page [http://www.stat.ucla.edu/~ywu/ABP/main.html](http://www.stat.ucla.edu/~ywu/ABP/main.html).

The training images and sounds are scaled so that the intensities are within the range $[-1, 1]$. We adopt the structure of the generator network of Radford et al. (2015) and Dosovitskiy et al. (2015), where the top-down network consists of multiple layers of deconvolution by linear superposition, ReLU non-linearity, and up-sampling, with tanh non-linearity at the bottom-layer (Radford et al., 2015).
Figure 2: Modeling texture patterns. Left: $224 \times 224$ observed image. Right: $448 \times 448$ generated image.
to make the signals fall within $[-1, 1]$. We also adopt batch normalization layers (Ioffe & Szegedy, 2015) following the now standard practice.

Throughout this paper, we use the alternating back-propagation algorithm with Langevin inference, i.e., Algorithm 2. We fix $\sigma = 0.3$. We use $L = 10$ or 30 steps for Langevin dynamics within each learning iteration, and the Langevin step size $\Delta$ is set at 0.1 or 0.3. We run $T = 600$ learning iterations, with learning rate .0001, and momentum .5. The learning algorithm produces the learned network parameters $W$ and the inferred latent factors $Z$ for each image $Y$ in the end. The synthesized images are obtained by $f(Z; W)$, where $Z$ is sampled from the prior distribution $N(0, I_d)$. 

Figure 3: Mixed texture pattern. Left two images: $224 \times 224$ observed images. Right: $448 \times 448$ generated image.

Figure 4: Modeling sound patterns. The first plot is the waveform of the training sound (the range is 0-5 seconds). The next three plots are the waveforms of the synthesized sounds (the range is 0-11 seconds).
5.1 Modeling texture patterns

We learn a separate model from each texture image. The images are collected from the Internet, and then resized to 224 × 224. The synthesized images are 448 × 448. Figures 1 and 2 show some examples. Figure 3 shows an example of learning the model from two training images.

The factors $Z$ at the top layer form a $\sqrt{d} \times \sqrt{d}$ image, with each pixel following $N(0, 1)$ independently. The $\sqrt{d} \times \sqrt{d}$ image $Z$ is then transformed to $Y$ by the top-down ConvNet. We use $d = 7^2$ in the learning stage for all the texture experiments. In order to obtain the synthesized image, we randomly sample a $14 \times 14 Z$ from $N(0, I)$, and then use the learned network $W$ to generate the 448 × 448 synthesized image $f(Z; W)$.

The training network is as follows. Starting from $7 \times 7$ Gaussian white noise image $Z$, the network has 5 layers of deconvolution with $5 \times 5$ kernels (i.e., linear superposition with $5 \times 5$ basis functions), with a up-sampling factor of 2 at each layer (i.e., the basis functions are 2 pixels apart). The number of channels in the first layer is 512 (i.e., 512 translation invariant basis functions), and is decreased by a factor 2 at each layer. The Langevin steps $L = 10$ with step size $\Delta = .1$.

5.2 Modeling sound patterns

We treat a sound signal as a one-dimensional texture image. The sound data are collected from the Internet. Each training signal is a 5 second clip with the sampling rate of 11025 Hertz and is represented as a $1 \times 60000$ vector. We learn a separate model from each sound signal.

The latent factors $Z$ form a sequence that follows $N(0, I_d)$, with $d = 6$. The top-down network consists of 4 layers of deconvolution with kernels of size $1 \times 25$, and up-sampling factor of 10. The number of channels in the first layer is 256, and decreases by a factor of 2 at each layer. For synthesis, we start from a longer Gaussian white noise sequence $Z$ with $d = 12$ and generate the synthesized sound using the learned parameters. Figure 4 shows the waveforms of the observed sound signal in the first row and the synthesized sound signals in the next three rows. The reader can listen to the sounds at [http://www.stat.ucla.edu/~yw/AAB/main.html](http://www.stat.ucla.edu/~yw/AAB/main.html).

5.3 Modeling object patterns

We model object patterns using the network structure that is essentially the same as the network for the texture model, except that we include a fully connected layer under the latent factors $Z$. The images are $64 \times 64$. We use ReLU with a leaking factor 0.2 (Maas et al., 2013; Xu et al., 2015) to avoid piecewise constant pieces in the ConvNet mapping and to make it more linear. The Langevin steps $L = 30$ with step size $\Delta = .3$.

In the first experiment, we learn a model where $Z$ has two components, i.e., $Z = (z_1, z_2)$, and $d = 2$. The training data are 11 images of 6 tigers and 5 lions. After training the model, we generate images using the learned top-down ConvNet for $(z_1, z_2) \in [-2, 2]^2$, where we discretize both $z_1$ and $z_2$ into 9 equally spaced values. Figure 5 displays the synthesized images on the $9 \times 9$ panel.

In the second experiment, we learn a model with $d = 100$ from 1000 face images randomly selected from the celebA dataset (Liu et al., 2015). Figure 6(a) displays the images generated by the learned model. (b) displays the interpolation results. The images at the four corners are generated by the $Z$ vectors of four images randomly selected from the training set. The images in the middle are obtained by first interpolating the $Z$’s of the four corner images using the sphere interpolation (Dinh et al., 2016) and then generating the images by the learned ConvNet.

6 Discussion

This paper explores an alternating back-propagation algorithm for unsupervised learning of the generative ConvNet model with continuous latent factors. Compared to supervised learning of the discriminative ConvNet powered by back-propagation, the unsupervised learning algorithm only adds an extra back-propagation stage for inferring latent factors. Moreover, this extra step is a by-product of the back-propagation of the learning step in terms of coding and computation.
Figure 5: Modeling object patterns. The synthesized images are generated by $Z = (z_1, z_2) \in [-2, 2]^2$. $Z$ is discretized into $9 \times 9$ values.

Figure 6: Modeling object patterns. Left: The synthesized images are generated by $Z \sim N(0, I_{100})$. Right: Interpolation. The images at the four corners are reconstructed from the inferred $Z$ vectors of four images randomly selected from the training set.
The ConvNet with latent factors is a non-linear generalization of the factor analysis model, where the loading matrix is replaced by the ConvNet transformation. The prior distribution of the latent factors can be changed to non-Gaussian distributions in order to incorporate more sophisticated features and structures.

**Code and data**

The code and training data can be downloaded from the project page: [http://www.stat.ucla.edu/~ywu/ABP/main.html](http://www.stat.ucla.edu/~ywu/ABP/main.html)

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