Spike-and-Slab Sparse Coding for Unsupervised Feature Discovery

Ian J. Goodfellow, Aaron Courville, Yoshua Bengio
Département d’informatique et de recherche opérationnelle
Université de Montréal
Montréal, QC H3T 1J4
{goodfeli@iro.,courvila@iro.,yoshua.bengio@umontreal.ca

Abstract

We consider the problem of using a factor model we call spike-and-slab sparse coding (S3C) to learn features for a classification task. The S3C model resembles both the spike-and-slab RBM and sparse coding. Since exact inference in this model is intractable, we derive a structured variational inference procedure and employ a variational EM training algorithm. Prior work on approximate inference for this model has not prioritized the ability to exploit parallel architectures and scale to enormous problem sizes. We present an inference procedure appropriate for use with GPUs which allows us to dramatically increase both the training set size and the amount of latent factors.

We demonstrate that this approach improves upon the supervised learning capabilities of both sparse coding and the ssRBM on the CIFAR-10 dataset. We evaluate our approach’s potential for semi-supervised learning on subsets of CIFAR-10. We use our method to win the NIPS 2011 Workshop on Challenges In Learning Hierarchical Models’ Transfer Learning Challenge.

1 The S3C model

The S3C model consists of latent binary spike variables \( h \in \{0,1\}^N \), latent real-valued slab variables \( s \in \mathbb{R}^N \), and real-valued \( D \)-dimensional visible vector \( v \in \mathbb{R}^D \) generated according to this process: \( \forall i \in \{1,\ldots,N\}, d \in \{1,\ldots,D\}, \)

\[
p(h_i = 1) = \sigma(b_i), \quad p(s_i \mid h_i) = \mathcal{N}(s_i \mid \mu_i, \alpha_{ii}^{-1}), \quad p(v_d \mid s, h) = \mathcal{N}(v_d \mid W_d (h \circ s), \beta_d^{-1})
\]

(1)

where \( \sigma \) is the logistic sigmoid function, \( b \) is a set of biases on the spike variables, \( \mu \) and \( W \) govern the linear dependence of \( s \) on \( h \) and \( v \) on \( s \) respectively, \( \alpha \) and \( \beta \) are diagonal precision matrices of their respective conditionals, and \( h \circ s \) denotes the element-wise product of \( h \) and \( s \).

To avoid overparameterizing the distribution, we constrain the columns of \( W \) to have unit norm, as in sparse coding. We restrict \( \alpha \) to be a diagonal matrix and \( \beta \) to be a diagonal matrix or a scalar. We refer to the variables \( h_i \) and \( s_i \) as jointly defining the \( i \)-th hidden unit, so that there are are total of \( N \) rather than \( 2N \) hidden units. The state of a hidden unit is best understood as \( h_i s_i \), that is, the spike variables gate the slab variables.

In the subsequent sections we motivate our use of S3C as a feature discovery algorithm by describing how this model occupies a middle ground between sparse coding and the ssRBM. The S3C model avoids many disadvantages that the ssRBM and sparse coding have when applied as feature discovery algorithms.

1.1 Comparison to sparse coding

Sparse coding has been widely used to discover features for classification (Raina et al. 2007). Recently Coates and Ng (2011a) showed that this approach achieves excellent performance on the CIFAR10 object recognition dataset.

Sparse coding (Olshausen and Field [1997]) describes a class of generative models where the observed data \( v \) is normally distributed given a set of continuous latent variables \( s \) and a dictionary...
matrix $W$: $v \sim \mathcal{N}(Ws, \sigma I)$. Sparse coding places a factorial prior on $s$ such as a Cauchy or Laplace distribution, chosen to encourage the posterior mode of $p(s \mid v)$ to be sparse. One can derive the S3C model from sparse coding by replacing the factorial Cauchy or Laplace prior with a spike-and-slab prior.

One drawback of sparse coding is that the latent variables are not merely encouraged to be sparse; they are encouraged to remain close to 0, even when they are active. This kind of regularization is not necessarily undesirable, but in the case of simple but popular priors such as the Laplace prior (corresponding to an $L_1$ penalty on the latent variables $s$), the degree of regularization on active units is confounded with the degree of sparsity. There is little reason to believe that in realistic settings, these two types of complexity control should be so tightly bound together. The S3C model avoids this issue by controlling the sparsity of units via the $b$ parameter that determines how likely each spike unit is to be active, while separately controlling the magnitude of active units via the $\mu$ and $\alpha$ parameters that govern the distribution over $s$. Sparse coding has no parameter analogous to $\mu$ and cannot control these aspects of the posterior independently.

Sparse coding is also difficult to integrate into a deep generative model of data such as natural images. While Yu et al. (2011) and Zeiler et al. (2009) have recently shown some success at learning hierarchical sparse coding, our goal is to integrate the feature extraction scheme into a proven generative model framework such as the deep Boltzmann Machine (Salakhutdinov and Hinton, 2009). Existing inference schemes known to work well in the DBM-type setting are all either sample-based or are based on variational approximations to the model posteriors, while sparse coding schemes typically employ MAP inference. Our use of variational inference makes the S3C framework well suited to integrate into the known successful strategies for learning and inference in DBM models. It is not obvious how one can employ a variational inference strategy to standard sparse coding with the goal of achieving sparse feature encoding.

1.2 Comparison to Restricted Boltzmann Machines

The S3C model also resembles another class of models commonly used for feature discovery: the RBM. An RBM (Smolensky, 1986) is an energy-based model defined through an energy function that describes the interactions between the observed data variables and a set of latent variables. It is possible to interpret the S3C as an energy-based model, by rearranging $p(v, s, h)$ to take the form

$$\exp\{-E(v, s, h)\} / Z,$$

with the following energy function:

$$E(v, s, h) = \frac{1}{2} \left( v - \sum_i W_i s_i h_i \right)^T \beta \left( v - \sum_i W_i s_i h_i \right) + \frac{1}{2} \sum_{i=1}^N \alpha_i (s_i - \mu_i h_i)^2 - \sum_{i=1}^N b_i h_i,$$

(2)

The ssRBM model family is a good starting point for S3C because it has demonstrated both reasonable performance as a feature discovery scheme and remarkable performance as a generative model (Courville et al., 2011). Within the ssRBM family, S3C’s closest relative is a variant of the $\mu$-ssRBM, defined by the following energy function:

$$E(v, s, h) = -\sum_{i=1}^N v^T \beta W_i h_i + \frac{1}{2} v^T \beta v + \frac{1}{2} \sum_{i=1}^N \alpha_i (s_i - \mu_i h_i)^2 - \sum_{i=1}^N b_i h_i,$$

(3)

where the variables and parameters are defined identically to the S3C. Comparison of equations 2 and 3 reveals that the simple addition of a latent factor interaction term $\frac{1}{2} (h \circ s)^T W^T \beta W (h \circ s)$ to the ssRBM energy function turns the ssRBM into the S3C model. With the inclusion of this term S3C moves from an undirected ssRBM model to the directed graphical model, described in equation 1. This change from undirected modeling to directed modeling has three important effects, that we describe in the following sections.

**The effect on the partition function:** The most immediate consequence of the transition to directed modeling is that the partition function becomes tractable. This changes the nature of learning algorithms that can be applied to the model, since most of the difficulty in training an RBM comes from estimating the gradient of the log partition function. The partition function of S3C is also guaranteed to exist for all possible settings of the model parameters, which is not true of the ssRBM.

**The effect on the posterior:** RBMs have a factorial posterior, but S3C and sparse coding have a complicated posterior due to the “explaining away” effect. This means that for RBMs, features defined by similar basis functions will have similar activations, while in directed models, similar features will compete so that only the most relevant feature will remain active. As shown by Coates...
Figure 1: (Left) $Q$ imposes a sparse distribution on $h$: $Q(h_i) < .01$ 91.8% of the time. The samples in this histogram are values of $Q(h_i)$ for 1600 different hidden units from a trained model applied to 100 different image patches. (Right) The inference procedure sparsifies the representation due to the explaining-away effect. $Q$ is initialized at the prior, which is very sparse. The data then drives $Q$ to become less sparse, but subsequent iterations make $Q$ become sparse again.

and Ng (2011a), the sparse Gaussian RBM is not a very good feature extractor – the set of basis functions $W$ learned by the RBM actually work better for supervised learning when these parameters are plugged into a sparse coding model than when the RBM itself is used for feature extraction. We think this is due to the factorial posterior. In the vastly overcomplete setting, being able to selectively activate a small set of features likely provides S3C a major advantage in discriminative capability.

The effect on the prior: The addition of the interaction term causes S3C to have a factorial prior. This probably makes it a poor generative model, but this is not a problem for the purpose of feature discovery.

2 Other Related work

The notion of a spike-and-slab prior was established in statistics by Mitchell and Beauchamp (1988). Outside the context of unsupervised feature discovery for supervised, semi-supervised and self-taught learning, the basic form of the S3C model (i.e. a spike-and-slab latent factor model) has appeared a number of times in different domains (Lücke and Sheikh (2011), Garritus and Olshausen, 2008, Mohamed et al. 2011, Titsias and Lázaro-Gredilla, 2011). To this literature, we contribute an inference scheme that scales to the kinds of object classifications tasks that we consider. We outline this inference scheme next.

3 Variational EM for S3C

Having explained why S3C is a powerful model for unsupervised feature discovery we turn to the problem of how to perform learning and inference in this model. Because computing the exact posterior distribution is intractable, we derive an efficient and effective inference mechanism and a variational EM learning algorithm.

We turn to variational EM (Saul and Jordan, 1996) because this algorithm is well-suited for models with latent variables whose posterior is intractable. It works by maximizing a variational lower bound on the log-likelihood called the energy functional (Neal and Hinton, 1999). More specifically, it is a variant of the EM algorithm (Dempster et al. 1977) with the modification that in the E-step, we compute a variational approximation to the posterior rather than the posterior itself. While our model admits a closed-form solution to the M-step, we found that online learning with small gradient steps on the M-step objective worked better in practice. We therefore focus our presentation on the E-step, given in Algorithm 1.

The goal of the variational E-step is to maximize the energy functional with respect to a distribution $Q$ over the unobserved variables. We can do this by selecting the $Q$ that minimizes the Kullback–Leibler divergence:

$$D_{KL}(Q(h, s)||P(h, s|v))$$

(4)
where \( Q(h, s) \) is drawn from a restricted family of distributions. This family can be chosen to ensure that \( Q \) is tractable.

Our E-step can be seen as analogous to the encoding step of the sparse coding algorithm. The key difference is that while sparse coding approximates the true posterior with a MAP point estimate of the latent variables, we approximate the true posterior with the distribution \( Q \). We use the family \( Q(h, s) = \Pi_i Q(h_i, s_i) \).

Observing that eq. (4) is an instance of the Euler-Lagrange equation \( \text{(Gelfand, 1963)} \), we find that the solution must take the form

\[
Q(h_i) = \hat{h}_i, \quad Q(s_i | h_i) = N(s_i | h_i \hat{s}_i, (\alpha_i + h_iW_i^T \beta W_i)^{-1})
\]

where \( \hat{h}_i \) and \( \hat{s}_i \) must be found by an iterative process. In a typical application of variational inference, the iterative process consists of sequentially applying fixed point equations that give the optimal value of the parameters \( \hat{h}_i \) and \( \hat{s}_i \) for one factor \( Q(h_i, s_i) \) given the value all of the other factors’ parameters. This is for example the approach taken by \( \text{Titsias and Lázaro-Gredilla (2011)} \) who independently developed a variational inference procedure for the same problem. This process is only guaranteed to decrease the KL divergence if applied to each factor sequentially, i.e. first updating \( \hat{h}_1 \) and \( \hat{s}_1 \) to optimize \( Q(h_1, s_1) \), then updating \( \hat{h}_2 \) and \( \hat{s}_2 \) to optimize \( Q(h_2, s_2) \), and so on. In a typical application of variational inference, the optimal values for each update are simply given by the solutions to the Euler-Lagrange equations. For S3C, we make three deviations from this standard approach.

Because we apply S3C to very large-scale problems, we need an algorithm that can fully exploit the benefits of parallel hardware such as GPUs. Sequential updates across all \( N \) factors require far too much runtime to be competitive in this regime.

We propose a different method that enables parallel updates to all units. First, we partially minimize the KL divergence with respect to \( \hat{s} \). The terms of the KL divergence that depend on \( \hat{s} \) make up a quadratic function so this can be minimized via conjugate gradient descent. We implement conjugate gradient descent efficiently by using the R-operator to perform Hessian-vector products rather than computing the entire Hessian explicitly \( \text{[Schraudolph, 2002]} \). This step is guaranteed to improve the KL divergence on each iteration.

We next update \( \hat{s} \) in parallel, shrinking the update by a damping coefficient. This approach is not guaranteed to decrease the KL divergence on each iteration but it is a widely applied approach that works well in practice \( \text{[Koller and Friedman, 2009]} \).

In practice we find that we can obtain a faster algorithm that reaches equally good solutions by replacing the conjugate gradient update to \( \hat{s} \) with a more heuristic approach. We use a parallel damped update on \( \hat{s} \) much like what we do for \( \hat{h} \). In this case we make an additional heuristic modification to the update rule which is made necessary by the unbounded nature of \( \hat{s} \). We clip the update to \( \hat{s} \) so that if \( \hat{s}_{\text{new}} \) has the opposite sign from \( \hat{s} \), its magnitude is at most \( \rho \hat{s} \). In all of our experiments we used \( \rho = 0.5 \) but any value in \( [0, 1] \) is sensible. This prevents a case where multiple mutually inhibitory units inhibit each other so strongly that rather than being driven to 0 they change sign and actually increase in magnitude. This case is a failure mode of the parallel updates that can result in \( \hat{s} \) amplifying without bound if clipping is not used.

We include some visualizations that demonstrate the effect of our E-step. Figure \( \text{[1]} \) (right) shows that it produces a sparse representation. Figure \( \text{[1]} \) (left) shows that the explaining-away effect incrementally makes the representation more sparse. Figure \( \text{[2]} \) (left) shows that the E-step increases the energy functional.

4 Results

We conducted experiments to evaluate the usefulness of S3C features for supervised learning and semi-supervised learning on CIFAR-10 \( \text{[Krizhevsky and Hinton, 2009]} \), a dataset consisting of color images of animals and vehicles. It contains ten labeled classes, with 5000 train and 1000 test examples per class.

For all experiments, we used the same procedure as \( \text{Coates and Ng (2011a)} \). CIFAR-10 consists of \( 32 \times 32 \) images. We train our feature extractor on \( 6 \times 6 \) contrast-normalized and ZCA-whitened patches from the training set. At test time, we extract features from all \( 6 \times 6 \) patches on an image, then
average-pool them. The average-pooling regions are arranged on a non-overlapping grid. Finally, we train a linear SVM on the pooled features.

Coates and Ng (2011a) used 1600 basis vectors in all of their sparse coding experiments. They post-processed the sparse coding feature vectors by splitting them into the positive and negative part for a total of 3200 features per average-pooling region. They average-pool on a $2 \times 2$ grid to a total of 12,800 features per image. We used $\mathbb{E}_Q[h]$ as our feature vector. This does not have a negative part, so using a $2 \times 2$ grid we would have only 6,400 features. In order to compare with similar sizes of feature vectors we used a $3 \times 3$ pooling grid for a total of 14,400 features.

### 4.1 CIFAR-10

On CIFAR-10, S3C achieves a test set accuracy of $78.3 \pm 0.9\%$ with 95% confidence (or $76.2 \pm 0.9\%$ when using a $2 \times 2$ grid). Coates and Ng (2011a) do not report test set accuracy for sparse coding with “natural encoding” (i.e., extracting features in a model whose parameters are all the same as in the model used for training) but sparse coding with different parameters for feature extraction than training achieves an accuracy of $78.8 \pm 0.9\%$ (Coates and Ng 2011a). Since we have not enhanced our performance by modifying parameters at feature extraction time these results seem to indicate that S3C is roughly equivalent to sparse coding for this classification task. S3C also outperforms ssRBMs, which require 4,096 basis vectors per patch and a $3 \times 3$ pooling grid to achieve $76.7 \pm 0.9\%$

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**Algorithm 1 Fixed-Point Inference**

```
Initialize $h^{(0)} = \sigma(b)$ and $\tilde{h}^{(0)} = \mu$. 

for $k = 0, K$ do
  Compute the individually optimal value $\hat{s}^*_i$ for each $i$ simultaneously:
  \[ h^*_i = \frac{\mu_i x_i + \alpha_i + W_i^T \beta \tilde{h}_i}{\beta \tilde{h}_i + W_i^T} \]
  Clip reflections by assigning
  \[ s^*_i = \mu_i \text{sign}(\hat{s}^*_i) \] if $|\hat{s}^*_i| > \rho |\hat{x}_i|$.
  Dump the updates by assigning
  \[ s^*_i = \hat{s}^*_i \] for all other $i$.

  Compute the individually optimal values for $h$:
  \[ h^{(k+1)} = \sigma \left( v - \sum_{j \neq i} W_j \hat{s}^{(k+1)}_j h_i^{(k)} + \frac{1}{2} W_i \hat{s}^{(k+1)}_i b_i \right)^T \beta W_i \hat{s}^{(k+1)}_i + b_i + \frac{1}{2} \log(\alpha_i + W_i^T \beta W_i) + \frac{1}{2} \log(\alpha_i) \]

  Dump the update for $\tilde{h}$:
  \[ \tilde{h}^{(k+1)} = \eta \tilde{h}^*_i + (1 - \eta) \tilde{h}^{(k)} \]

end for
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**Figure 2:** (Left) The energy functional of a batch of 5000 image patches increases during the E-step. (Right) Semi-supervised classification accuracy on CIFAR-10. In both cases the hyperparameters for the unsupervised stage were optimized for performance on the full CIFAR-10 dataset, not re-optimized for each point on the learning curve.
accuracy. All of these approaches are close to the state of the art of 82.0 ± 0.8 %, which used a three-layer network [Coates and Ng, 2011b]. We also used CIFAR-10 to evaluate S3C’s semi-supervised learning performance by training the SVM on small subsets of the CIFAR-10 training set, but using features that were learned on the entire CIFAR-10 train set. The results, summarized in Figure 2(right) show that S3C is most advantageous for medium amounts of labeled data. S3C features thus include an aspect of flexible regularization—they improve generalization for smaller training sets yet do not cause underfitting on larger ones.

5 Transfer Learning Challenge

For the NIPS 2011 Workshop on Challenges in Learning Hierarchical Models [Le et al., 2011], the organizers proposed a transfer learning competition. This competition used a dataset consisting of 32 × 32 color images, including 100,000 unlabeled examples, 50,000 labeled examples of 100 object classes not present in the test set, and 120 labeled examples of 10 object classes present in the test set. The test set was not made public until after the competition. We chose to disregard the 50,000 labels and treat this as a semi-supervised learning task. We applied the same approach as on CIFAR-10 and won the competition, with a test set accuracy of 48.6 %.

6 Conclusion

We have motivated the use of the S3C model for unsupervised feature discovery. We have described a variational approximation scheme that makes it feasible to perform learning and inference in large-scale S3C models. Finally, we have demonstrated that S3C is an effective feature discovery algorithm for supervised, semi-supervised, and self-taught learning.

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