Abstract

Bayesian optimization has been demonstrated as an effective methodology for the global optimization of functions with expensive evaluations. Its strategy relies on querying a distribution over functions defined by a relatively cheap surrogate model. The ability to accurately model this distribution over functions is critical to the effectiveness of Bayesian optimization, and is typically fit using Gaussian processes (GPs). However, since GPs scale cubically with the number of observations, it has been challenging to handle objectives whose optimization requires a large number of evaluations, and as such, massively parallelizing the optimization.

In this work, we explore the use of neural networks as an alternative to Gaussian processes to model distributions over functions. We show that performing adaptive basis function regression with a neural network as the parametric form performs competitively with state-of-the-art GP-based approaches, but scales linearly with the number of data rather than cubically. This allows us to achieve a previously intractable degree of parallelism, which we use to rapidly search over large spaces of models. We achieve state-of-the-art results on benchmark object recognition tasks using convolutional neural networks, and image caption generation using multimodal neural language models.

1. Introduction

Recently, the field of machine learning has seen unprecedented growth due to a new wealth of data, increases in computational power, new algorithms, and a plethora of exciting new applications. As researchers tackle more ambitious problems, the models they use are also becoming more sophisticated. However, the growing complexity of machine learning models inevitably comes with the introduction of additional hyperparameters. These range from design decisions, such as the shape of a neural network architecture, to optimization parameters, such as learning rates, to regularization hyperparameters such as weight decay. Proper setting of these hyperparameters is critical for performance on difficult problems.

There are many methods for optimizing over hyperparameter settings, ranging from simplistic procedures like grid or random search (Bergstra & Bengio, 2012), to more sophisticated model-based approaches using random forests (Hutter et al., 2011) or Gaussian processes (Snoek et al., 2012). Bayesian optimization is a natural framework for model-based global optimization of noisy, expensive black-box functions. It offers a principled approach to modeling uncertainty, which allows exploration and exploitation to be naturally bal-
anced during the search. Perhaps the most commonly used model for Bayesian optimization is the Gaussian process (GP) due to its simplicity and flexibility in terms of conditioning and inference.

However, a major drawback of GP-based Bayesian optimization is that inference time grows cubically in the number of observations, due to the need to solve a linear system with a dense covariance matrix. For problems with a very small number of hyperparameters, this has not been an issue, as the minimum is often discovered before the cubic scaling renders further evaluations prohibitive. As the complexity of machine learning models grows, however, the size of the search space grows as well, along with the number of hyperparameter configurations that need to be evaluated before a solution of sufficient quality is found. Fortunately, as models have grown in complexity, computation has become significantly more accessible and it is now possible to train many models in parallel using relatively inexpensive compute clusters. A natural solution to the hyperparameter search problem is to therefore combine large-scale parallelism with a scalable Bayesian optimization method. The cubic scaling of the GP, however, has made it infeasible to pursue this approach.

The goal of this work is to develop a method for scaling Bayesian optimization, while still maintaining its desirable flexibility and characterization of uncertainty. To that end, we propose the use of neural networks to learn an adaptive set of basis functions for Bayesian linear regression. We refer to this approach as Deep Networks for Global Optimization (DNGO). Unlike a standard Gaussian process, DNGO scales linearly with the number of function evaluations—which, in the case of hyperparameter optimization, corresponds to the number of models trained—and is amenable to stochastic gradient training. Although it may seem that we are merely moving the problem of setting the hyperparameters of the model being tuned to setting them for the tuner itself, we show that for a suitable set of design choices it is possible to create a robust, scalable, and effective Bayesian optimization system that generalizes across many global optimization problems.

We demonstrate the effectiveness of DNGO on a number of difficult problems, including benchmark problems for Bayesian optimization, convolutional neural networks for object recognition, and multi-modal neural language models models for image caption generation. We find hyperparameter configurations that achieve state-of-the-art results of 6.37% and 27.4% on CIFAR-10 and CIFAR-100 respectively, and BLEU scores of 25.1 and 26.7 on the Microsoft COCO 2014 dataset using a single model and a 2-model ensemble respectively.

2. Background and Related Work

2.1. Bayesian Optimization

Bayesian optimization is a well-established strategy for the global optimization of noisy, expensive black-box functions (Mockus et al., 1978). For an in-depth review, see Lizotte (2008), Brochu et al. (2010) and Osborne et al. (2009). Bayesian optimization relies on the construction of a probabilistic model that defines a distribution over objective functions from the input space to the objective of interest. Conditioned on a prior over the functional form and a set of \( N \) observations of input-target pairs \( \{(x_n, y_n)\}_{n=1}^N \), the relatively cheap posterior over functions is then queried to reason about where to seek the optimum of the expensive function of interest. The promise of a new experiment is quantified using an acquisition function, which, applied to the posterior mean and variance, expresses a trade-off between exploration and exploitation. Bayesian optimization proceeds by performing a proxy optimization over this acquisition function in order to determine the next input to evaluate.

Recent innovation has resulted in significant progress in Bayesian optimization, including elegant theoretical results (Srinivas et al., 2010; Bull, 2011; de Freitas et al., 2012), multitask and transfer optimization (Krause & Ong, 2011; Swersky et al., 2013; Bard et al., 2013) and the application to diverse tasks such as sensor set selection (Garnett et al., 2010), the tuning of adaptive Monte Carlo (Mahendran et al., 2012) and robotic gait control (Calandra et al., 2014b).

Typically, Gaussian processes have been used to construct the distribution over functions used in Bayesian optimization, due to their flexibility, well-calibrated uncertainty, and analytic properties (Jones, 2001; Osborne et al., 2009). Recent work has sought to improve the performance of the GP approach through accommodating higher dimensional problems (Wang et al., 2013; Djolonga et al., 2013), input non-stationarities (Snoek et al., 2014) and initialization through meta-learning (Feurer et al., 2015). Random forests, which scale linearly with the data, have also been used successfully for algorithm configuration by Hutter et al. (2011) with empirical estimates of model uncertainty.

More specifically, Bayesian optimization seeks to solve the minimization problem

\[
\mathbf{x}^* = \arg\min_{\mathbf{x} \in \mathbf{X}} f(\mathbf{x}),
\]

where \( f(\mathbf{x}) \) is the objective function to be minimized.
where we take $\mathcal{X}$ to be a compact subset of $\mathbb{R}^K$. In our work, we build upon the standard GP-based approach of Jones (2001) which uses a GP surrogate and the expected improvement acquisition function (Mockus et al., 1978). For model hyperparameters $\Theta$, let $\sigma^2(x; \Theta) = \Sigma(x, x; \Theta)$ be the marginal predictive variance of the probabilistic model, $\mu(x; \{x_n, y_n\}, \Theta)$ be the predictive mean, and define

$$
\gamma(x) = \frac{f(x_{\text{best}}) - \mu(x; \{x_n, y_n\}, \Theta)}{\sigma(x; \{x_n, y_n\}, \Theta)},
$$

(2)

where $f(x_{\text{best}})$ is the lowest observed value. The expected improvement criterion is defined as

$$
a_{\text{EI}}(x; \{x_n, y_n\}, \Theta) = \sigma(x; \{x_n, y_n\}, \Theta) [\gamma(x)\Phi(\gamma(x)) + \mathcal{N}(\gamma(x); 0, 1)].
$$

(3)

Here $\Phi(\cdot)$ is the cumulative distribution function of a standard normal, and $\mathcal{N}(\cdot; 0, 1)$ is the density of a standard normal. Note that numerous alternate acquisition functions and combinations thereof have been proposed (Kushner, 1964; Srinivas et al., 2010; Hoffman et al., 2011), which could be used without affecting the analytic properties of our approach.

### 3. Adaptive Basis Regression with Deep Neural Networks

The idea of applying Bayesian methods to neural networks has a rich history in machine learning (MacKay, 1992; Hinton & van Camp, 1993; Buntine & Weigend, 1991; Neal, 1995; De Freitas, 2003). The goal of Bayesian neural networks is to uncover the full posterior distribution over the network weights in order to capture uncertainty, to act as a regularizer, and to provide a framework for model comparison. The full posterior is, however, intractable for most forms of neural networks, necessitating expensive approximate inference or Markov chain Monte Carlo simulation. More recently, full or approximate Bayesian inference has been considered for small pieces of the overall architecture. For example, in similar spirit to this work, Lázaro-Gredilla & Figueiras-Vidal (2010); Hinton & Salakhutdinov (2008) and Calandra et al. (2014a) considered inference over just the last layer of a neural network. Other examples can be found in Kingma & Welling (2014); Rezende et al. (2014) and Mnih & Gregor (2014), where a neural network is used in a variational approximation to the posterior distribution over the latent variables of a directed generative neural network.

As such, we take a pragmatic approach and add a Bayesian linear regressor to the last hidden layer of a deep neural network, marginalizing only the output weights of the net while using a point estimate for the remaining parameters. This results in adaptive basis regression, a well-established statistical technique which scales linearly in the number of observations, and cubically in the basis function dimensionality. This allows us to explicitly trade off evaluation time and model capacity. As such, we form the basis using the very flexible and powerful non-linear functions defined by the neural network.

First of all, without loss of generality and assuming compact support for each input dimension, we scale the input space to the unit hypercube. We denote by $[\phi_1(\cdot), \ldots, \phi_D(\cdot)]^\top$ the vector of outputs from the last hidden layer of the network, trained on inputs and targets $D := \{(x_n, y_n)\}_{n=1}^N \subset \mathbb{R}^K \times \mathbb{R}$. We take these to be our set of basis functions. In addition, define $\Phi$ to be the design matrix arising from the data and this basis, where $\Phi_{nd} = \phi_d(x_n)$ is the output design matrix, and $y$ the stacked target vector.

These basis functions are parameterized via the weights and biases of the deep neural network, and these parameters are trained via backpropagation and stochastic gradient descent with momentum. In this training phase, a linear output layer is also fit. This procedure can be viewed as a maximum a posteriori (MAP) estimate of all parameters in the network. Once this “basis function neural network” has been trained, we replace the MAP-parameterized output layer with a Bayesian linear regressor that captures uncertainty in the weights. See Section 3.1.2 for a more elaborate explanation of this choice.
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3.1. Model details

Here we elaborate on various choices made in the design of the model.

3.1.1. Network architecture

A natural concern with the use of deep networks is that they often require significant effort to tune and tailor to specific problems. One can consider adjusting the architecture and tuning the hyperparameters of the neural network as itself a difficult hyperparameter optimization problem. An additional challenge is that we aim to create an approach that generalizes across optimization problems. We found that design decisions such as the type of activation function used significantly altered the performance of the Bayesian optimization routine. For example, in Figure 2 we see that the commonly used rectified linear (ReLU) function leads to very poor estimates of uncertainty, which causes the Bayesian optimization routine to explore excessively. Since the bounded tanh function results in smooth functions with realistic variance, we use this nonlinearity in this work; however, if the smoothness assumption needs to be relaxed, a combination of rectified linear functions with a tanh function only on the last layer can also be used in order to bound the basis.

In order to tune any remaining hyperparameters, such as the width of the hidden layers and the amount of regularization, we used GP-based Bayesian optimization. For each of one to four layers we ran Bayesian optimization using the Spearmint (Snoek et al., 2014) package to minimize the average relative loss on a series of benchmark global optimization problems. We tuned a global learning rate, momentum, layer sizes, L2 normalization penalties for each set of weights and dropout rates (Hinton et al., 2012) for each layer. Interestingly, the optimal configuration featured no dropout and very modest L2 normalization. We suspect that dropout, despite having an approximate correction term, causes noise in the predicted mean resulting in a loss of precision. The optimizer instead preferred to restrict capacity via narrow layer width. Namely, the optimal architecture is a deep and narrow network with 3 hidden layers and approximately 50 hidden units per layer. We use the same architecture throughout all of our empirical evaluation, and this architecture is illustrated in Figure 2(d).

3.1.2. Marginal likelihood versus MAP estimate

The standard empirical Bayesian approach to adaptive basis regression is to maximize the marginal likelihood with respect to the parameters of the basis (see...
3.1.3. Quadratic Prior

One of the advantages of Bayesian optimization is that it provides natural avenues for incorporating prior information about the objective function and search space. For example, when choosing the boundaries of the search space, a typical assumption has been that the optimal solution lies somewhere in the interior of the input space. However, by the curse of dimensionality, most of the volume of the space lies very close to its boundaries.

As such, we select a mean function $\eta(x)$ (see Equation 4) to reflect our subjective prior beliefs that the function is coarsely approximated by a convex quadratic function centered in the bounded search region, i.e.,

$$\eta(x) = \lambda + (x - c)^T \Lambda (x - c)$$

where $c$ is the center of the quadratic, $\lambda$ is an offset and $\Lambda$ is a diagonal scaling matrix. We place a Gaussian prior with mean 0.5 (the center of the unit hypercube) on $c$, horseshoe (Carvalho et al., 2009) priors on the diagonal elements $\Lambda_{kk} \forall k \in \{1, \ldots, K\}$ and integrate out $\lambda$, $\Lambda$ and $c$ using slice sampling over the marginal likelihood.

The horseshoe is a so-called one-group prior for inducing sparsity and is a somewhat unusual choice for the weights of a regression model. Here we choose it because 1) it has support only on the positive reals, leading to convex functions, and 2) it has a large spike at zero with a heavy tail, resulting in strong shrinkage for small values while preserving large ones. This last effect is important for handling model misspecification as it allows the quadratic effect to disappear and become a simple offset if necessary.

3.2. Incorporating input space constraints

Many problems of interest have complex, possibly unknown bounds, or exhibit undefined behavior in some regions of the input space. These regions can be characterized as constraints on the search space. Recent work (Gelbart et al., 2014; Snoek, 2013; Gramacy & Lee, 2010) has developed approaches for modeling unknown constraints in GP-based Bayesian optimization by learning a constraint classifier and then discounting expected improvement by the probability of constraint violation.

More specifically, define $c_n \in \{0, 1\}$ to be a binary indicator of the validity of input $x_n$. Also, denote the sets of valid and invalid inputs as $\mathcal{V} = \{(x_n, y_n) \mid c_n = 1\}$ and $\mathcal{I} = \{(x_n, y_n) \mid c_n = 0\}$, respectively. Note that $\mathcal{D} = \mathcal{V} \cup \mathcal{I}$. Lastly, let $\Psi$ be the collection of constraint hyperparameters. The modified expected im-

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Figure 2. A comparison of the predictive mean and uncertainty learned by the model when using 2(a) only tanh, 2(c) only rectified linear (ReLU) activation functions or 2(b) ReLU’s but a tanh on the last hidden layer. The shaded regions correspond to standard deviation envelopes around the mean. The choice of activation function significantly modifies the basis functions learned by the model. Although the ReLU, which is the standard for deep neural networks, is highly flexible, its unbounded activation leads to extremely large uncertainty estimates. Subfigure 2(d) illustrates the overall architecture of the DNGO model. Dashed lines correspond to weights that are marginalized.
Table 1. Evaluation of DNGO on global optimization benchmark problems versus scalable (TPE, SMAC) and non-scalable (Spearmint) Bayesian optimization methods. All problems are minimization problems. For each problem, each method was run 10 times to produce error bars.

| Experiment                  | # Evals | SMAC          | TPE            | Spearmint       | DNGO          |
|-----------------------------|---------|---------------|----------------|-----------------|---------------|
| Branin (0.398)              | 200     | 0.655 ± 0.27  | 0.526 ± 0.13   | **0.398 ± 0.00**| **0.399 ± 0.002** |
| Hartmann6 (-3.322)          | 200     | −2.977 ± 0.11 | −2.823 ± 0.18  | −3.**3166 ± 0.02** | −3.289 ± 0.002 |
| Logistic Regression         | 100     | 8.6 ± 0.9     | 8.2 ± 0.6      | **6.88 ± 0.00**  | **6.89 ± 0.04**  |
| LDA (On grid)               | 50      | 1269.6 ± 2.9  | 1271.5 ± 3.5   | **1266.2 ± 0.1** | **1266.2 ± 0.0** |
| SVM (On grid)               | 100     | **24.1 ± 0.1**| 24.2 ± 0.0     | **24.1 ± 0.1**   | **24.1 ± 0.1** |

Table 1 Evaluation of DNGO on global optimization benchmark problems versus scalable (TPE, SMAC) and non-scalable (Spearmint) Bayesian optimization methods. All problems are minimization problems. For each problem, each method was run 10 times to produce error bars.

To that end, given currently running jobs with inputs \( \{ x_j \}_{j=1}^J \), the marginalized acquisition function \( a_{MCEI}(\cdot; D, \Theta, \Psi) \) is given by

\[
a_{MCEI}(\cdot; D, \Theta, \Psi) = \int a_{CEI}(\cdot; D, \Theta, \Psi) \, d\Theta d\Psi.
\]

When this strategy is applied to a GP, the cost of computing EI for a candidate point becomes cubic in the size of the augmented dataset. This restricts both the number of running experiments that can be tolerated, as well as the number of fantasy sets used for marginalization. With DNGO it is possible to scale both of these up to accommodate a much higher degree of parallelism.

Finally, following the approach of Snoek (2013) we integrate out the hyperparameters of the model to obtain our final integrated acquisition function. For each iteration of the optimization routine we pick the next input, \( x^* \), to evaluate according to

\[
x^* = \arg\max_x a_{MCEI}(x; D, \{ x_j \}_{j=1}^J),
\]

where

\[
a_{MCEI}(x; D, \{ x_j \}_{j=1}^J) = \int a_{MCEI}(x; D, \Theta, \Psi) \, d\Theta d\Psi.
\]
Figure 3. Sample test images and generated captions from the best LBL model on the COCO 2014 dataset. The first two captions sensibly describe the contents of their respective images, while the third is offensively inaccurate.

this comes at the cost of a more heuristic treatment of uncertainty. By contrast, DNGO provides a balance between scalability and the Bayesian marginalization of model parameters and hyperparameters.

To demonstrate the effectiveness of our approach, we compare DNGO to these scalable model-based optimization variants, as well as the input-warped Gaussian process method of Snoek et al. (2014) on the benchmark set of continuous problems from the HPOLib package (Eggensperger et al., 2013). As Table 1 shows, DNGO significantly outperforms SMAC and TPE, and is competitive with the Gaussian process approach. This shows that, despite vast improvements in scalability, DNGO retains the statistical efficiency of the Gaussian process method in terms of the number of evaluations required to find the minimum.

4.2. Image Caption Generation

In this experiment, we explore the effectiveness of DNGO on a practical and expensive problem where highly parallel evaluation is necessary to make progress in a reasonable amount of time. We consider the task of image caption generation using multi-modal neural language models. Specifically, we optimize the hyperparameters of the log-bilinear model (LBL) from Kiros et al. (2014) to optimize the BLEU score of a validation set from the recently released COCO dataset (Lin et al., 2014). From our experiments, each evaluation of this model took an average of 26.6 hours.

We optimize learning parameters such as learning rate, momentum and batch size; regularization parameters like dropout and weight decay for word and image representations; and architectural parameters such as the context size, whether to use the additive or multiplicative version, the size of the word embeddings and the multi-modal representation size. The final parameter is the number of factors, which is only relevant for the multiplicative model. This adds an interesting challenge, since it is only relevant for half of the hyperparameter space. This gives a total of 11 hyperparameters. Even though this number seems small, this problem offers a number of challenges which render its optimization quite difficult. For example, in order to not lose any generality, we choose broad box constraints for the hyperparameters; this, however, renders most of the volume of the model space infeasible.

Table 2. Image caption generation results using BLEU-4 on the Microsoft COCO 2014 test set. Regularized and ensembled LSTM results are reported in Zaremba et al. (2015). The baseline LBL tuned by a human expert and the Soft and Hard Attention models are reported in (Xu et al., 2015). Using a DNGO optimized LBL model achieves the state-of-the-art results on this task. We see that ensembling our top models resulting from the optimization further improves results significantly. We noticed that there were distinct multiple local optima in the hyperparameter space, which may explain the dramatic improvement from ensembling a small number of models.

| Method                     | Test BLEU |
|---------------------------|-----------|
| Human Expert LBL          | 24.3      |
| Regularized LSTM          | 24.3      |
| Soft-Attention LSTM       | 24.3      |
| 10 LSTM ensemble          | 24.4      |
| Hard-Attention LSTM       | 25.0      |
| Single LBL                | 25.1      |
| 2 LBL ensemble            | 25.9      |
| 3 LBL ensemble            | 26.7      |

1Details are provided in the supplementary material.
In addition, quite a few of the hyperparameters are categorical, which introduces severe non-stationarities in the objective surface.

Nevertheless, one of the advantages of a scalable method is the ability to highly parallelize hyperparameter optimization. In this way, high quality settings can be found after only a few sequential steps. To test DNGO in this scenario, we optimize the log-bilinear model with up to 800 parallel evaluations.

Running between 300 and 800 experiments in parallel (determined by cluster availability), we proposed and evaluated approximately 1800 experiments—the equivalent of almost 2000 CPU days—in less than one week. Using the BLEU-4 metric, we optimized the validation set performance and the best LBL model found by DNGO outperforms recently proposed models using LSTM recurrent neural networks (Hochreiter & Schmidhuber, 1997; Zaremba et al., 2015; Xu et al., 2015) on the test set. This is remarkable, as the LBL is a relatively simple approach. Ensembling this top model with the second and third best (under the validation metric) LBL models resulted in a test-set BLEU score\(^2\) of 26.7, significantly outperforming the LSTM-based approaches. We noticed that there were distinct multiple local optima in the hyperparameter space, which may explain the dramatic improvement from ensembling a small number of models. We show some qualitative examples of generated captions on test images in Figure 3.

4.3. Deep Convolutional Neural Networks

Finally, we use DNGO on a pair of highly competitive deep learning visual object recognition benchmark problems. We tune the hyperparameters of a deep convolutional neural network on the CIFAR-10 and CIFAR-100 datasets. Our approach is to establish a single, generic architecture, and specialize it to various tasks via individualized hyperparameter tuning. As such, for both datasets, we employed the same architecture, which can be found in Table 3.

For this architecture, we tuned the momentum, learning rate, \(\mathcal{L}_2\) weight decay coefficients, dropout rates, standard deviations of the random i.i.d. Gaussian weight initializations, and corruption bounds for various data augmentations: global perturbations of hue, saturation and value, random scalings, input pixel dropout and random horizontal reflections. We optimized these over a validation set of 10,000 examples drawn from the training set, running each network for 200 epochs. See Figure 4 for a visualization of the hyperparameter tuning procedure.

We performed the optimization on a cluster of Intel\textsuperscript{®} Xeon Phi\textsuperscript{TM} coprocessors, with 40 jobs running in parallel. We ran our experiments using a kernel library that has been highly optimized for efficient computation on the Intel\textsuperscript{®} Xeon Phi\textsuperscript{TM} coprocessor. We are going to release this library for public use.

For the optimal hyperparameter configuration found, we then ran a final experiment for 350 epochs on the entire training set, and report its result.

| Method       | CIFAR-10 | CIFAR-100 |
|--------------|----------|-----------|
| Maxout       | 9.38%    | 38.57%    |
| DropConnect  | 9.32%    | N/A       |
| Network in network | 8.81% | 35.68% |
| Deeply supervised | 7.97% | 34.57% |
| Tuned CNN    | 6.37%    | 27.4%     |
| Human error  | 6.0%     | N/A       |

\(^2\)We have verified that our BLEU score evaluation is consistent across reported results. We will incorporate other baseline results when the COCO evaluation server is running. We used a beam search decoding for our test predictions with the LBL model.

\(\text{Table 4. We use our algorithm to optimize validation set error as a function of various hyperparameters of a convolutional neural network. We report the test errors of the models with the optimal hyperparameter configurations, as compared to current state-of-the-art results.}\)
Following this, our optimal models for CIFAR-10 and CIFAR-100 achieved test errors of 6.37% and 27.4% respectively. These, to our knowledge, represent the state-of-the-art for these datasets. For perspective, the human manual classification error on CIFAR-10 is 6.0%. A comparison to current state-of-the-art results (Goodfellow et al., 2013; Wan et al., 2013; Lin et al., 2013; Lee et al., 2014) can be found in Table 4.

A comprehensive overview of the setup, the tuning and the optimum configuration can be found in the supplementary material.

5. Conclusion

In this paper, we introduced deep networks for global optimization, or DNGO, which enables efficient optimization of noisy, expensive black-box functions. While this model maintains desirable properties of the GP such as tractability and principled management of uncertainty, it greatly improves its scalability from cubic to linear as a function of the number of observations. We demonstrate that while this model allows efficient computation, its performance is nevertheless competitive with existing approaches.

While adaptive basis regression with neural networks provides one approach to the enhancement of scalability, other models may also present promise. One interesting line of work, for example, would be to introduce a similar methodology by instead employing the sparse Gaussian process as the underlying probabilistic model (Snelson & Ghahramani, 2005; Titsias, 2009; Hensman et al., 2013).

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A. Convolutional neural network experiment specifications

In this section we elaborate on the details of the network training and the meta-optimization. In the following subsections we elaborate on the hyperparametrization scheme. The priors on the hyperparameters as well as their optimal configurations for the two datasets can be found in Table 5.

A.1. Data augmentation

We corrupt each input in a number of ways. Below we describe our parametrization of these corruptions.

**HSV** We shift the hue, saturation and value fields of each input by global constants \( b_H \sim U(-B_H, B_H) \), \( b_S \sim U(-B_S, B_S) \), \( b_V \sim U(-B_V, B_V) \). Similarly, we globally stretch the saturation and value fields by global constants \( a_S \sim U(\frac{1}{1+A_S}, 1 + A_S) \), \( a_V \sim U(\frac{1}{1+A_V}, 1 + A_V) \).

**Scalings** Each input is scaled by some factor \( s \sim U(1, 1 + S) \).

**Translations** We crop each input to size \( 27 \times 27 \), where the window is chosen randomly and uniformly.

**Horizontal reflections** Each input is reflected horizontally with a probability of 0.5.

**Pixel dropout** Each input element is dropped independently and identically with some random probability \( D_0 \).

A.2. Initialization and training procedure

We initialize the weights of each convolution layer \( m \) with i.i.d zero-mean Gaussians with standard deviation \( \frac{\sqrt{2}}{\sqrt{F_m}} \) where \( F_m \) is the number of parameters per filter for that layer. We chose this parametrization to produce activations whose variances are invariant to filter dimensionality. We use the same standard deviation for all layers but the input, for which we dedicate its own hyperparameter \( \sigma_I \) as it oftentimes varies in scale from deeper layers in the network.

We train the model using the standard stochastic gradient descent and momentum optimizer. We use minibatch size of 128, and tune the momentum and learning rate, which we parametrize as \( 1 - 0.1^M \) and \( 0.1^L \) respectively. We anneal the learning rate by a factor of 0.1 at epochs 130 and 190. We terminate the training after 200 epochs.

We regularize the weights of all layers with weight decay coefficient \( W \). We apply dropout on the outputs of the max pooling layers, and tune these rates \( D_1, D_2 \) separately.

A.3. Testing procedure

We evaluate the performance of the learned model by averaging its log-probability predictions on 100 samples drawn from the input corruption distribution, with masks drawn from the unit dropout distribution.

B. Multimodal neural language model hyperparameters

B.1. Description of the hyperparameters

We optimize a total of 11 hyperparameters of the log-bilinear model (LBL). Below we explain what these hyperparameters refer to.

**Model** The LBL model has two variants, an additive model where the image features are incorporated via an additive bias term, and a multiplicative that uses a factored weight tensor to control the interaction between modalities.

**Context size** The goal of the LBL is to predict the next word given a sequence of words. The context size dictates the number of words in this sequence.

**Learning rate, momentum, batch size** These are optimization parameters used during stochastic gradient learning of the LBL model parameters. The optimization over learning rate is carried out in log-space, but the proposed learning rate is exponentiated before being passed to the training procedure.

**Hidden layer size** Controls the size of the joint hidden representation for words and images.

**Embedding size** Words are represented by feature embeddings rather than one-hot vectors. This is the dimensionality of the embedding.

**Dropout** A regularization parameter that determines the amount of dropout to be added to the hidden layer.

**Context decay, Word decay** \( L_2 \) regularization on the input and output weights respectively. Like the learning rate, these are optimized in log-space as they vary over several orders of magnitude.

**Factors** The rank of the weight tensor. Only relevant for the multiplicative model.
| Hyperparameter       | Notation | Support of prior | CIFAR-10 Optimum | CIFAR-100 Optimum |
|----------------------|----------|------------------|------------------|-------------------|
| Momentum             | $M$      | $[0.5, 2]$       | 1.6242           | 1.3339            |
| Learning rate        | $L$      | $[1, 4]$         | 2.7773           | 2.1205            |
| Initialization dev.  | $\sigma_I$ | $[0.5, 1.5]$  | 0.83359          | 1.5570            |
| Input initialization dev. | $\sigma$  | $[0.01, 1]$   | 0.025370         | 0.13556           |
| Hue shift            | $B_H$    | $[0.45]$         | 31.992           | 19.282            |
| Saturation scale     | $A_S$    | $[0.5]$          | 0.31640          | 0.30780           |
| Saturation shift     | $B_S$    | $[0.5]$          | 0.10546          | 0.14695           |
| Value scale          | $A_S$    | $[0.5]$          | 0.13671          | 0.13668           |
| Value shift          | $B_S$    | $[0.5]$          | 0.24140          | 0.010960          |
| Pixel dropout        | $D_0$    | $[0.3]$          | 0.19921          | 0.00056598        |
| Scaling              | $S$      | $[0.3]$          | 0.24140          | 0.12463           |
| L2 weight decay      | $W$      | $[2, 5]$         | 4.2734           | 3.1133            |
| Dropout 1            | $D_1$    | $[0.7]$          | 0.082031         | 0.081494          |
| Dropout 2            | $D_2$    | $[0.7]$          | 0.67265          | 0.38364           |

Table 5. Specification of the hyperparametrization scheme, and optimal hyperparameter configurations found.

| Hyperparameter   | Support of prior | Notes            | COCO Optimum |
|------------------|------------------|------------------|--------------|
| Model            | {additive,multiplicative} |                  | additive     |
| Context size     | $[3, 25]$        |                  | 5            |
| Learning rate    | $[0.001, 10]$    | Log-space        | 0.43193      |
| Momentum         | $[0, 0.9]$       |                  | 0.23269      |
| Batch size       | $[20, 200]$      |                  | 40           |
| Hidden layer size| $[100, 2000]$    |                  | 441          |
| Embedding size   | $\{50, 100, 200\}$ |              | 100          |
| Dropout          | $[0, 0.7]$       |                  | 0.14847      |
| Word decay       | $[10^{-9}, 10^{-3}]$ | Log-space      | 2.98456$^{-7}$|
| Context decay    | $[10^{-9}, 10^{-3}]$ | Log-space    | 1.09181$^{-8}$|
| Factors          | $[50, 200]$      | Multiplicative model only | -            |

Table 6. Specification of the hyperparametrization scheme, and optimal hyperparameter configurations found for the multimodal neural language model. For parameters marked log-space, the log is given to the Bayesian optimization routine and the result is exponentiated before being passed into the multimodal neural language model for training. Square brackets denote a range of parameters, while curly braces denote a set of options.