Metric-Free Natural Gradient for Joint-Training of Boltzmann Machines

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Abstract

This paper introduces the Metric-Free Natural Gradient (MFNG) algorithm for training Boltzmann Machines. Similar in spirit to the Hessian-Free method of Martens [8], our algorithm belongs to the family of truncated Newton methods and exploits an efficient matrix-vector product to avoid explicitly storing the natural gradient metric $L$. This metric is shown to be the expected second derivative of the log-partition function (under the model distribution), or equivalently, the covariance of the vector of partial derivatives of the energy function. We evaluate our method on the task of joint-training a 3-layer Deep Boltzmann Machine and show that MFNG does indeed have faster per-epoch convergence compared to Stochastic Maximum Likelihood with centering, though wall-clock performance is currently not competitive.

1 Introduction

Boltzmann Machines (BM) have become a popular method in Deep Learning for performing feature extraction and probability modeling. The emergence of these models as practical learning algorithms stems from the development of efficient training algorithms, which estimate the negative log-likelihood gradient by either contrastive [4] or stochastic [18, 19] approximations. However, the success of these models has for the most part been limited to the Restricted Boltzmann Machine (RBM) [6], whose architecture allows for efficient exact inference. Unfortunately, this comes at the cost of the model’s representational capacity, which is limited to a single layer of latent variables. The Deep Boltzmann Machine (DBM) [15] addresses this by defining a joint energy function over multiple disjoint layers of latent variables, where interactions within a layer are prohibited. While this affords the model a rich inference scheme incorporating top-down feedback, it also makes training much more difficult, requiring until recently an initial greedy layer-wise pretraining scheme. Since, Montavon and Muller [9] have shown that this difficulty stems from an ill-conditioning of the Hessian matrix, which can be addressed by a simple reparameterization of the DBM energy function, a trick called centering (an analogue to centering and skip-connections found in the deterministic neural network literature [17, 14]). As the barrier to joint-training is overcoming a challenging optimization problem, it is apparent that second-order gradient methods might prove to be more effective than simple stochastic gradient methods. This should prove especially important as we consider models with increasingly complex posteriors or higher-order interactions between latent variables.

To this end, we explore the use of the Natural Gradient [2], which seems ideally suited to the stochastic nature of Boltzmann Machines. Our paper is structured as follows. Section 2 provides a detailed derivation of the natural gradient, including its specific form for BMs. While most of these equations

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Joint-training refers to the act of jointly optimizing $\theta$ (the concatenation of all model parameters, across all layers of the DBM) through maximum likelihood. This is in contrast to [15], where joint-training is preceded by a greedy layer-wise pretraining strategy.
have previously appeared in [3], our derivation aims to be more accessible as it attempts to derive the natural gradient from basic principles, while minimizing references to Information Geometry. Section 5 represents the true contribution of the paper: a practical natural gradient algorithm for BMs which exploits the persistent Markov chains of Stochastic Maximum Likelihood (SML) [18], with a Hessian-Free (HF) like algorithm [8]. The method, named Metric-Free Natural Gradient (MFNG) (in recognition of the similarities of our method to HF), avoids explicitly storing the natural gradient metric \( L \) and uses a linear solver to perform the required matrix-vector product \( L^{-1} E_q [\nabla \log p_\theta] \). Preliminary experimental results on DBMs are presented in Section 4, with the discussion appearing in Section 5.

### 2 The Natural Gradient

#### 2.1 Motivation and Derivation

The main insight behind the natural gradient is that the space of all probability distributions \( \mathcal{P} = \{ p_\theta(x); \theta \in \Theta, x \in \chi \} \) forms a Riemannian manifold. Learning, which typically proceeds by iteratively adapting the parameters \( \theta \) to fit an empirical distribution \( q \), thus traces out a path along this manifold. An immediate consequence is that following the direction of steepest descent in the original Euclidean parameter space does not correspond to the direction of steepest descent along \( \mathcal{P} \). To do so, one needs to account for the metric describing the local geometry of the manifold, which is given by the Fisher Information matrix \( F \), shown in Equation 4. While this metric is typically derived from Information Geometry, a derivation more accessible to a machine learning audience can be obtained as follows.

The natural gradient aims to find the search direction \( \Delta \theta \) which minimizes a given objective function, such that the Kullback–Leibler divergence \( KL(p_\theta \parallel p_{\theta+\Delta \theta}) \) remains constant throughout optimization. This constraint ensures that we make constant progress regardless of the curvature of the manifold \( \mathcal{P} \) and enforces an invariance to the parameterization of the model. The natural gradient for maximum likelihood can thus be formalized as:

\[
\nabla_N := \Delta \theta^* \leftarrow \arg\min_{\Delta \theta} E_q \left[ -\log p_{\theta+\Delta \theta}(x) \right] \quad \text{s.t.} \quad KL(p_\theta \parallel p_{\theta+\Delta \theta}) = \text{const.} \tag{1}
\]

In order to derive a useful parameter update rule, we will consider the KL divergence under the assumption \( \Delta \theta \rightarrow 0 \). We also assume we have a discrete and bounded domain \( \chi \) over which we define the probability mass function \( p_\theta \). Taking the Taylor series expansion of \( \log p_{\theta+\Delta \theta} \) around \( \theta \), and denoting \( \nabla f \) as the column vector of partial derivatives with \( \frac{\partial f}{\partial \theta_i} \) as the \( i \)-th entry, and \( \nabla^2 f \) the Hessian matrix with \( \frac{\partial^2 f}{\partial \theta_i \partial \theta_j} \) in position \((i, j)\), we have:

\[
KL(p_\theta \parallel p_{\theta+\Delta \theta}) \approx \sum_x p_\theta \log p_\theta - \sum_x p_\theta \left[ \log p_\theta + (\nabla \log p_\theta)^T \Delta \theta + \frac{1}{2} \Delta \theta^T (\nabla^2 \log p_\theta) \Delta \theta \right] \\
= \frac{1}{2} \Delta \theta^T E_p \left[ -\nabla^2 \log p_\theta \right] \Delta \theta \tag{2}
\]

with the transition stemming from the fact that \( \sum_x p_\theta \frac{\partial \log p_\theta}{\partial \theta_i} = \frac{\partial}{\partial \theta_i} \sum_x p_\theta(x) = 0 \). Replacing the objective function of Equation 1 by its first-order Taylor expansion and rewriting the constraint as a Lagrangian, we arrive at the following formulation for \( L(\theta, \Delta \theta) \), the loss function which the natural gradient seeks to minimize.

\[
L(\theta, \Delta \theta) = E_q \left[ -\log p_\theta \right] + E_q \left[ -\nabla \log p_\theta \right]^T \Delta \theta + \lambda \frac{1}{2} \Delta \theta^T E_p \left[ -\nabla^2 \log p_\theta \right] \Delta \theta.
\]

Setting \( \frac{\partial L}{\partial \Delta \theta} \) to zero yields the natural gradient direction \( \nabla_N \):

\[
\nabla_N = L^{-1} E_q [\nabla \log p_\theta] \quad \text{with} \quad L = E_p \left[ -\nabla^2 \log p_\theta \right] \quad \text{or equivalently} \quad L = E_p [\nabla \log p_\theta \nabla^T \log p_\theta] \tag{3}
\]

2When clear from context, we will drop the argument of \( p_\theta \) to save space.
While its form is reminiscent of the Newton direction, the natural gradient multiplies the estimated gradient by the inverse of the expected Hessian of \( \log p_\theta \) (Equation 3) or equivalently by the Fisher Information matrix (FIM, Equation 4). The equivalence between both expressions can be shown trivially, with the details appearing in the Appendix. We stress that both of these expectations are computed with respect to the model distribution, and thus computing the metric \( L \) does not involve the empirical distribution in any way. The FIM for Boltzmann Machines is thus not equal to the uncentered covariance of the maximum likelihood gradients. In the following, we pursue our derivation from the form given in Equation 4.

2.2 Natural Gradient for Boltzmann Machines

**Derivation.** Boltzmann machines define a joint distribution over a vector of binary random variables \( x \in \{0, 1\}^N \) by way of an energy function \( E(x) = -\sum_{k<l} W_{kl} x_k x_l - \sum_k b_k x_k \), with weight matrix \( W \in \mathbb{R}^{N \times N} \) and bias vector \( b \in \mathbb{R}^N \). Energy and probability are related by the Boltzmann distribution, such that \( p(x) = \frac{1}{Z} \exp(-E(x)) \), with \( Z \) the partition function defined by 

\[
Z = \sum_x \exp(-E(x)).
\]

Starting from the expression of \( L \) found in Equation 3, we can derive the natural gradient metric for Boltzmann Machines.

\[
L^{(BM)} = \mathbb{E}_{p_\theta} [\nabla^2 E(x) + \nabla^2 \log Z] = \mathbb{E}_{p_\theta} [\nabla^2 \log Z]
\]

The natural gradient metric for first-order BMs takes on a surprisingly simple form: it is the expected Hessian of the log-partition function. With a few lines of algebra (whose details are presented in the Appendix), we can rewrite it as follows:

\[
L^{(BM)} = \mathbb{E}_{p_\theta} \left[ (\nabla E(x) - \mathbb{E}_{p_\theta} [\nabla E(x)])^T (\nabla E(x) - \mathbb{E}_{p_\theta} [\nabla E(x)]) \right]
\]  

Equation 5

\( L^{(BM)} \) is thus given by the covariance of \( \nabla E \), measured under the model distribution \( p_\theta \). Concretely, if we denote \( W_{kl} \) and \( W_{mn} \) as the i and j-th parameters of the model respectively, the entry \( L_{ij} \) will take on the value 

\[
-\mathbb{E} [x_k x_l x_m x_n] + \mathbb{E} [x_k x_l] \mathbb{E} [x_m x_n].
\]

**Discussion.** When computing the Taylor expansion of the KL divergence in Equation 2, we glossed over an important detail. Namely, how to handle latent variables in \( p_\theta(x) \), a topic first discussed in [1]. If \( x = [v, h] \), we could just as easily have derived the natural gradient by considering the constraint \( KL(\sum_h p_\theta(v, h) \| \sum_h p_\theta+\Delta \theta(v, h)) = \text{const.} \) Alternatively, since the distinction between visible and hidden units is entirely artificial (since the KL divergence does not involve the empirical distribution), we may simply wish to consider the distribution obtained by analytically integrating out a maximal number of random variables. In a DBM, this would entail marginalizing over all odd or even layers, a strategy employed with great success in the context of AIS [15]. In this work however, we only consider the metric obtained by considering the KL divergence between the full joint distributions \( p_\theta \) and \( p_\theta+\Delta \theta \).

3 Metric-Free Natural Gradient Implementation

We can compute the natural gradient \( \nabla N \) by first replacing the expectations of Equation 5 by a finite sample approximation. We can do this efficiently by reusing the model samples generated by the persistent Markov chains of SML. Given the size of the matrix being estimated however, we expect this method to require a larger number of chains than is typically used. The rest of the method is similar to the Hessian-Free (HF) algorithm of Martens [8]: we exploit an efficient matrix-vector implementation combined with a linear-solver, such as Conjugate Gradient or MinRes[12], to solve the system \( L \hat{y} = \mathbb{E}_q [\nabla \log p_\theta] \) for \( y \in \mathbb{R}^N \). Additionally, we replace the expectation on the rhs. of this previous equation by an average computed over a mini-batch of training examples (sampled from the empirical distribution \( q \)), as is typically done in the stochastic learning setting.

For Boltzmann Machines, the matrix-vector product \( L\hat{y} \) can be computed in a straightforward manner, without recourse to Pearlmutter’s R-operator [13]. Starting from a sampling approximation to Equation 5 we simply push the dot product inside of the expectation as follows:
By first computing the matrix-vector product \( \theta \): parameters of the model.
\( N := | \theta | \).
\( X^+ \): mini-batch of training examples, with \( X^+ = \{ x_m; m \in [1, M] \} \).
\( Z_{old}^- \): previous state of Markov chains, with \( Z = \{ z_m := (v_m, h_m^{(1)}, h_m^{(2)}); m \in [1, M] \} \).

- Generate positive phase samples \( Z^+ = \{ z^+_m := (x_m, h^{(1)+}_m, h^{(2)+}_m); m \in [1, M] \} \).
- Initializing \( M \) Markov chains from state \( Z_{old}^- \), generate negative phase samples \( Z_{new}^- \).
- Compute the vectors \( s^+_m = \frac{\partial E(z^+_m)}{\partial \theta} \) and \( s^-_m = \frac{\partial E(z^-_m)}{\partial \theta} \), \( \forall m \).
- Compute negative log-likelihood gradient as \( g = \frac{1}{M} \sum_m (s^+_m - s^-_m) \).
- Denote \( S \in \mathbb{R}^{M \times N} \) as the matrix with rows \( s^-_m \) and \( \bar{S} = \frac{1}{M} \sum_m s^-_m \).

\# Solve the system \( Ly = g \) for \( y \), given \( L = (S - \bar{S})^T (S - \bar{S}) \) and an initial zero vector.
\# computeLy is a function which performs equation \[6\] without instantiating \( L \).
- \( \nabla_N \theta \leftarrow \text{CGSolve\text{(computeLy, } S, g, \text{zeros}(N))} \)

\[ L^{(BM)} y \approx (S - \bar{S})^T \left( (S - \bar{S}) y \right) \]  
\[
\text{with } \quad S \in \mathbb{R}^{M \times N}, \text{ the matrix with entries } s_{mj} = \frac{\partial E(x_m)}{\partial \theta_j} \\
\text{and } \quad \bar{S} \in \mathbb{R}^N, \text{ the vector with entries } s_j = \frac{1}{M} \sum_ms_{mj} \\
\text{and } \quad x_m \sim p_\theta(x), \ m \in [1, M].
\]

By first computing the matrix-vector product \( (S - \bar{S})y \), we can easily avoid computing the full \( N \times N \) matrix \( L \). Indeed, the result of this operation is a vector of length \( M \), which is then left-multiplied by a matrix of dimension \( N \times M \), yielding the matrix-vector product \( Ly \in \mathbb{R}^N \). A single iteration of the MFNG is presented in Algorithm \[1\]. A full open-source implementation is also available online \[6\].

## 4 Experiments

We performed a proof-of-concept experiment to determine whether our Metric-Free Natural Gradient (MFNG) algorithm is suitable for joint-training of complex Boltzmann Machines. To this end, we compared our method to Stochastic Maximum Likelihood and a diagonal approximation of MFNG on a 3-layer Deep Boltzmann Machine trained on MNIST \[7\]. All algorithms were run in conjunction with the centering strategy of Montavon and Muller \[9\], which proved crucial to successfully joint-train all layers of the DBM (even when using MFNG) \[10\]. We chose a small 3-layer DBM with 784-400-100 units at the first, second and third layers respectively, to be comparable to \[10\]. Hyper-parameters were varied as follows. For inference, we ran 5 iterations of either mean-field as implemented in \[15\] or Gibbs sampling. The learning rate was kept fixed during training and chosen from the set \( \{ 5 \times 10^{-3}, 10^{-3}, 10^{-4} \} \). For MinRes, we set the damping coefficient to 0.1 and used a fixed tolerance of \( 10^{-5} \) (used to determine convergence). Finally, we tested all algorithms on minibatch sizes of either 25, 128 or 256 elements \[6\]. Finally, since we are comparing optimization algorithms, hyper-parameters were chosen based on the training set likelihood (though we still report the associated test errors). All experiments used the MinRes linear solver, both for its speed and its ability to return pseudo-inverses when faced with ill-conditioning.

\[1\] https://github.com/gdesjardins/MFNG
\[2\] The centering coefficients were initialized as in \[9\], but were otherwise held fixed during training.
\[3\] We expect larger minibatch sizes to be preferable, however simulating this number of Markov chains in parallel (on top of all other memory requirements) was sufficient to hit the memory bottlenecks of GPUs.
Figure 1: Estimated model likelihood as a function of (left) epochs and (right) CPU-time for MFNG, its diagonal approximation (MFNG-diag) and SML. All methods were run in conjunction with the DBM centering trick [9], with centering coefficients held fixed during training. Our grid search yielded the following hyper-parameters: batch size of $256/128$ for MFNG(-diag)/SGD; 5 steps of mean-field / sampling-based inference for MFNG(-diag)/SGD and a learning rate of $5 \cdot 10^{-3}$.

Figure 1 (left) shows the likelihood as estimated by Annealed Importance Sampling [15, 11] as a function of the number of epochs. Under this metric, MFNG achieves the fastest convergence, obtaining a training/test set likelihood of $-71.26/\overline{72.84}$ nats after 94 epochs. In comparison, MFNG-diag obtains $-73.22/\overline{74.05}$ nats and SML $-80.12/\overline{79.71}$ nats in 100 epochs. The picture changes however when plotting likelihood as a function of CPU-time, as shown in Figure 1 (right). Given a wall-time of 8000s for MFNG and SML, and 5000s for MFNG-diag, SML is able to perform upwards of 1550 epochs, resulting in an impressive likelihood score of $-64.94/\overline{67.73}$. Note that these results were obtained on the binary-version of MNIST (thresholded at 0.5) in order to compare to [10]. These results are therefore not directly comparable to [15], which binarizes the dataset through sampling (by treating each pixel activation as the probability $p_i$ of a Bernouilli distribution).

Figure 2 shows a breakdown of the algorithm runtime, for various components of the algorithm. These statistics were collected in the early stages of training, but are generally representative of the bigger picture. While the linear solver clearly dominates the runtime, there are a few interesting observations to make. For small models and batch sizes greater than 256, a single evaluation of $L_y$ appears to be of the same order of magnitude as a gradient evaluation. In all cases, this cost is smaller than that of sampling, which represents a non-negligible part of the total computational budget. This suggests that MFNG could become especially attractive for models which are expensive to sample from. Overall however, restricting the number of CG/MinRes iterations appears key to computational performance, which can be achieved by increasing the damping factor $\alpha$. How this affects convergence in terms of likelihood is left for future work.

5 Discussion and Future Work

While the wall-clock performance of MFNG is not currently competitive with SML, we believe there are still many avenues to explore to improve computational efficiency. Firstly, we performed almost no optimization of the various MinRes hyper-parameters. In particular, we ran the algorithm to convergence with a fixed tolerance of $10^{-5}$. While this typically resulted in relatively few iterations (around 15), this level of precision might not be required (especially given the stochastic nature of

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6While we do not report error margins for AIS likelihood estimates, the numbers proved robust to changes in the number of particles and temperatures being simulated. To obtain such robust estimates, we implemented all the tricks described in Salakhutdinov and Hinton [15] and [16]: a zero-weight base-rate model whose biases are set by maximum likelihood; interpolating distributions $p_i \propto p_A^{1-\beta_i} p_B^{\beta_i}$, with $p_B$ the target distribution; and finally analytical integration of all odd-layers.

7This discrepancy will be resolved in the next revision.
the algorithm). Additionally, it could be worth exploiting the same strategy as HF where the linear solver is initialized by the solution found in the previous iteration. This may prove much more efficient than the current approach of initializing the solver with a zero vector. Pre-conditioning is also a well-known method for accelerating the convergence speed of linear solvers [5]. Our implementation used a simple diagonal regularization of $L$. The Jacobi preconditioner could be implemented easily however by computing the diagonal of $L$ in a first-pass.

Finally, while our single experiment offers little evidence in support of either conclusion, it may very well be possible that MFNG is simply not computationally efficient for DBMs, compared to SML with centering. In this case, it would be worth applying the method to either (i) models with known ill-conditioning, such as factored 3-rd order Boltzmann Machines or (ii) models and distributions exhibiting complex posterior distributions. In such scenarios, we may wish to maximize the use of the positive phase statistics (which were obtained at a high computational cost) by performing larger jumps in parameter space. It remains to be seen how this would interact with SML, where the burn-in period of the persistent chains is directly tied to the magnitude of $\Delta \theta$.

Appendix

We include the following derivations for completeness.

5.1 Expected Hessian of $\log Z$ and Fisher Information.

\[
\mathbb{E}_{p_\theta} \left[ - \frac{\partial^2 \log p(x)}{\partial \theta_i \partial \theta_j} \right] = \mathbb{E}_{p_\theta} \left[ \frac{1}{p(x)^2} \frac{\partial p(x)}{\partial \theta_j} \frac{\partial p(x)}{\partial \theta_i} - \frac{1}{p(x)} \frac{\partial^2 p(x)}{\partial \theta_i \partial \theta_j} \right]
\]
\[
= \mathbb{E}_{p_\theta} \left[ \frac{1}{p(x)} \frac{\partial p(x)}{\partial \theta_i} \frac{1}{p(x)} \frac{\partial p(x)}{\partial \theta_j} - \frac{1}{p(x)} \frac{\partial^2 p(x)}{\partial \theta_i \partial \theta_j} \right]
\]
\[
= \mathbb{E}_{p_\theta} \left[ \frac{\partial \log p(x)}{\partial \theta_i} \frac{\partial \log p(x)}{\partial \theta_j} \right] - \sum_x p(x) \frac{\partial^2 p(x)}{\partial \theta_i \partial \theta_j}
\]
\[
= \mathbb{E}_{p_\theta} \left[ \frac{\partial \log p(x)}{\partial \theta_i} \frac{\partial \log p(x)}{\partial \theta_j} \right] - \sum_x \frac{\partial^2 p(x)}{\partial \theta_i \partial \theta_j} - \sum_x \frac{\partial^2 p(x)}{\partial \theta_i \partial \theta_j}
\]
\[
= \mathbb{E}_{p_\theta} \left[ \frac{\partial \log p(x)}{\partial \theta_i} \frac{\partial \log p(x)}{\partial \theta_j} \right] - \frac{\partial^2}{\partial \theta_i \partial \theta_j}
\]
5.2 Derivation of Equation

\[
\log p(x) = -E(x) - \log Z
\]
\[
\frac{\partial \log p(x)}{\partial \theta_i} = -\frac{\partial E(x)}{\partial \theta_i} - \frac{1}{Z} \sum_x \frac{\partial}{\partial \theta_i} [\exp(-E(x))]
\]
\[
\mathbb{E}_p \left[ -\frac{\partial^2 \log p(x)}{\partial \theta_i \partial \theta_j} \right] = \mathbb{E}_p \left[ \left( \frac{\partial E(x)}{\partial \theta_i} - \mathbb{E}_p \left[ \frac{\partial E(x)}{\partial \theta_i} \right] \right) \left( \frac{\partial E(x)}{\partial \theta_j} - \mathbb{E}_p \left[ \frac{\partial E(x)}{\partial \theta_j} \right] \right) \right] - \mathbb{E}_p \left[ \frac{\partial E(x)}{\partial \theta_i} \right] \mathbb{E}_p \left[ \frac{\partial E(x)}{\partial \theta_j} \right]
\]

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